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1. Tuning Parameters for the Q-tof-2

The instrument was scanned from 50 Daltons to 1020 Daltons in 2 seconds, with a 123 S pusher time. W-mode was used in the +ESI mode with a resolution of about 17500 (peak width at half-height). The source was heated at 80 degrees and the electrospray probe temperature was set at 150 degrees. The cone voltage was 35 V. The argon pressure in the collision cell was optimized for maximum resolution. The settings below were used to optimize sensitivity for small molecules.

MS profile:

Mass	Dwell Time	Ramp Time
45	10	80
400	10	0
400		

Rf settings:

	Gain	Offset
Transport Rf	3	0.2
Collision Rf	3	0.2

Calibration:

Calibration Solution: 40 mg of sodium acetate trihydrate (Sigma) and 2 mg of acetamide were dissolved in 5 mL of Mobile Phase A (5% methanol, 95% water, 12.5 mM ammonium acetate, 12.5 mM acetic acid). After vortexing to dissolve the compounds, 5 mL of Mobile Phase B (95% methanol, 5% water, 12.5 mM ammonium acetate, 12.5 mM acetic acid) was added. This solution was subsequently diluted 1:10 with additional Mobile Phase B.

4 L of Calibration Solution was injected into the Q-tof-2. A third order calibration curve was obtained using the MassLynx 3.51 software. The calibration accuracy was verified using a second injection of 4 L of Calibration Solution. [The masses of the sodium acetate clusters used for calibration were not corrected for the mass of the missing electron, and the calibration curve was thus shifted by the mass of one electron; the calculated masses from MassLynx 3.5 likewise are shifted by one electron.]

Accurate Mass Product Ion Spectra:

Compounds were injected into the mass spectrometer and the spectra were recorded. The collision gas pressure was optimized for resolution. The cone energy was set at 35V for all work. Product ion spectra were obtained for most compounds using alternating scans at three different collision energies: 20 V, 25V, and 30V. Some of the experimental details are summarized in Table 2.

Absolute intensities were kept below 150 counts/second, so no corrections (N_p) were made for multiple ions hitting the detector at the same time. To maximize accuracy, all parameters used for obtaining data were identical to the parameters used in calibrating the Q-tof-2, except for collision energy. For example, cone voltage, scan time, and scan range were kept constant.

2. Conditions used to obtain the spectra.

Compound	Conc.	•L inj Quattro II	Quattro II Cone voltage	Coll. Energy Quattro II	mL inj Q-tof-2	Q-tof-2 collision energies Functions 1, 2, and 3		
xemilofiban	25ng/uL	10	70	20	10	20	30	25
orbofiban	25ng/uL	10	70	20	10	20	30	25
D	25ng/uL	10	70	20	2	20	30	25
B	1ug/uL	2	35	12	2	10	8	12
Leu-enkeph	25ng/uL	10	70	20	20	35	30	25
A	25ng/uL	10	70	20	10	20	30	25
E	25ng/uL	10	70	20	10	20	30	25
C	140ng/uL	7	70	20	20	20	30	25

3. Configurations

Number of Cells	Number of Configurations	Number of Cell Combinations ($2^n - 1$)	Maximum Number of Fragments Fitting at Least 1 Model
1	1	1	1
2	1	3	3
3	1	7	6
4	2	15	11
5	3	31	20

5-Cell Connectivity Chart

(1 = works; 0 = does not work)

Binary Fragment				W	Y	X	Binary Fragment				W	Y	X
12345							12345						
1	00001	1	1	1			16	10000	1	1	1		
2	00010	1	1	1			17	10001	0	0	0		
3	00011	1	0	0			18	10010	0	0	0		
4	00100	1	1	1			19	10011	0	0	0		
5	00101	0	1	0			20	10100	0	0	0		
6	00110	1	0	0			21	10101	0	0	0		
7	00111	1	0	0			22	10110	0	0	0		
8	01000	1	1	1			23	10111	0	0	0		
9	01001	0	0	1			24	11000	1	1	1		
10	01010	0	1	1			25	11001	0	0	1		
11	01011	0	0	1			26	11010	0	1	1		
12	01100	1	1	1			27	11011	0	0	1		
13	01101	0	1	1			28	11100	1	1	1		
14	01110	1	1	1			29	11101	0	1	1		
15	01111	1	1	1			30	11110	1	1	1		
							31	11111	1	1	1		
							max frags:				15	17	20

Works for none: fragments 17 to 23;

W only: fragments 3, 6, and 7; Y only: fragment 5;

X only: fragments 9,11,25, and 27;

X and Y: fragments 10,13,26,and 29

4. Cells as sums/differences of neutralized fragment ions

5-cell 6 hits can require up to 4 sums/differences to define a cell.

ion 1:	A	B	C	D	E
ion 2:					E
ion 3:				D	E
ion 4:	A				
ion 5:		B	C		
ion 6:			C	D	

B can be calculated in two ways, both require a sum/difference of 4 ions:

$$B = (B+C) + (D+E) - (C+D) - E = \text{ion 5} + \text{ion 3} - \text{ion 6} - \text{ion 2}$$

$$B = ((A+B+C+D+E) - (C+D) - E - A = \text{ion 1} - \text{ion 6} - \text{ion 2} - \text{ion 4}$$

Both formulae require using differences of 4 ions. B is a hidden cell. There is no simpler way to calculate B.

—

The table below illustrates that with 12 masses (all masses from the spectrum of xemilofiban) it is possible to generate every positive integer between 1 and 358, the molecular weight of xemilofiban, using sums/differences of 1,2,3, or 4 ions. In the table below, 1 means add the following integer, – means subtract the following integer, and 0 means ignore the following integer.

1	1	217	-	216	0	118	0	95
2	-	217	1	124	0	118	1	95
3	1	216	0	124	-	118	-	95
4	1	217	0	124	-	118	-	95
5	1	175	-	141	-	124	1	95
6	0	135	1	124	-	118	0	95
7	-	223	1	135	0	118	1	95

8	1	223	-	175	-	135	1	95
9	-	177	1	175	1	135	-	124
10	1	223	0	124	-	118	-	95
11	1	135	-	124	0	118	0	95
12	-	135	1	124	1	118	-	95
13	-	200	0	124	1	118	1	95
14	-	216	1	135	0	118	1	95
15	-	200	1	175	1	135	-	95
16	1	216	-	177	-	118	1	95
17	1	135	0	124	-	118	0	95
18	1	216	-	175	-	118	1	95
19	-	200	1	124	0	118	1	95
20	-	216	1	141	0	118	1	95
21	1	358	-	124	-	118	-	95
22	-	217	1	216	1	118	-	95
23	0	135	0	124	1	118	-	95
24	1	217	-	216	1	118	-	95
25	-	217	1	124	1	118	0	95
26	-	216	1	124	1	118	0	95
27	-	177	1	175	1	124	-	95
28	1	175	-	124	-	118	1	95
29	0	135	1	124	0	118	-	95
30	1	177	-	124	-	118	1	95
31	1	177	-	175	1	124	-	95
32	-	358	1	177	1	118	1	95
33	-	223	1	216	1	135	-	95
34	1	135	-	124	1	118	-	95
35	1	141	-	135	1	124	-	95
36	-	177	0	124	1	118	1	95
37	-	216	1	135	1	118	0	95
38	-	175	0	124	1	118	1	95
39	1	216	-	177	0	118	0	95
40	1	135	0	124	0	118	-	95

41	1	216	-	175	0	118	0	95
42	-	177	1	124	0	118	1	95
43	-	216	1	141	1	118	0	95
44	-	175	1	124	0	118	1	95
45	1	216	-	200	1	124	-	95
46	1	135	1	124	-	118	-	95
47	-	223	1	175	0	118	1	95
48	1	200	-	175	1	118	-	95
49	-	223	1	177	0	118	1	95
50	-	223	1	216	1	175	-	118
51	1	175	-	124	0	118	0	95
52	1	141	1	124	-	118	-	95
53	1	177	-	124	0	118	0	95
54	-	216	1	175	0	118	1	95
55	-	175	1	135	0	118	1	95
56	-	216	1	177	0	118	1	95
57	1	175	0	124	-	118	0	95
58	1	216	-	135	-	118	1	95
59	1	177	0	124	-	118	0	95
60	-	216	1	141	1	135	0	95
61	-	175	1	141	0	118	1	95
62	1	216	-	177	1	118	-	95
63	1	141	1	135	-	118	-	95
64	1	216	-	175	1	118	-	95
65	-	177	1	124	1	118	0	95
66	-	216	1	200	1	177	-	95
67	-	175	1	124	1	118	0	95
68	1	216	-	177	1	124	-	95
69	1	216	-	124	-	118	1	95
70	1	217	-	124	-	118	1	95
71	1	223	-	175	1	118	-	95
72	-	141	0	124	1	118	1	95
73	-	223	1	216	1	175	-	95

74	1	175	-	124	1	118	-	95
75	1	216	-	141	0	118	0	95
76	1	177	-	124	1	118	-	95
77	-	216	1	175	1	118	0	95
78	-	135	0	124	1	118	1	95
79	-	216	1	177	1	118	0	95
80	1	175	0	124	0	118	-	95
81	1	216	-	135	0	118	0	95
82	1	177	0	124	0	118	-	95
83	-	216	1	175	1	124	0	95
84	-	135	1	124	0	118	1	95
85	-	216	1	177	1	124	0	95
86	1	175	1	124	-	118	-	95
87	-	223	1	175	1	135	0	95
88	1	177	1	124	-	118	-	95
89	0	135	-	124	1	118	1	95
90	-	175	1	141	1	124	0	95
91	1	175	1	135	-	124	-	95
92	1	216	-	124	0	118	0	95
93	1	217	-	124	0	118	0	95
94	-	217	1	216	0	118	1	95
95	0	135	0	124	0	118	1	95
96	1	217	-	216	0	118	1	95
97	1	175	1	135	-	118	-	95
98	1	216	0	124	-	118	0	95
99	1	200	-	124	1	118	-	95
100	-	216	1	175	1	141	0	95
101	0	135	1	124	-	118	1	95
102	-	216	1	200	1	118	0	95
103	1	175	1	141	-	118	-	95
104	1	216	-	135	1	118	-	95
105	1	200	0	124	0	118	-	95
106	1	135	-	124	0	118	1	95

107	-	135	1	124	1	118	0	95
108	-	216	1	200	1	124	0	95
109	1	216	1	135	-	124	-	118
110	1	216	-	135	1	124	-	95
111	1	200	1	124	-	118	-	95
112	1	135	0	124	-	118	1	95
113	1	358	-	216	-	124	1	95
114	-	223	1	124	1	118	1	95
115	1	216	-	124	1	118	-	95
116	1	217	-	124	1	118	-	95
117	-	217	1	216	1	118	0	95
118	0	135	0	124	1	118	0	95
119	1	217	-	216	1	118	0	95
120	-	217	1	124	1	118	1	95
121	1	216	0	124	0	118	-	95
122	1	217	0	124	0	118	-	95
123	-	217	1	216	1	124	0	95
124	0	135	1	124	0	118	0	95
125	-	223	1	135	1	118	1	95
126	1	177	-	175	1	124	0	95
127	1	216	1	124	-	118	-	95
128	1	217	1	124	-	118	-	95
129	1	135	-	124	1	118	0	95
130	1	141	-	135	1	124	0	95
131	-	217	1	135	1	118	1	95
132	-	216	1	135	1	118	1	95
133	1	217	1	135	-	124	-	95
134	1	223	1	124	-	118	-	95
135	1	135	0	124	0	118	0	95
136	1	216	-	175	0	118	1	95
137	-	200	1	124	1	118	1	95
138	1	216	1	135	-	118	-	95
139	1	358	-	124	0	118	-	95

140	1	216	-	200	1	124	0	95
141	1	135	1	124	-	118	0	95
142	1	358	-	216	0	118	0	95
143	1	200	-	175	1	118	0	95
144	1	216	1	141	-	118	-	95
145	1	358	0	124	-	118	-	95
146	1	175	-	124	0	118	1	95
147	0	135	1	124	1	118	-	95
148	1	177	-	124	0	118	1	95
149	1	200	-	175	1	124	0	95
150	1	217	1	175	-	124	-	118
151	1	223	1	141	-	118	-	95
152	1	175	0	124	-	118	1	95
153	1	223	1	200	-	175	-	95
154	1	177	0	124	-	118	1	95
155	-	216	1	141	1	135	1	95
156	1	200	1	175	-	124	-	95
157	1	216	-	177	1	118	0	95
158	1	135	0	124	1	118	-	95
159	1	216	-	175	1	118	0	95
160	-	177	1	124	1	118	1	95
161	1	216	1	175	-	135	-	95
162	-	175	1	124	1	118	1	95
163	1	216	-	177	1	124	0	95
164	1	135	1	124	0	118	-	95
165	-	223	1	175	1	118	1	95
166	1	223	-	175	1	118	0	95
167	-	223	1	177	1	118	1	95
168	1	223	1	175	-	135	-	95
169	1	175	-	124	1	118	0	95
170	1	141	1	124	0	118	-	95
171	1	177	-	124	1	118	0	95
172	-	216	1	175	1	118	1	95

173	-	175	1	135	1	118	1	95
174	-	216	1	177	1	118	1	95
175	1	175	0	124	0	118	0	95
176	1	216	-	135	0	118	1	95
177	1	177	0	124	0	118	0	95
178	1	216	1	175	-	118	-	95
179	-	175	1	141	1	118	1	95
180	1	216	1	177	-	118	-	95
181	1	175	1	124	-	118	0	95
182	-	223	1	175	1	135	1	95
183	1	177	1	124	-	118	0	95
184	-	223	1	177	1	135	1	95
185	1	223	1	175	-	118	-	95
186	1	175	1	135	-	124	0	95
187	1	216	-	124	0	118	1	95
188	1	217	-	124	0	118	1	95
189	1	200	-	135	1	124	0	95
190	-	200	1	177	1	118	1	95
191	-	216	1	177	1	135	1	95
192	1	175	1	135	-	118	0	95
193	1	216	0	124	-	118	1	95
194	1	200	-	124	1	118	0	95
195	-	216	1	175	1	141	1	95
196	-	141	1	124	1	118	1	95
197	-	216	1	200	1	118	1	95
198	1	175	0	124	1	118	-	95
199	1	216	-	135	1	118	0	95
200	1	177	0	124	1	118	-	95
201	1	217	-	216	1	200	0	95
202	-	135	1	124	1	118	1	95
203	1	216	1	200	-	118	-	95
204	1	175	1	124	0	118	-	95
205	1	216	-	135	1	124	0	95

206	1	177	1	124	0	118	-	95
207	-	141	1	135	1	118	1	95
208	-	175	1	141	1	124	1	118
209	1	223	1	216	-	135	-	95
210	1	216	-	124	1	118	0	95
211	1	217	-	124	1	118	0	95
212	-	217	1	216	1	118	1	95
213	0	135	0	124	1	118	1	95
214	1	217	-	216	1	118	1	95
215	1	175	1	135	0	118	-	95
216	1	216	0	124	0	118	0	95
217	1	217	0	124	0	118	0	95
218	-	217	1	216	1	124	1	95
219	0	135	1	124	0	118	1	95
220	1	217	1	216	-	118	-	95
221	1	175	1	141	0	118	-	95
222	1	216	1	124	-	118	0	95
223	1	200	0	124	1	118	-	95
224	1	135	-	124	1	118	1	95
225	1	141	-	135	1	124	1	95
226	1	223	1	216	-	118	-	95
227	1	223	1	217	-	118	-	95
228	1	217	1	135	-	124	0	95
229	1	200	1	124	0	118	-	95
230	1	135	0	124	0	118	1	95
231	1	217	-	216	1	135	1	95
232	1	177	-	175	1	135	1	95
233	1	216	1	135	-	118	0	95
234	1	358	-	124	0	118	0	95
235	1	216	-	200	1	124	1	95
236	1	135	1	124	-	118	1	95
237	1	358	-	216	0	118	1	95
238	1	200	-	175	1	118	1	95

239	1	216	0	124	1	118	-	95
240	1	217	0	124	1	118	-	95
241	1	216	1	200	-	175	0	95
242	0	135	1	124	1	118	0	95
243	1	223	-	216	1	141	1	95
244	1	200	-	175	1	124	1	95
245	1	216	1	124	0	118	-	95
246	1	217	1	124	0	118	-	95
247	1	175	-	141	1	118	1	95
248	1	223	1	200	-	175	0	95
249	1	177	-	141	1	118	1	95
250	1	216	1	175	-	141	0	95
251	1	200	1	175	-	124	0	95
252	1	223	1	124	0	118	-	95
253	1	135	0	124	1	118	0	95
254	1	216	-	175	1	118	1	95
255	1	177	-	135	1	118	1	95
256	1	216	1	135	0	118	-	95
257	1	358	-	124	1	118	-	95
258	1	216	-	177	1	124	1	95
259	1	135	1	124	0	118	0	95
260	1	358	-	216	1	118	0	95
261	1	223	-	175	1	118	1	95
262	1	216	1	141	0	118	-	95
263	1	358	0	124	0	118	-	95
264	1	175	-	124	1	118	1	95
265	1	141	1	124	0	118	0	95
266	1	177	-	124	1	118	1	95
267	1	216	1	175	-	124	0	95
268	1	217	1	175	-	124	0	95
269	1	358	1	124	-	118	-	95
270	1	175	0	124	0	118	1	95
271	1	216	-	175	1	135	1	95

272	1	177	0	124	0	118	1	95
273	1	216	1	175	-	118	0	95
274	1	217	1	175	-	118	0	95
275	1	216	1	177	-	118	0	95
276	1	175	1	124	-	118	1	95
277	1	358	-	216	1	135	0	95
278	1	177	1	124	-	118	1	95
279	1	223	-	216	1	177	1	95
280	1	358	1	135	-	118	-	95
281	1	175	1	135	-	124	1	95
282	1	135	1	124	1	118	-	95
283	1	177	1	135	-	124	1	95
284	1	200	-	135	1	124	1	95
285	-	216	1	200	1	177	1	124
286	1	358	1	141	-	118	-	95
287	1	175	1	135	-	118	1	95
288	1	141	1	124	1	118	-	95
289	1	200	-	124	1	118	1	95
290	1	223	-	175	1	124	1	118
291	1	358	1	175	-	124	-	118
292	1	216	1	200	-	124	0	95
293	1	175	0	124	1	118	0	95
294	1	216	-	135	1	118	1	95
295	1	177	0	124	1	118	0	95
296	1	216	1	175	0	118	-	95
297	1	217	1	175	0	118	-	95
298	1	216	1	177	0	118	-	95
299	1	175	1	124	0	118	0	95
300	1	216	-	135	1	124	1	95
301	1	177	1	124	0	118	0	95
302	1	358	1	216	-	177	-	95
303	1	223	1	175	0	118	-	95
304	1	223	1	216	-	135	0	95

305	1	216	-	124	1	118	1	95
306	1	217	-	124	1	118	1	95
307	1	223	-	135	1	124	1	95
308	1	223	-	216	1	177	1	124
309	1	217	1	216	-	124	0	95
310	1	175	1	135	0	118	0	95
311	1	216	0	124	0	118	1	95
312	1	217	0	124	0	118	1	95
313	1	216	1	177	-	175	1	95
314	1	358	1	175	-	124	-	95
315	1	217	1	216	-	118	0	95
316	1	175	1	141	0	118	0	95
317	1	216	1	124	-	118	1	95
318	1	200	0	124	1	118	0	95
319	1	358	-	216	1	177	0	95
320	1	358	1	175	-	118	-	95
321	1	216	1	200	0	118	-	95
322	1	175	1	124	1	118	-	95
323	1	217	1	135	-	124	1	95
324	1	177	1	124	1	118	-	95
325	1	223	-	216	1	200	1	118
326	1	200	1	177	-	175	1	124
327	1	175	1	141	1	135	-	124
328	1	216	1	135	-	118	1	95
329	1	358	-	124	0	118	1	95
330	1	223	-	135	1	124	1	118
331	1	200	1	177	-	141	1	95
332	1	358	1	216	-	124	-	118
333	1	175	1	135	1	118	-	95
334	1	216	0	124	1	118	0	95
335	1	217	0	124	1	118	0	95
336	1	216	1	200	-	175	1	95
337	0	135	1	124	1	118	1	95

338	1	217	1	216	0	118	-	95
339	1	175	1	141	1	118	-	95
340	1	216	1	124	0	118	0	95
341	1	217	1	124	0	118	0	95
342	1	358	-	216	1	200	0	95
343	1	223	1	200	-	175	1	95
344	1	223	1	216	0	118	-	95
345	1	358	1	200	-	118	-	95
346	1	200	1	175	-	124	1	95
347	1	200	1	124	1	118	-	95
348	1	135	0	124	1	118	1	95
349	1	223	1	177	-	175	1	124
350	1	217	-	177	1	175	1	135
351	1	216	1	135	0	118	0	95
352	1	358	-	124	1	118	0	95
353	1	216	1	177	-	135	1	95
354	1	135	1	124	0	118	1	95
355	1	358	-	216	1	118	1	95
356	1	358	1	217	-	124	-	95
357	1	216	1	141	0	118	0	95
358	1	358	0	124	0	118	0	95

5. Compound B: Inputting Different molecular formulae/ Isotope Ratios

Section A: MaxDefect of Cells was about 2.5 milliDaltons

Elemental Composition Used: C₂₈H₃₄N₂O₁₃S₁Cl₀F₀

MaxDefect 25

Solution Number 1

Linear Fit 2 Coverage 100

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell C:	16	14	2	3	1	0	0	314	720	722
Cell B:	6	10	0	5	0	0	0	162	530	525
Cell A:	6	10	0	5	0	0	0	162	530	525

Frag Composition		Mass	LSdefect	CalcDefect	MeasDefect
1	A	162	530	525	540
2	C	314	720	722	730
3	AB	324	1060	1050	1060
4	A C	476	1250	1247	1250
5	ABC	638	1780	1772	1780

Best Permutation: CAB

Best Permutation: BAC

Elemental Composition Used: C₂₉H₃₀N₆O₉S₁Cl₀F₀

MaxDefect 25

Solution Number 1

Linear Fit 2 Coverage 100

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell C:	16	14	2	3	1	0	0	314	720	722
Cell B:	7	6	4	1	0	0	0	162	530	541
Cell A:	6	10	0	5	0	0	0	162	530	525

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	A	162	530	525	540
2	C	314	720	722	730
3	AB	324	1060	1066	1060
4	A C	476	1250	1247	1250
5	ABC	638	1780	1788	1780

Best Permutation: CAB

Best Permutation: BAC

Solution Number 2

Linear Fit 2 Coverage 100

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell C:	16	14	2	3	1	0	0	314	720	722
Cell B:	6	10	0	5	0	0	0	162	530	525
Cell A:	7	6	4	1	0	0	0	162	530	541

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	A	162	530	541	540
2	C	314	720	722	730
3	AB	324	1060	1066	1060
4	A C	476	1250	1263	1250
5	ABC	638	1780	1788	1780

Best Permutation: CAB

Best Permutation: BAC

Elemental Composition Used: C32H26N6O9S0Cl0F0

MaxDefect 25

Solution Number 1

Linear Fit 1 Coverage 100

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell C:	24	10	0	1	0	0	0	314	730	729
Cell B:	2	6	6	3	0	0	0	162	520	501
Cell A:	6	10	0	5	0	0	0	162	540	525

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	A	162	540	525	540
2	C	314	730	729	730
3	AB	324	1060	1026	1060
4	BC	476	1250	1230	1250
5	ABC	638	1790	1755	1780

Best Permutation: CBA

Best Permutation: ABC

Elemental Composition Used: C32H34N2O8S2Cl0F0

MaxDefect 25

Solution Number 1

Linear Fit 1	Coverage 100									
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell C:	16	14	2	3	1	0	0	314	730	722
Cell B:	10	10	0	0	1	0	0	162	520	501
Cell A:	6	10	0	5	0	0	0	162	540	525

Frag Composition	Mass	LSdefect	CalcDefect	MeasDefect
------------------	------	----------	------------	------------

1	A	162	540	525	540
2	C	314	730	722	730
3	AB	324	1060	1026	1060
4	BC	476	1250	1223	1250
5	ABC	638	1790	1748	1780

Best Permutation: CBA

Best Permutation: ABC

Elemental Composition Used: C24H34N2O18S0Cl0F0

MaxDefect 25

Solution Number 1

Linear Fit 1	Coverage 100									
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell C:	12	14	2	8	0	0	0	314	730	746
Cell B:	6	10	0	5	0	0	0	162	520	525

Cell A:	6	10	0	5	0	0	0	162	540	525
---------	---	----	---	---	---	---	---	-----	-----	-----

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	A	162	540	525	540
2	C	314	730	746	730
3	AB	324	1060	1050	1060
4	BC	476	1250	1271	1250
5	ABC	638	1790	1796	1780

Best Permutation: CBA

Best Permutation: ABC

Elemental Composition Used: C24H30N8O11S1Cl0F0

MaxDefect 25

Solution Number 1

Linear Fit 2 Coverage 100

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell C:	12	10	8	1	1	0	0	314	720	698
Cell B:	6	10	0	5	0	0	0	162	530	525
Cell A:	6	10	0	5	0	0	0	162	530	525

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	A	162	530	525	540
---	---	-----	-----	-----	-----

2	C	314	720	698	730
3	AB	324	1060	1050	1060
4	A C	476	1250	1223	1250
5	ABC	638	1780	1748	1780

Best Permutation: CAB

Best Permutation: BAC

Elemental Composition Used: C30H26N10O5S1Cl0F0

MaxDefect 25

Solution Number 1

Linear Fit 2	Coverage 100									
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell C:	16	14	2	3	1	0	0	314	720	722
Cell B:	7	6	4	1	0	0	0	162	530	541
Cell A:	7	6	4	1	0	0	0	162	530	541

Frag Composition	Mass	LSdefect	CalcDefect	MeasDefect
------------------	------	----------	------------	------------

1	A	162	530	541	540
2	C	314	720	722	730
3	AB	324	1060	1082	1060
4	A C	476	1250	1263	1250
5	ABC	638	1780	1804	1780

Best Permutation: CAB

Best Permutation: BAC

Section B: **MaxDefect of Cells was about 1.0 milliDaltons**

Elemental Composition Used: C28H34N2O13S1Cl0F0

MaxDefect 10

Solution Number 1

Linear Fit 2

Coverage 100

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell C:	16	14	2	3	1	0	0	314	720	722
Cell B:	6	10	0	5	0	0	0	162	530	525
Cell A:	6	10	0	5	0	0	0	162	530	525

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	A	162	530	525	540
2	C	314	720	722	730
3	AB	324	1060	1050	1060
4	A C	476	1250	1247	1250
5	ABC	638	1780	1772	1780

Best Permutation: CAB

Best Permutation: BAC

Elemental Composition Used: C29H30N6O9S1Cl0F0

MaxDefect 10

Solution Number 1

Linear Fit 1

Coverage 100

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell C:	16	14	2	3	1	0	0	314	730	722
Cell B:	6	10	0	5	0	0	0	162	520	525
Cell A:	7	6	4	1	0	0	0	162	540	541

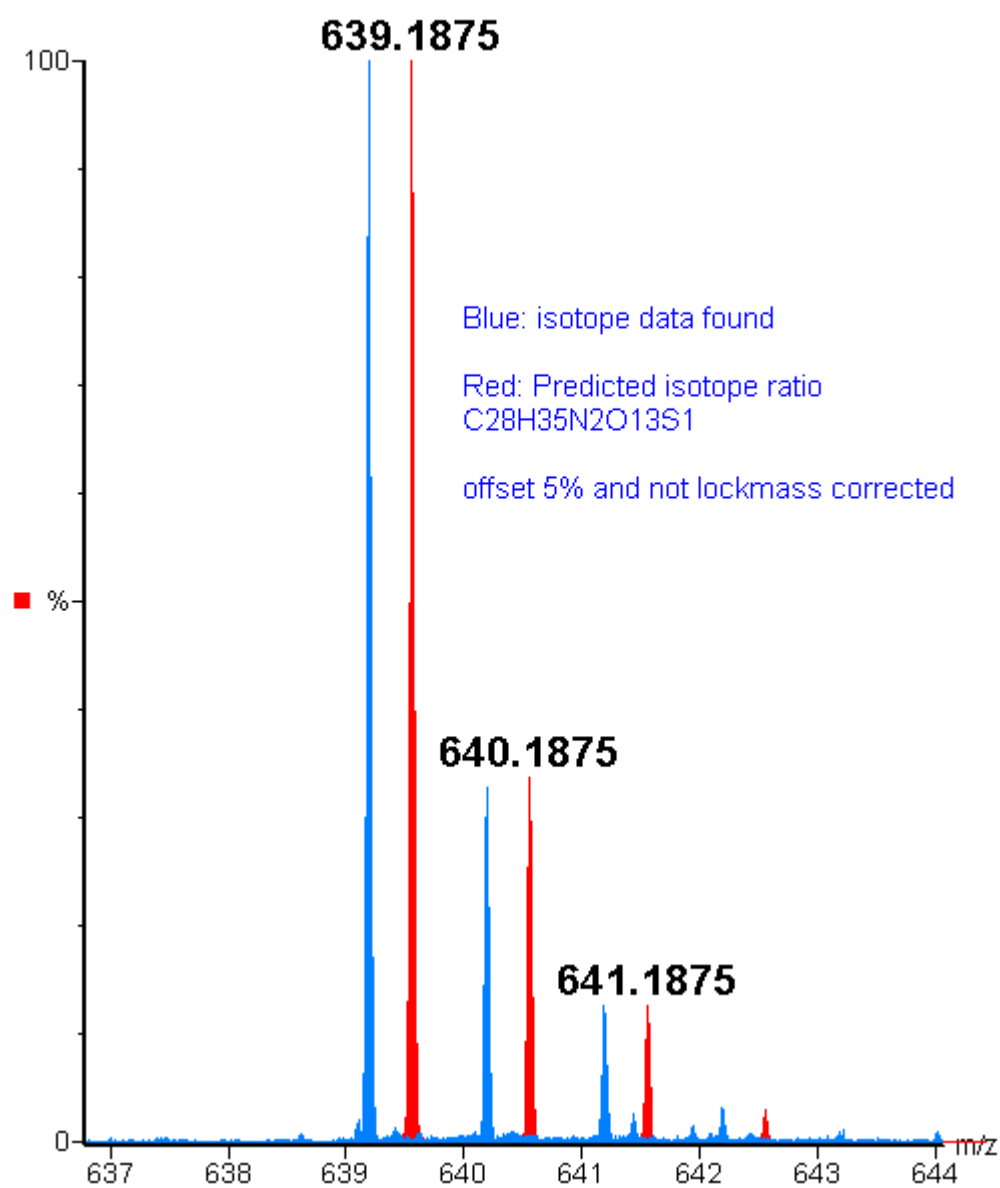
Frag Composition Mass

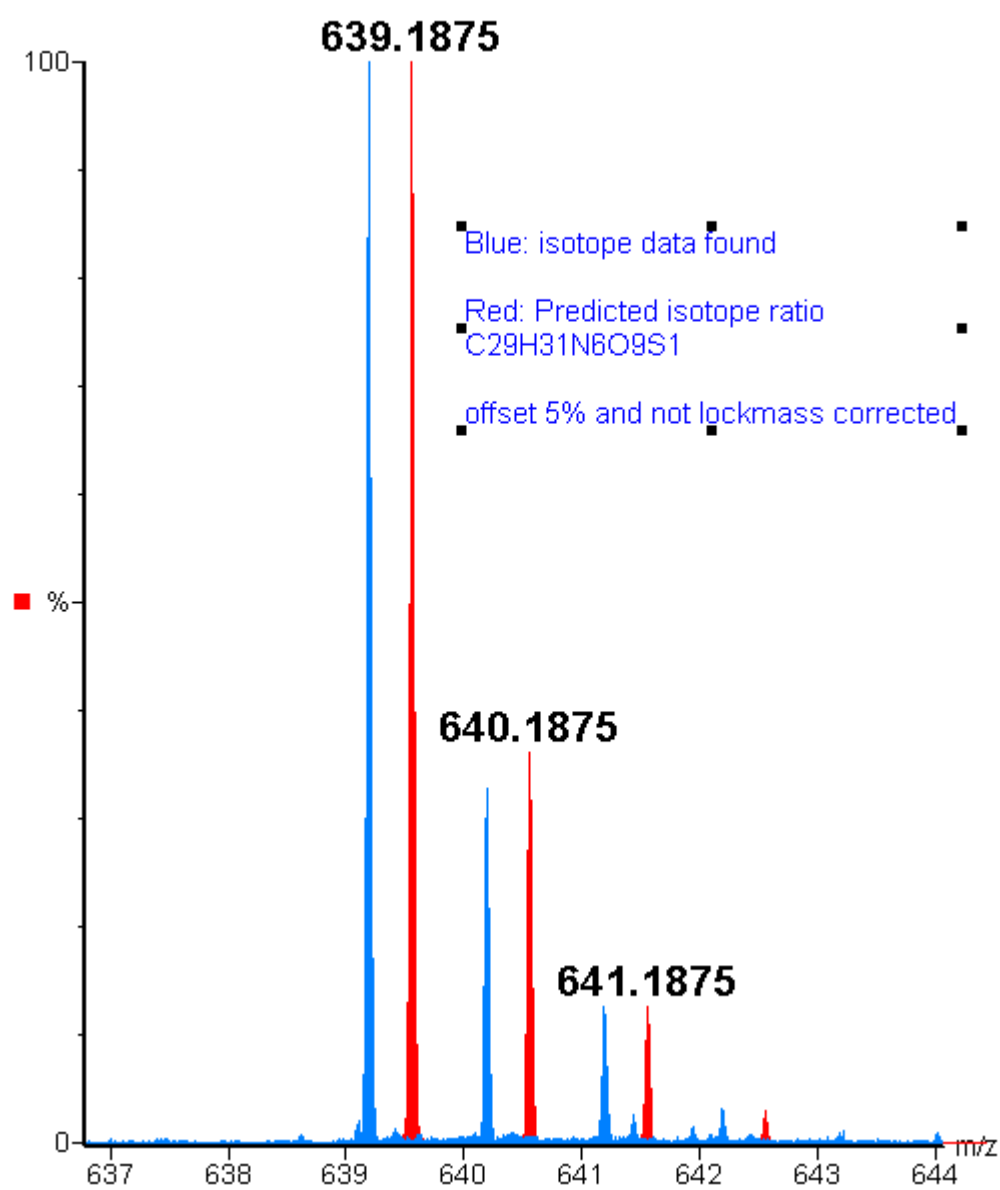
LSdefect CalcDefect MeasDefect

1	A	162	540	541	540
2	C	314	730	722	730
3	AB	324	1060	1066	1060
4	BC	476	1250	1247	1250
5	ABC	638	1790	1788	1780

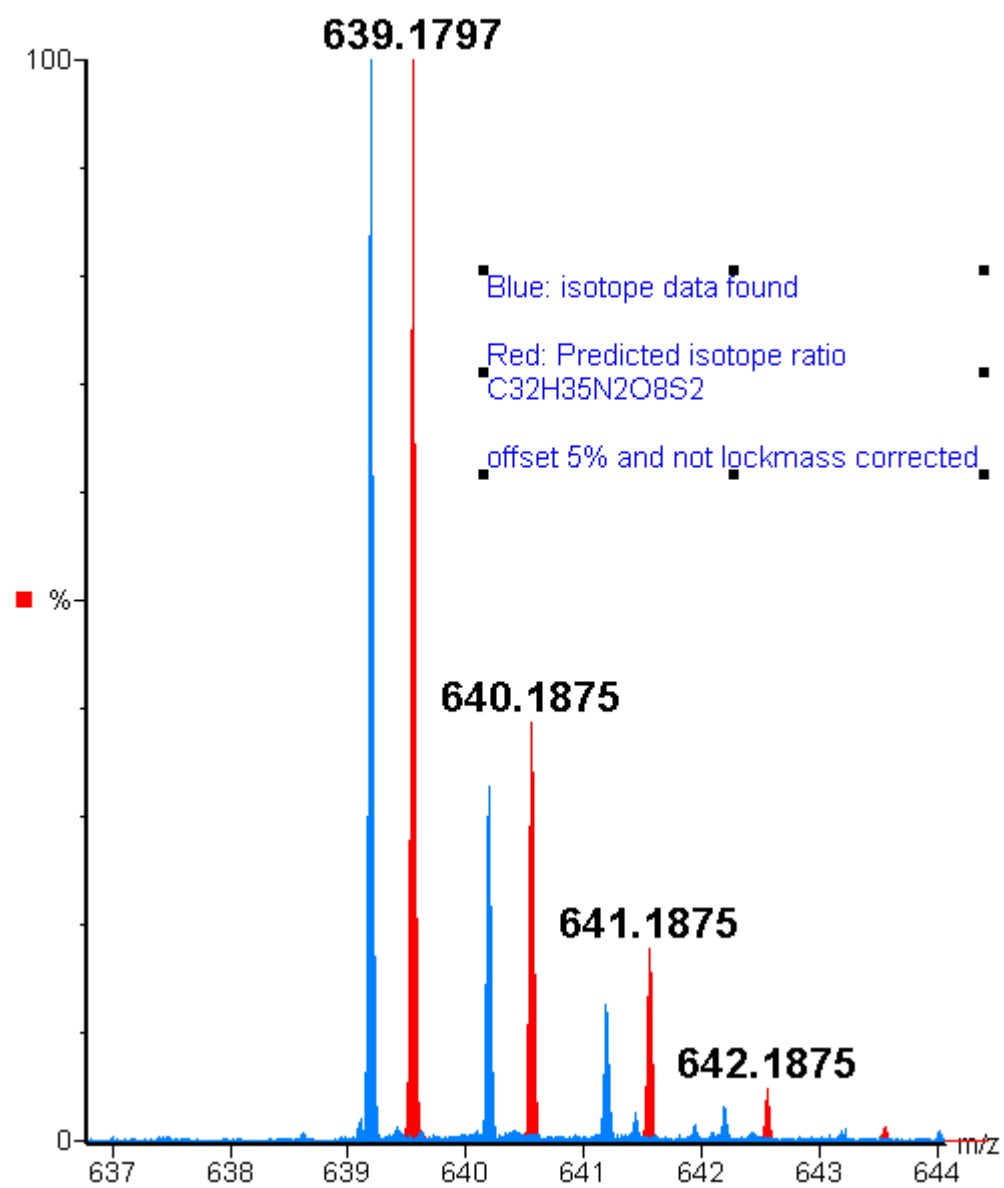
Best Permutation: CBA

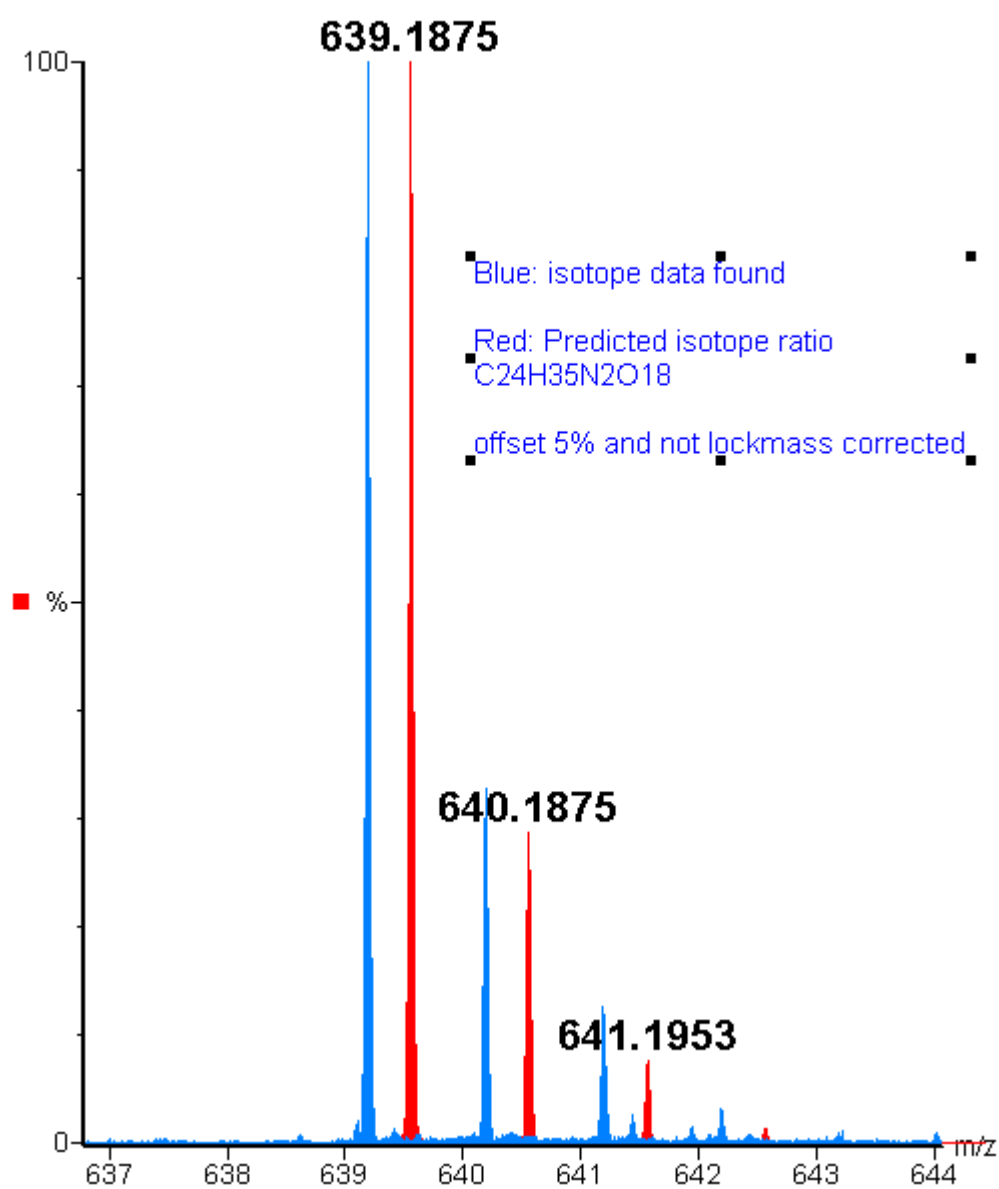
Best Permutation: ABC

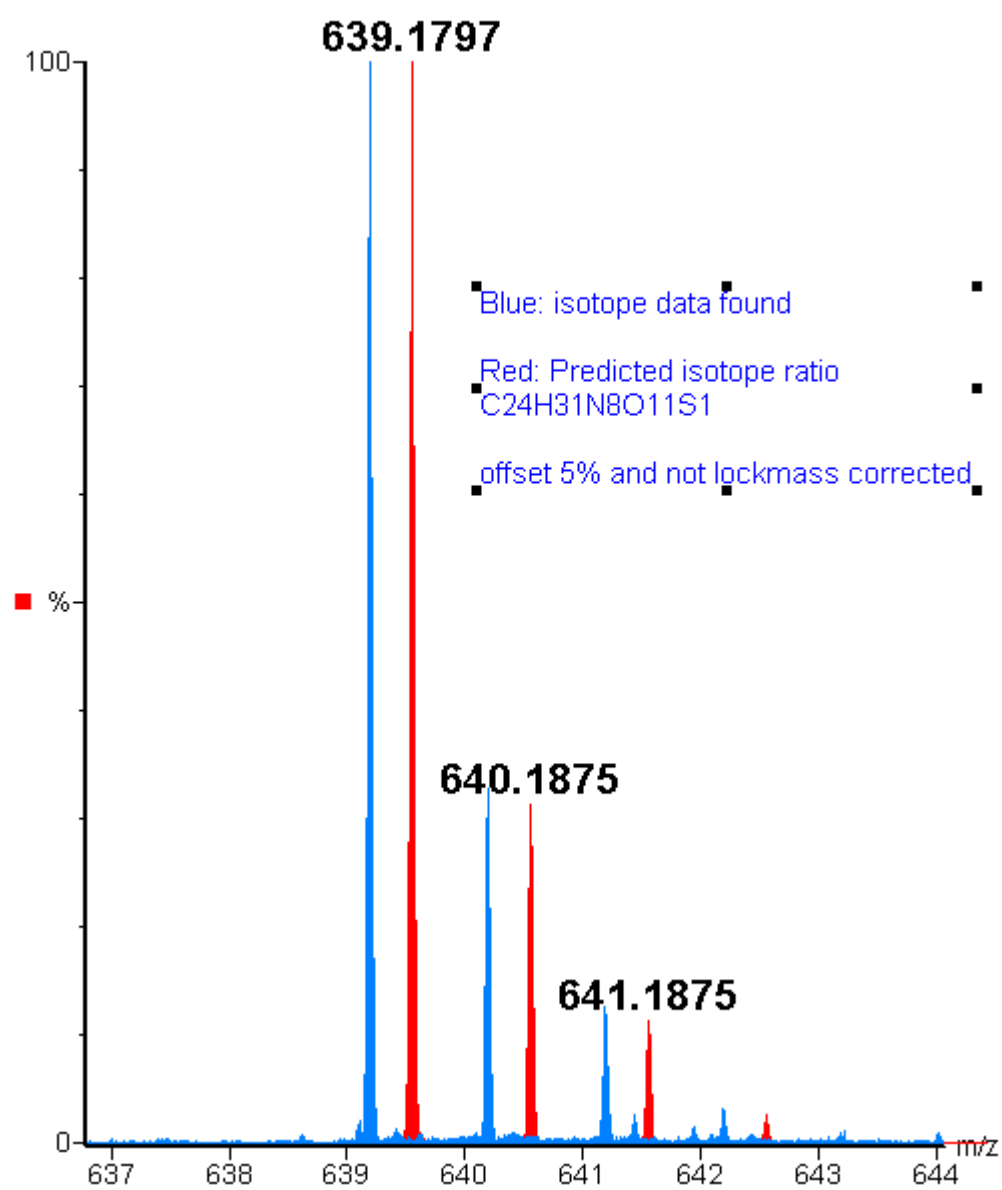


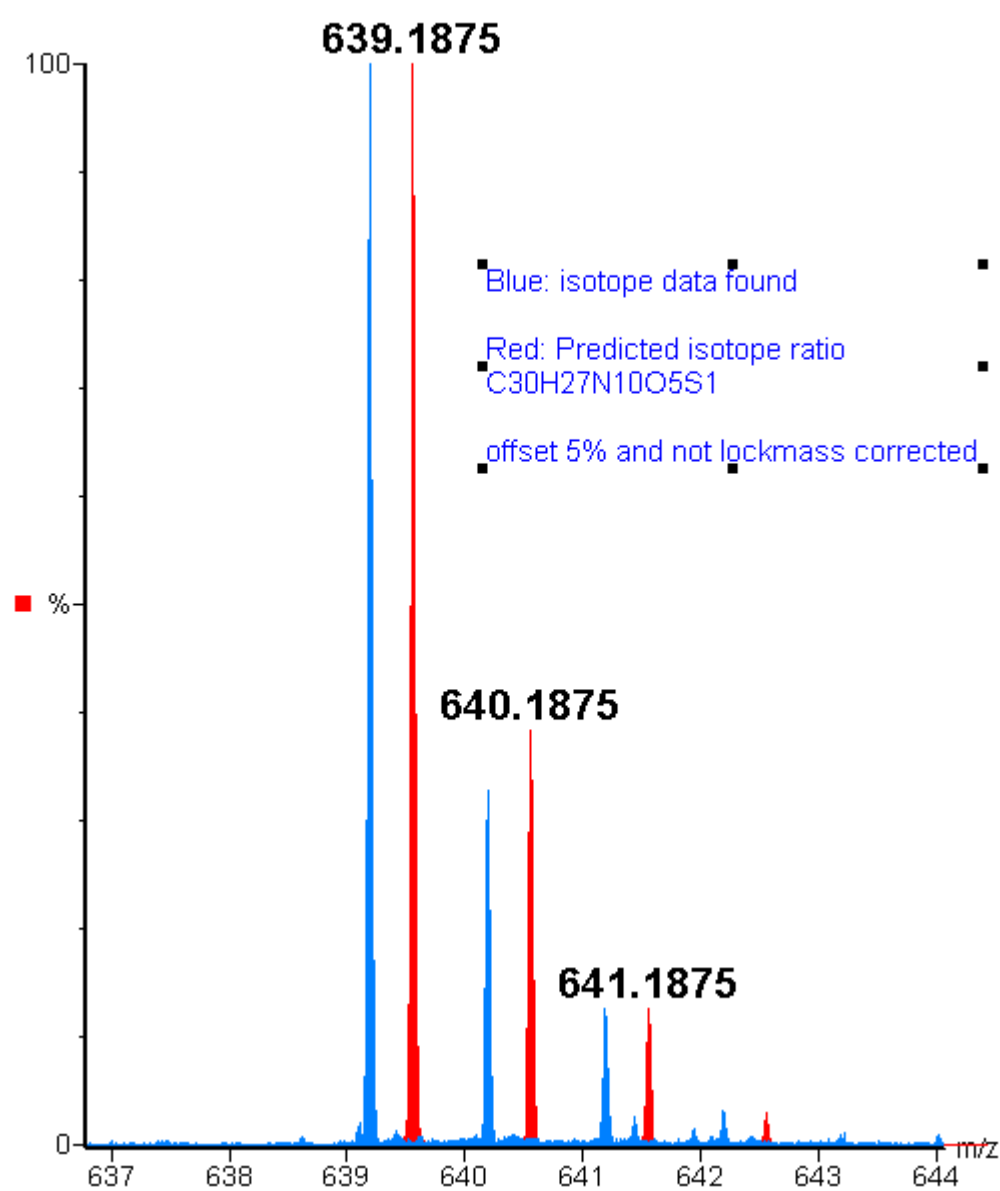












6. Xemilofiban

CID-MSMS data

218

201

0

201

119

0

178

96

0

136

119

0

MS/MS Spectrum

96.0445

2

119.0600

2

125.0603

3

136.0878

47

142.0868

2

176.0721

3

178.0508

17

201.0668

19

217.1096

2

218.0934

100

224.0929

6

359.1720

0

Elemental Composition Used: C₁₈H₂₂N₄O₄S₀Cl₀F₀ Data File: xemilofiban.dat

Minimum Hits Required: 6

Least Square Error per Hit: 5

Maximum Mass Error Accepted: 25

Minimum Coverage in Percent: 65

Compound's MW: 358 Total Number of Ions: 12

95.0367	95	37
118.0522	118	52
124.0525	124	52
135.0800	135	80
141.0790	141	79
175.0643	175	64
177.0430	177	43
200.0590	200	59
216.1018	216	102
217.0856	217	86
223.0851	223	85

358.1642 358 164

Solution Number 1

Linear Fit 3	Coverage 78									
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	8	0	2	0	0	0	124	530	522
Cell D:	7	6	2	0	0	0	0	118	530	530
Cell C:	4	2	0	2	0	0	0	82	60	54
Cell B:	0	3	1	0	0	0	0	17	260	265
Cell A:	0	3	1	0	0	0	0	17	270	265

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
1	D	118	530	530	520
2	E	124	530	522	520
3	A D	135	800	795	800
4	B E	141	790	787	790
5	CD	200	590	584	590
6	A CD	217	860	849	860
7	BC E	223	850	841	850
8	ABCDE	358	1650	1636	1640
9		95	0	0	0
10		175	0	0	0
11		177	0	0	0
12		216	0	0	0

Model Used: W Best Permutation: EBCDA

Model Used: W Best Permutation: BECDA

Model Used: W Best Permutation: ADCEB

Model Used: W Best Permutation: ADCBE

Solution Number 2

Linear Fit 4		Coverage 78								
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	9	3	0	0	0	0	135	800	795
Cell D:	4	2	0	2	0	0	0	82	50	54
Cell C:	5	2	0	1	0	0	0	78	120	105
Cell B:	2	6	0	1	0	0	0	46	410	417
Cell A:	0	3	1	0	0	0	0	17	260	265

Frag Composition		Mass	LSdefect CalcDefect MeasDefect		
1	E	135	800	795	800
2	DE	217	850	849	860
3	BC	124	530	522	520
4	A C	95	380	370	370
5	A CD	177	430	424	430
6	ABC	141	790	787	790
7	ABCD	223	840	841	850
8	ABCDE	358	1640	1636	1640
9		118	0	0	0
10		175	0	0	0
11		200	0	0	0
12		216	0	0	0

Model Used: W Best Permutation: EDACB

Model Used: Y Best Permutation: BCDAE

Model Used: Y Best Permutation: ACDBE

Model Used: W Best Permutation: BCADE

Solution Number 3

Linear Fit 3		Coverage 90								
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	6	2	0	0	0	0	118	530	530
Cell D:	5	5	1	1	0	0	0	95	370	370
Cell C:	4	2	0	2	0	0	0	82	60	54
Cell B:	2	6	0	1	0	0	0	46	420	417
Cell A:	0	3	1	0	0	0	0	17	260	265

Frag Composition			Mass	LSdefect	CalcDefect	MeasDefect
1	E		118	530	530	520
2	D		95	370	370	370
3	C E		200	590	584	590
4	CD		177	430	424	430
5	B D		141	790	787	790
6	BCD		223	850	841	850
7	A E		135	790	795	800
8	A C E		217	850	849	860
9	ABCDE		358	1640	1636	1640
10			124	0	0	0
11			175	0	0	0
12			216	0	0	0

Model Used: W Best Permutation: AECDB

Model Used: W Best Permutation: BDCEA

Solution Number 4

Linear Fit 3		Coverage 78								
	C	H	N	O	S	Cl	F	mass	defect	calcdefect

Cell E:	7	6	2	0	0	0	0	118	520	530
Cell D:	6	7	1	0	0	0	0	93	580	577
Cell C:	4	2	0	2	0	0	0	82	60	54
Cell B:	1	4	0	2	0	0	0	48	210	210
Cell A:	0	3	1	0	0	0	0	17	270	265

Frag Composition Mass			LSdefect	CalcDefect	MeasDefect
1	E	118	520	530	520
2	C E	200	580	584	590
3	CD	175	640	631	640
4	B D	141	790	787	790
5	BCD	223	850	841	850
6	A E	135	790	795	800
7	A C E	217	850	849	860
8	ABCDE	358	1640	1636	1640
9		95	0	0	0
10		124	0	0	0
11		177	0	0	0
12		216	0	0	0

Model Used: W Best Permutation: AECDB

Model Used: W Best Permutation: BDCEA

Total partitions of 5 cells: 1506841

Partitions accounting for less than 6 fragments: 1494296

Number of partitions with required number of fragments: 12545

Number of linked cells rejected: 851

Number of partitions failing least squares criterion: 926

Number of partitions not matching any model: 1940

Number of partitions with contradictory CID-MSMS data: 89

Number of partitions failing MinimumCoverage test: 9743

Number of partitions not fitting the elemental data: 124

Number of partitions duplicated by multisign: 1132

Number of partitions having multiple elemental compositions: 0

Number of Solutions: 4

7. Compound A

CID-MS/MS Data

218

201

0

196

100

97

0

136

119

0

MS/MS Spectrum

97.0282

2

100.0397

5

119.0613

2

136.0881

52

160.0977

3

168.0668

3

176.0707

2

178.0521

2

196.0616

31

201.0670

12

218.0935

100

224.0943

4

242.1040

5

331.1403

3

359.1710

2

377.1826

0

Elemental Composition Used: C₁₈H₂₄N₄O₅S₀Cl₀F₀ Data File: CompoundA.dat

Minimum Hits Required: 6

Least Square Error per Hit: 5

Maximum Mass Error Accepted: 25

Minimum Coverage in Percent: 65

Compound's MW: 376 Total Number of Ions: 16

96.0204 96 20

99.0319 99 32

118.0535 118 53

135.0803 135 80

159.0899 159 90
 167.0590 167 59
 175.0629 175 63
 177.0443 177 44
 195.0538 195 54
 200.0592 200 59
 217.0857 217 86
 223.0865 223 86
 241.0962 241 96
 330.1325 330 132
 358.1632 358 163
 376.1748 376 175

Solution Number 1

Linear Fit 7		Coverage 66								
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	13	1	3	0	0	0	159	910	892
Cell D:	7	3	1	0	0	0	0	101	260	265
Cell C:	4	2	0	2	0	0	0	82	50	54
Cell B:	0	3	1	0	0	0	0	17	280	265
Cell A:	0	3	1	0	0	0	0	17	270	265

Frag Composition		Mass	LSdefect	CalcDefect	MeasDefect
1	A C	99	320	319	320
2	A D	118	530	530	530
3	AB D	135	810	795	800
4	E	159	910	892	900
5	A CD	200	580	584	590

6	ABCD	217	860	849	860
7	C E	241	960	946	960
8	ABCDE	376	1770	1741	1750
9		96	0	0	0
10		167	0	0	0
11		175	0	0	0
12		177	0	0	0
13		195	0	0	0
14		223	0	0	0
15		330	0	0	0
16		358	0	0	0

Model Used: W Best Permutation: ECADB

Model Used: Y Best Permutation: DACBE

Model Used: W Best Permutation: BDACE

Model Used: Y Best Permutation: BACDE

Solution Number 2

Linear Fit 5

Coverage 66

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	10	0	3	0	0	0	142	650	627
Cell D:	7	6	2	0	0	0	0	118	530	530
Cell C:	4	2	0	2	0	0	0	82	60	54
Cell B:	0	3	1	0	0	0	0	17	260	265
Cell A:	0	3	1	0	0	0	0	17	260	265

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	A C	99	320	319	320
2	D	118	530	530	530

3	B D	135	790	795	800
4	A E	159	910	892	900
5	CD	200	590	584	590
6	A CD	217	850	849	860
7	A C E	241	970	946	960
8	ABCDE	376	1760	1741	1750
9		96	0	0	0
10		167	0	0	0
11		175	0	0	0
12		177	0	0	0
13		195	0	0	0
14		223	0	0	0
15		330	0	0	0
16		358	0	0	0

Model Used: W Best Permutation: EACDB

Model Used: W Best Permutation: BDCAE

Solution Number 3

Linear Fit 4

Coverage 74

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	9	3	0	0	0	0	135	800	795
Cell D:	5	4	0	2	0	0	0	96	200	210
Cell C:	4	2	0	2	0	0	0	82	60	54
Cell B:	2	6	0	1	0	0	0	46	430	417
Cell A:	0	3	1	0	0	0	0	17	270	265

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	E	135	800	795	800
---	---	-----	-----	-----	-----

2	D	96	200	210	200
3	C E	217	860	849	860
4	A C	99	330	319	320
5	A CD	195	530	529	540
6	A CDE	330	1330	1324	1320
7	AB D	159	900	892	900
8	ABCD	241	960	946	960
9	ABCDE	376	1760	1741	1750
10		118	0	0	0
11		167	0	0	0
12		175	0	0	0
13		177	0	0	0
14		200	0	0	0
15		223	0	0	0
16		358	0	0	0

Model Used: W Best Permutation: ECADB

Model Used: Y Best Permutation: DACBE

Model Used: W Best Permutation: BDACE

Model Used: Y Best Permutation: BACDE

Solution Number 4

Linear Fit 10	Coverage 74									
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	9	3	0	0	0	0	135	790	795
Cell D:	5	7	1	2	0	0	0	113	460	475
Cell C:	4	2	0	2	0	0	0	82	70	54
Cell B:	2	4	0	0	0	0	0	28	320	312
Cell A:	0	2	0	1	0	0	0	18	100	105

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	E	135	790	795	800
2	C E	217	860	849	860
3	CD	195	530	529	540
4	CDE	330	1320	1324	1320
5	BCD	223	850	841	860
6	BCDE	358	1640	1636	1630
7	AB D	159	880	892	900
8	ABCD	241	950	946	960
9	ABCDE	376	1740	1741	1750
10		96	0	0	0
11		99	0	0	0
12		118	0	0	0
13		167	0	0	0
14		175	0	0	0
15		177	0	0	0
16		200	0	0	0

Model Used: W Best Permutation: ECDBA

Model Used: Y Best Permutation: BDCAE

Model Used: Y Best Permutation: ADCBE

Model Used: W Best Permutation: ABDCE

Solution Number 5

Linear Fit 10	Coverage 76									
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	9	3	0	0	0	0	135	780	795
Cell D:	5	7	1	2	0	0	0	113	470	475
Cell C:	4	0	0	1	0	0	0	64	-40	-51

Cell B:	2	6	0	1	0	0	0	46	420	417
Cell A:	0	2	0	1	0	0	0	18	120	105

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	E	135	780	795	800
2	B D	159	890	892	900
3	CD	177	430	424	440
4	A CD	195	550	529	540
5	A C E	217	860	849	860
6	BCD	223	850	841	860
7	ABCD	241	970	946	960
8	A CDE	330	1330	1324	1320
9	BCDE	358	1630	1636	1630
10	ABCDE	376	1750	1741	1750
11		96	0	0	0
12		99	0	0	0
13		118	0	0	0
14		167	0	0	0
15		175	0	0	0
16		200	0	0	0

Model Used: Y Best Permutation: ECDAB

Model Used: Y Best Permutation: ACDEB

Solution Number 6

Linear Fit 9	Coverage 76									
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	9	3	0	0	0	0	135	790	795
Cell D:	5	5	1	1	0	0	0	95	360	370

Cell C:	4	2	0	2	0	0	0	82	70	54
Cell B:	2	6	0	1	0	0	0	46	430	417
Cell A:	0	2	0	1	0	0	0	18	110	105

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	E	135	790	795	800
2	C E	217	860	849	860
3	CD	177	430	424	440
4	BCD	223	860	841	860
5	BCDE	358	1650	1636	1630
6	A CD	195	540	529	540
7	A CDE	330	1330	1324	1320
8	AB D	159	900	892	900
9	ABCD	241	970	946	960
10	ABCDE	376	1760	1741	1750
11		96	0	0	0
12		99	0	0	0
13		118	0	0	0
14		167	0	0	0
15		175	0	0	0
16		200	0	0	0

Model Used: Y Best Permutation: BDCAE

Model Used: Y Best Permutation: ADCBE

Solution Number 7

Linear Fit 6 Coverage 69

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	9	3	0	0	0	0	135	800	795

Cell D:	5	7	1	2	0	0	0	113	490	475
Cell C:	3	2	0	1	0	0	0	54	100	105
Cell B:	2	6	0	1	0	0	0	46	410	417
Cell A:	1	0	0	1	0	0	0	28	-50	-51

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	E	135	800	795	800
2	CD	167	590	580	590
3	B D	159	900	892	900
4	A C E	217	850	849	860
5	A CD	195	540	529	540
6	A CDE	330	1340	1324	1320
7	ABCD	241	950	946	960
8	ABCDE	376	1750	1741	1750
9		96	0	0	0
10		99	0	0	0
11		118	0	0	0
12		175	0	0	0
13		177	0	0	0
14		200	0	0	0
15		223	0	0	0
16		358	0	0	0

Model Used: Y Best Permutation: ECDAB

Model Used: W Best Permutation: EACDB

Model Used: Y Best Permutation: ACDEB

Model Used: W Best Permutation: BDCAE

Solution Number 8

Linear Fit 4 Coverage 69

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	9	3	0	0	0	0	135	790	795
Cell D:	4	7	1	1	0	0	0	85	540	526
Cell C:	4	2	0	2	0	0	0	82	60	54
Cell B:	2	6	0	1	0	0	0	46	420	417
Cell A:	1	0	0	1	0	0	0	28	-60	-51

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
1	E	135	790	795	800
2	C E	217	850	849	860
3	CD	167	600	580	590
4	A CD	195	540	529	540
5	A CDE	330	1330	1324	1320
6	AB D	159	900	892	900
7	ABCD	241	960	946	960
8	ABCDE	376	1750	1741	1750
9		96	0	0	0
10		99	0	0	0
11		118	0	0	0
12		175	0	0	0
13		177	0	0	0
14		200	0	0	0
15		223	0	0	0
16		358	0	0	0

Model Used: W Best Permutation: ECDAB

Model Used: Y Best Permutation: BDCAE

Model Used: Y Best Permutation: ADCBE

Model Used: W Best Permutation: BADCE

Solution Number 9

Linear Fit 5

Coverage 66

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	9	3	0	0	0	0	135	800	795
Cell D:	4	2	0	2	0	0	0	82	50	54
Cell C:	4	2	0	2	0	0	0	82	60	54
Cell B:	2	6	0	1	0	0	0	46	430	417
Cell A:	1	5	1	0	0	0	0	31	410	421

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	E	135	800	795	800
2	ABC	159	900	892	900
3	A CD	195	520	529	540
4	C E	217	860	849	860
5	ABCD	241	950	946	960
6	A CDE	330	1320	1324	1320
7	ABCDE	376	1750	1741	1750
8		96	0	0	0
9		99	0	0	0
10		118	0	0	0
11		167	0	0	0
12		175	0	0	0
13		177	0	0	0
14		200	0	0	0
15		223	0	0	0
16		358	0	0	0

Model Used: X Best Permutation: ECDBA

Model Used: X Best Permutation: ECDAB
 Model Used: X Best Permutation: ECBDA
 Model Used: XY Best Permutation: ECADB
 Model Used: X Best Permutation: ECBAD
 Model Used: XY Best Permutation: ECABD
 Model Used: X Best Permutation: DCEBA
 Model Used: X Best Permutation: DCEAB
 Model Used: X Best Permutation: BCEDA
 Model Used: X Best Permutation: ACEDB
 Model Used: X Best Permutation: BCEAD
 Model Used: X Best Permutation: ACEBD
 Model Used: X Best Permutation: DCBEA
 Model Used: XY Best Permutation: DCAEB
 Model Used: X Best Permutation: BCDEA
 Model Used: X Best Permutation: ACDEB
 Model Used: XY Best Permutation: BCAED
 Model Used: X Best Permutation: ACBED
 Model Used: X Best Permutation: DCBAE
 Model Used: X Best Permutation: DCABE
 Model Used: Y Best Permutation: DACBE
 Model Used: X Best Permutation: BCDAE
 Model Used: X Best Permutation: ACDBE
 Model Used: X Best Permutation: BCADE
 Model Used: X Best Permutation: ACBDE
 Model Used: Y Best Permutation: BACDE

Solution Number 10

Linear Fit 2	Coverage 66								
	C	H	N	O	S	Cl	F	mass	defect calcdefect

Cell E:	5	7	1	2	0	0	0	113	470	475
Cell D:	6	4	2	0	0	0	0	104	390	374
Cell C:	4	2	0	2	0	0	0	82	60	54
Cell B:	2	6	0	1	0	0	0	46	430	417
Cell A:	1	5	1	0	0	0	0	31	400	421

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	A D	135	790	795	800
2	B E	159	900	892	900
3	C E	195	530	529	540
4	DE	217	860	849	860
5	BC E	241	960	946	960
6	A CDE	330	1320	1324	1320
7	ABCDE	376	1750	1741	1750
8		96	0	0	0
9		99	0	0	0
10		118	0	0	0
11		167	0	0	0
12		175	0	0	0
13		177	0	0	0
14		200	0	0	0
15		223	0	0	0
16		358	0	0	0

Model Used: Y Best Permutation: CEDBA

Model Used: Y Best Permutation: BEDCA

Solution Number 11

Linear Fit 7 Coverage 69

C	H	N	O	S	Cl	F	mass	defect	calcdefect
---	---	---	---	---	----	---	------	--------	------------

Cell E:	5	7	1	2	0	0	0	113	470	475
Cell D:	6	7	1	0	0	0	0	93	580	577
Cell C:	4	2	0	2	0	0	0	82	60	54
Cell B:	2	6	0	1	0	0	0	46	440	417
Cell A:	1	2	2	0	0	0	0	42	210	218

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	C E	195	530	529	540
2	CD	175	640	631	630
3	B E	159	910	892	900
4	BC E	241	970	946	960
5	A D	135	790	795	800
6	A CD	217	850	849	860
7	A CDE	330	1320	1324	1320
8	ABCDE	376	1760	1741	1750
9	96	0	0	0	
10	99	0	0	0	
11	118	0	0	0	
12	167	0	0	0	
13	177	0	0	0	
14	200	0	0	0	
15	223	0	0	0	
16	358	0	0	0	

Model Used: W Best Permutation: BECDA

Model Used: W Best Permutation: ADCEB

Total partitions of 5 cells: 1973903

Partitions accounting for less than 6 fragments: 1937303
Number of partitions with required number of fragments: 36600
Number of linked cells rejected: 349
Number of partitions failing least squares criterion: 876
Number of partitions not matching any model: 717
Number of partitions with contradictory CID-MSMS data: 39
Number of partitions failing MinimumCoverage test: 35310
Number of partitions not fitting the elemental data: 76
Number of partitions duplicated by multisign: 778
Number of partitions having multiple elemental compositions: 0

8. Compound B

MS/MS data

477

315

0

325

163

0

MS/MS Spectrum

163.0614

5

315.0807

100

325.1135

16

477.1330

18

639.1859

0

9. Compound C

CID-MS/MS data

336

218

201

136

0

218

201

0

201

119

0

136

119

0

MS/MS Spectrum

119.0601

5

136.0869

63

176.0724

3

201.0660

34

218.0923

95

336.1459

100

337.1257

2

353.1722

0

Elemental Composition Used: C18H20N6O2S0Cl0F0 Data File: CompoundC.dat

Minimum Hits Required: 6

Least Square Error per Hit: 5

Maximum Mass Error Accepted: 25

Minimum Coverage in Percent: 65

Compound's MW: 352 Total Number of Ions: 8

118.0523	118	52
135.0791	135	79
175.0646	175	65
200.0582	200	58
217.0845	217	84
335.1381	335	138
336.1179	336	118
352.1644	352	164

Solution Number 1

Linear Fit 3 Coverage 94

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	6	2	0	0	0	0	118	550	530
Cell D:	7	6	2	0	0	0	0	118	530	530

Cell C:	4	2	0	2	0	0	0	82	50	54
Cell B:	0	3	1	0	0	0	0	17	260	265
Cell A:	0	3	1	0	0	0	0	17	260	265

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
1	D	118	530	530	520
2	A D	135	790	795	790
3	CD	200	580	584	580
4	A CD	217	840	849	840
5	A CDE	335	1390	1379	1380
6	ABCDE	352	1650	1644	1640
7		175	0	0	0
8		336	0	0	0

Model Used: Y Best Permutation: ECDBA

Model Used: W Best Permutation: ECDAB

Model Used: W Best Permutation: EADCB

Model Used: Y Best Permutation: EADBC

Model Used: XY Best Permutation: ADECB

Model Used: WXY Best Permutation: CDAEB

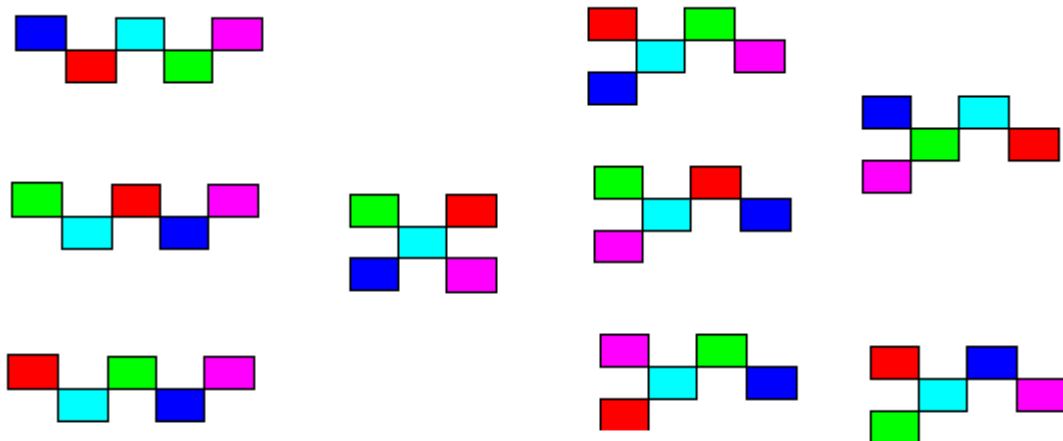
Model Used: WXY Best Permutation: ADCEB

Model Used: XY Best Permutation: CDABE

Model Used: XY Best Permutation: BDCAE

Note: Redundant Configurations have been removed for clarity.

Below are some graphically represented configurations:



Total partitions of 5 cells: 1371422

Partitions accounting for less than 6 fragments: 1369668

Number of partitions with required number of fragments: 1754

Number of linked cells rejected: 898

Number of partitions failing least squares criterion: 19

Number of partitions not matching any model: 422

Number of partitions with contradictory CID-MSMS data: 1205

Number of partitions failing MinimumCoverage test: 0

Number of partitions not fitting the elemental data: 0

Number of partitions duplicated by multisign: 791

Number of partitions having multiple elemental compositions: 0

10. Compound D

CID-MS/MS data

412

342

254

184

166

140

0

342

254

184

166

0

254

184

166

0

MS/MS Spectrum

140.1087

7

166.1241

88

184.1349

14

236.1657

35

254.1760

48

324.2178

21

340.2131

2

342.2289

78

412.2699

100

430.2801

9

500.3222

0

Elemental Composition Used: C26H45N1O8S0Cl0F0

Data File: CompoundD.dat

Minimum Hits Required: 6

Least Square Error per Hit: 5

Maximum Mass Error Accepted: 25

Minimum Coverage in Percent: 65

Compound's MW: 499 Total Number of Ions: 11

139.1009 139 101

165.1163 165 116

183.1271 183 127

235.1579 235 158

253.1682 253 168

323.2100 323 210

339.2053 339 205

341.2211 341 221

411.2621 411 262

429.2723 429 272

499.3144 499 314

Solution Number 1

Linear Fit 4 Coverage 70

C	H	N	O	S	Cl	F	mass	defect	calcdefect
---	---	---	---	---	----	---	------	--------	------------

Cell E:	14	21	1	2	0	0	0	235	1570	1567
Cell D:	4	8	0	2	0	0	0	88	510	522
Cell C:	4	8	0	2	0	0	0	88	520	522
Cell B:	4	6	0	1	0	0	0	70	420	417
Cell A:	0	2	0	1	0	0	0	18	120	105

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	E	235	1570	1567	1580
2	A E	253	1690	1672	1680
3	AB E	323	2110	2089	2100
4	A C E	341	2210	2194	2210
5	ABC E	411	2630	2611	2620
6	A CDE	429	2720	2716	2720
7	ABCDE	499	3140	3133	3140
8		139	0	0	0
9		165	0	0	0
10		183	0	0	0
11		339	0	0	0

Model Used: X Best Permutation: EADCB

Model Used: X Best Permutation: EADBC

Model Used: X Best Permutation: EACDB

Model Used: X Best Permutation: EABDC

Model Used: XY Best Permutation: EACBD

Model Used: X Best Permutation: EABCD

Model Used: X Best Permutation: DECBA

Model Used: X Best Permutation: DECAB

Model Used: X Best Permutation: DEBCA

Model Used: XY Best Permutation: DEACB

Model Used: X Best Permutation: DEBAC

Model Used: XY Best Permutation: DEABC
Model Used: X Best Permutation: CEDBA
Model Used: X Best Permutation: CEDAB
Model Used: X Best Permutation: BEDCA
Model Used: X Best Permutation: AEDCB
Model Used: X Best Permutation: BEDAC
Model Used: X Best Permutation: AEDBC
Model Used: X Best Permutation: CEBDA
Model Used: XY Best Permutation: CEADB
Model Used: X Best Permutation: BECDA
Model Used: X Best Permutation: AECDB
Model Used: XY Best Permutation: BEADC
Model Used: X Best Permutation: AEBDC
Model Used: X Best Permutation: CEBAD
Model Used: XY Best Permutation: CEABD
Model Used: XY Best Permutation: BECAD
Model Used: XY Best Permutation: AECBD
Model Used: WXY Best Permutation: BEACD
Model Used: X Best Permutation: AEBCD
Model Used: W Best Permutation: DCEAB
Model Used: XY Best Permutation: DAECB
Model Used: XY Best Permutation: DAEBC
Model Used: XY Best Permutation: CAEDB
Model Used: XY Best Permutation: BAEDC
Model Used: XY Best Permutation: CAEBD
Model Used: WXY Best Permutation: BAECD
Model Used: W Best Permutation: DCAEB
Model Used: X Best Permutation: DACEB
Model Used: X Best Permutation: DABEC
Model Used: X Best Permutation: CADEB

Model Used: X Best Permutation: BADEC

Model Used: X Best Permutation: CABED

Model Used: XY Best Permutation: BACED

Model Used: X Best Permutation: DACBE

Model Used: X Best Permutation: DABCE

Model Used: X Best Permutation: CADBE

Model Used: X Best Permutation: BADCE

Model Used: X Best Permutation: CABDE

Model Used: X Best Permutation: BACDE

Solution Number 2

Linear Fit 4

Coverage 66

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	10	17	1	2	0	0	0	183	1260	1255
Cell D:	4	8	0	2	0	0	0	88	530	522
Cell C:	4	8	0	2	0	0	0	88	520	522
Cell B:	4	6	0	1	0	0	0	70	420	417
Cell A:	4	6	0	1	0	0	0	70	420	417

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	E	183	1260	1255	1270
2	A E	253	1680	1672	1680
3	AB E	323	2100	2089	2100
4	A C E	341	2200	2194	2210
5	ABC E	411	2620	2611	2620
6	A CDE	429	2730	2716	2720
7	ABCDE	499	3150	3133	3140
8		139	0	0	0

9	165	0	0	0
10	235	0	0	0
11	339	0	0	0

Model Used: X Best Permutation: EADCB

Model Used: X Best Permutation: EADBC

Model Used: X Best Permutation: EACDB

Model Used: X Best Permutation: EABDC

Model Used: XY Best Permutation: EACBD

Model Used: X Best Permutation: EABCD

Model Used: X Best Permutation: DECBA

Model Used: X Best Permutation: DECAB

Model Used: X Best Permutation: DEBCA

Model Used: XY Best Permutation: DEACB

Model Used: X Best Permutation: DEBAC

Model Used: XY Best Permutation: DEABC

Model Used: X Best Permutation: CEDBA

Model Used: X Best Permutation: CEDAB

Model Used: X Best Permutation: BEDCA

Model Used: X Best Permutation: AEDCB

Model Used: X Best Permutation: BEDAC

Model Used: X Best Permutation: AEDBC

Model Used: X Best Permutation: CEBDA

Model Used: XY Best Permutation: CEADB

Model Used: X Best Permutation: BECDA

Model Used: X Best Permutation: AECDB

Model Used: XY Best Permutation: BEADC

Model Used: X Best Permutation: AEBDC

Model Used: X Best Permutation: CEBAD

Model Used: XY Best Permutation: CEABD

Model Used: XY Best Permutation: BECAD

Model Used: XY Best Permutation: AECBD
 Model Used: WXY Best Permutation: BEACD
 Model Used: X Best Permutation: AEBCD
 Model Used: W Best Permutation: DCEAB
 Model Used: XY Best Permutation: DAECB
 Model Used: XY Best Permutation: DAEBC
 Model Used: XY Best Permutation: CAEDB
 Model Used: XY Best Permutation: BAEDC
 Model Used: XY Best Permutation: CAEBD
 Model Used: WXY Best Permutation: BAECD
 Model Used: W Best Permutation: DCAEB
 Model Used: X Best Permutation: DACEB
 Model Used: X Best Permutation: DABEC
 Model Used: X Best Permutation: CADEB
 Model Used: X Best Permutation: BADEC
 Model Used: X Best Permutation: CABED
 Model Used: XY Best Permutation: BACED
 Model Used: X Best Permutation: DACBE
 Model Used: X Best Permutation: DABCE
 Model Used: X Best Permutation: CADBE
 Model Used: X Best Permutation: BADCE
 Model Used: X Best Permutation: CABDE
 Model Used: X Best Permutation: BACDE

Solution Number 3

Linear Fit 7	Coverage 88									
	C	H	N	O	S	Cl	F	mass	LSdefect	calcdefect
Cell E:	10	15	1	1	0	0	0	165	1160	1150
Cell D:	4	8	0	2	0	0	0	88	520	522

Cell C:	4	8	0	2	0	0	0	88	540	522
Cell B:	4	8	0	2	0	0	0	88	510	522
Cell A:	4	6	0	1	0	0	0	70	410	417

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	E	165	1160	1150	1160
2	A E	235	1570	1567	1580
3	B E	253	1670	1672	1680
4	AB E	323	2080	2089	2100
5	BC E	341	2210	2194	2210
6	ABC E	411	2620	2611	2620
7	BCDE	429	2730	2716	2720
8	ABCDE	499	3140	3133	3140
9		139	0	0	0
10		183	0	0	0
11		339	0	0	0

Model Used: X Best Permutation: DECBA

Model Used: X Best Permutation: DECAB

Model Used: X Best Permutation: DEBCA

Model Used: X Best Permutation: DEACB

Model Used: XY Best Permutation: DEBAC

Model Used: X Best Permutation: DEABC

Model Used: X Best Permutation: CEDBA

Model Used: X Best Permutation: CEDAB

Model Used: X Best Permutation: BEDCA

Model Used: X Best Permutation: AEDCB

Model Used: X Best Permutation: BEDAC

Model Used: X Best Permutation: AEDBC

Model Used: X Best Permutation: CEBDA

Model Used: X Best Permutation: CEADB
 Model Used: X Best Permutation: BECDA
 Model Used: X Best Permutation: AECDB
 Model Used: X Best Permutation: BEADC
 Model Used: XY Best Permutation: AEBDC
 Model Used: XY Best Permutation: CEBAD
 Model Used: X Best Permutation: CEABD
 Model Used: XY Best Permutation: BECAD
 Model Used: XY Best Permutation: AECBD
 Model Used: X Best Permutation: BEACD
 Model Used: WXY Best Permutation: AEBCD
 Model Used: Y Best Permutation: DBECA
 Model Used: Y Best Permutation: CBEDA
 Model Used: W Best Permutation: DCBEA

Solution Number 4

Linear Fit 2		Coverage 70								
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	10	13	1	0	0	0	0	147	1050	1045
Cell D:	4	10	0	3	0	0	0	106	630	627
Cell C:	4	8	0	2	0	0	0	88	520	522
Cell B:	4	8	0	2	0	0	0	88	520	522
Cell A:	4	6	0	1	0	0	0	70	420	417

Frag Composition		Mass	LSdefect	CalcDefect	MeasDefect
1	B E	235		1570	1567
2	DE	253		1680	1672
3	A DE	323		2100	2089

4	B DE	341	2200	2194	2210
5	AB DE	411	2620	2611	2620
6	BCDE	429	2720	2716	2720
7	ABCDE	499	3140	3133	3140
8		139	0	0	0
9		165	0	0	0
10		183	0	0	0
11		339	0	0	0

Model Used: X Best Permutation: DECBA

Model Used: X Best Permutation: DECAB

Model Used: X Best Permutation: DEBCA

Model Used: X Best Permutation: DEACB

Model Used: XY Best Permutation: DEBAC

Model Used: X Best Permutation: DEABC

Model Used: XY Best Permutation: CEDBA

Model Used: X Best Permutation: CEDAB

Model Used: XY Best Permutation: BEDCA

Model Used: X Best Permutation: AEDCB

Model Used: XY Best Permutation: BEDAC

Model Used: XY Best Permutation: AEDBC

Model Used: X Best Permutation: CEBDA

Model Used: X Best Permutation: CEADB

Model Used: X Best Permutation: BECDA

Model Used: X Best Permutation: AECDB

Model Used: X Best Permutation: BEADC

Model Used: XY Best Permutation: AEBDC

Model Used: X Best Permutation: CEBAD

Model Used: X Best Permutation: CEABD

Model Used: X Best Permutation: BECAD

Model Used: X Best Permutation: AECBD

Model Used: X Best Permutation: BEACD
 Model Used: X Best Permutation: AEBCD
 Model Used: Y Best Permutation: CDEAB
 Model Used: Y Best Permutation: ADECB
 Model Used: W Best Permutation: ADEBC
 Model Used: W Best Permutation: CBEDA

Total partitions of 5 cells: 8646698

Partitions accounting for less than 6 fragments: 8641866

Number of partitions with required number of fragments: 4832

Number of linked cells rejected: 694

Number of partitions failing least squares criterion: 0

Number of partitions not matching any model: 180

Number of partitions with contradictory CID-MSMS data: 978

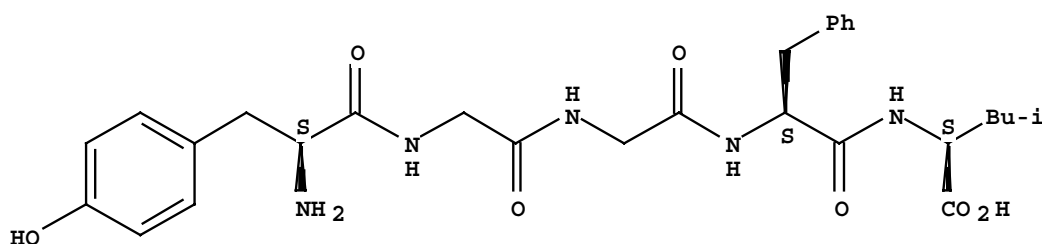
Number of partitions failing MinimumCoverage test: 3405

Number of partitions not fitting the elemental data: 2

Number of partitions duplicated by multiple assignments: 431

Number of partitions having multiple elemental compositions: 0

11. Leucine enkephalin



MSMS data

278

221

177

136

120

0

397

323

278

234

221

177

136

120

0

278

136

0

MSMS Spectrum

120.0813

9

132.1034

2

136.0766

7

177.1033

15

205.0983

22

221.0932

16

234.1250

5

262.1204

15

278.1141

72

279.1709

26

323.1399

3

336.1931

7

347.2091

4

375.2062

5

380.1626

5

393.2147

5

397.1881

100

425.1826

23

443.1948

3

465.2513

2

493.2454

3

510.2717

6.2

538.2664

5

556.2791

0

Spectrum of leucine enkephalin

Elemental Composition Used: C₂₈H₃₇N₅O₇S₀Cl₀F₀ Data File: leuenki.dat

Minimum Hits Required: 6

Least Square Error per Hit: 5

Maximum Mass Error Accepted: 25

Minimum Coverage in Percent: 50

Compound's MW: 555 Total Number of Ions: 24

119.0735 119 73

131.0956 131 96

135.0688 135 69

176.0955 176 95

204.0905 204 90

220.0854 220 85

233.1172 233 117

261.1126 261 113

277.1063 277 106

278.1631 278 163

322.1321 322 132

335.1853 335 185

346.2013 346 201
 374.1984 374 198
 379.1548 379 155
 392.2069 392 207
 396.1803 396 180
 424.1748 424 175
 442.1870 442 187
 464.2435 464 243
 492.2376 492 238
 509.2639 509 264
 537.2586 537 259
 555.2713 555 271

Solution Number 1

Linear Fit 5		Coverage 55								
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	11	12	2	3	0	0	0	220	860	845
Cell D:	7	13	1	3	0	0	0	159	900	892
Cell C:	8	9	1	0	0	0	0	119	730	733
Cell B:	2	0	0	1	0	0	0	40	-40	-51
Cell A:	0	3	1	0	0	0	0	17	250	265

Frag Composition		Mass	LSdefect	CalcDefect	MeasDefect
1	C	119	730	733	730
2	ABC	176	940	947	950
3	E	220	860	845	850
4	AB E	277	1070	1059	1060
5	CD	278	1630	1625	1630

6	ABCD	335	1840	1839	1850
7	BC E	379	1550	1527	1550
8	ABC E	396	1800	1792	1800
9	ABCDE	555	2700	2684	2710
10		131	0	0	0
11		135	0	0	0
12		204	0	0	0
13		233	0	0	0
14		261	0	0	0
15		322	0	0	0
16		346	0	0	0
17		374	0	0	0
18		392	0	0	0
19		424	0	0	0
20		442	0	0	0
21		464	0	0	0
22		492	0	0	0
23		509	0	0	0
24		537	0	0	0

Model Used: Y Best Permutation: EBCAD

Model Used: Y Best Permutation: ABCED

Solution Number 2

Linear Fit 5

Coverage 52

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	13	13	3	3	0	0	0	259	940	954
Cell D:	6	13	1	2	0	0	0	131	960	943
Cell C:	8	9	1	0	0	0	0	119	740	733
Cell B:	1	0	0	1	0	0	0	28	-60	-51

Cell A: 0 2 0 1 0 0 0 18 120 105

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	D	131	960	943	960
2	C	119	740	733	730
3	CDE	509	2640	2630	2640
4	BCD	278	1640	1625	1630
5	BCDE	537	2580	2579	2590
6	A E	277	1060	1059	1060
7	A C E	396	1800	1792	1800
8	ABC E	424	1740	1741	1750
9	ABCDE	555	2700	2684	2710
10		135	0	0	0
11		176	0	0	0
12		204	0	0	0
13		220	0	0	0
14		233	0	0	0
15		261	0	0	0
16		322	0	0	0
17		335	0	0	0
18		346	0	0	0
19		374	0	0	0
20		379	0	0	0
21		392	0	0	0
22		442	0	0	0
23		464	0	0	0
24		492	0	0	0

Model Used: Y Best Permutation: DCEBA

Model Used: Y Best Permutation: BCEDA

Solution Number 3

Linear Fit 8

Coverage 52

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	9	11	1	3	0	0	0	181	730	736
Cell D:	6	13	1	2	0	0	0	131	940	943
Cell C:	8	9	1	0	0	0	0	119	730	733
Cell B:	4	4	2	1	0	0	0	96	340	323
Cell A:	1	0	0	1	0	0	0	28	-40	-51

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	D	131	940	943	960
2	C	119	730	733	730
3	B E	277	1070	1059	1060
4	BC E	396	1800	1792	1800
5	BCD	346	2010	1999	2010
6	A CD	278	1630	1625	1630
7	ABC E	424	1760	1741	1750
8	ABCD	374	1970	1948	1980
9	ABCDE	555	2700	2684	2710
10		135	0	0	0
11		176	0	0	0
12		204	0	0	0
13		220	0	0	0
14		233	0	0	0
15		261	0	0	0
16		322	0	0	0
17		335	0	0	0

18	379	0	0	0
19	392	0	0	0
20	442	0	0	0
21	464	0	0	0
22	492	0	0	0
23	509	0	0	0
24	537	0	0	0

Model Used: Y Best Permutation: DCBAE

Model Used: Y Best Permutation: ACBDE

Solution Number 4

	Linear Fit 9							Coverage 56		
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	5	6	2	3	0	0	0	142	390	377
Cell D:	8	9	1	1	0	0	0	135	680	682
Cell C:	6	13	1	2	0	0	0	131	960	943
Cell B:	8	9	1	0	0	0	0	119	720	733
Cell A:	1	0	0	1	0	0	0	28	-40	-51

Frag Composition		Mass	LSdefect	CalcDefect	MeasDefect
1	D	135	680	682	690
2	DE	277	1070	1059	1060
3	C	131	960	943	960
4	B	119	720	733	730
5	B E	261	1110	1110	1130
6	B DE	396	1790	1792	1800
7	BC E	392	2070	2053	2070
8	AB DE	424	1750	1741	1750

9	ABC	278	1640	1625	1630
10	ABCDE	555	2710	2684	2710
11		176	0	0	0
12		204	0	0	0
13		220	0	0	0
14		233	0	0	0
15		322	0	0	0
16		335	0	0	0
17		346	0	0	0
18		374	0	0	0
19		379	0	0	0
20		442	0	0	0
21		464	0	0	0
22		492	0	0	0
23		509	0	0	0
24		537	0	0	0

Model Used: Y Best Permutation: CBEAD

Model Used: Y Best Permutation: ABECD

Solution Number 5

Linear Fit 10

Coverage 53

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	5	6	2	3	0	0	0	142	390	377
Cell D:	8	9	1	1	0	0	0	135	680	682
Cell C:	8	9	1	0	0	0	0	119	740	733
Cell B:	6	11	1	1	0	0	0	113	830	838
Cell A:	1	2	0	2	0	0	0	46	70	54

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	D	135	680	682	690
2	DE	277	1070	1059	1060
3	C	119	740	733	730
4	C E	261	1130	1110	1130
5	CDE	396	1810	1792	1800
6	BC E	374	1960	1948	1980
7	BCDE	509	2640	2630	2640
8	A CDE	442	1880	1846	1870
9	ABC	278	1640	1625	1630
10	ABCDE	555	2710	2684	2710
11		131	0	0	0
12		176	0	0	0
13		204	0	0	0
14		220	0	0	0
15		233	0	0	0
16		322	0	0	0
17		335	0	0	0
18		346	0	0	0
19		379	0	0	0
20		392	0	0	0
21		424	0	0	0
22		464	0	0	0
23		492	0	0	0
24		537	0	0	0

Model Used: Y Best Permutation: BCEAD

Model Used: Y Best Permutation: ACEBD

Solution Number 6

Linear Fit 4 Coverage 52

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	13	1	3	0	0	0	159	900	892
Cell D:	8	9	1	1	0	0	0	135	680	682
Cell C:	8	9	1	0	0	0	0	119	730	733
Cell B:	2	3	1	2	0	0	0	73	170	163
Cell A:	3	3	1	1	0	0	0	69	220	214

Frag Composition		Mass	LSdefect	CalcDefect	MeasDefect
1	D	135	680	682	690
2	C	119	730	733	730
3	C E	278	1630	1625	1630
4	A D	204	900	896	900
5	AB D	277	1070	1059	1060
6	ABC	261	1120	1110	1130
7	ABCD	396	1800	1792	1800
8	ABCDE	555	2700	2684	2710
9		131	0	0	0
10		176	0	0	0
11		220	0	0	0
12		233	0	0	0
13		322	0	0	0
14		335	0	0	0
15		346	0	0	0
16		374	0	0	0
17		379	0	0	0
18		392	0	0	0
19		424	0	0	0
20		442	0	0	0

21	464	0	0	0
22	492	0	0	0
23	509	0	0	0
24	537	0	0	0

Model Used: W Best Permutation: ECBAD

Model Used: Y Best Permutation: DACBE

Model Used: W Best Permutation: DABCE

Model Used: Y Best Permutation: BACDE

Total partitions of 5 cells: 14641666

Partitions accounting for less than 6 fragments: 14265615

Number of partitions with required number of fragments: 376051

Number of linked cells rejected: 512

Number of partitions failing least squares criterion: 2571

Number of partitions not matching any model: 113

Number of partitions with contradictory CID-MSMS data: 21

Number of partitions failing MinimumCoverage test: 374327

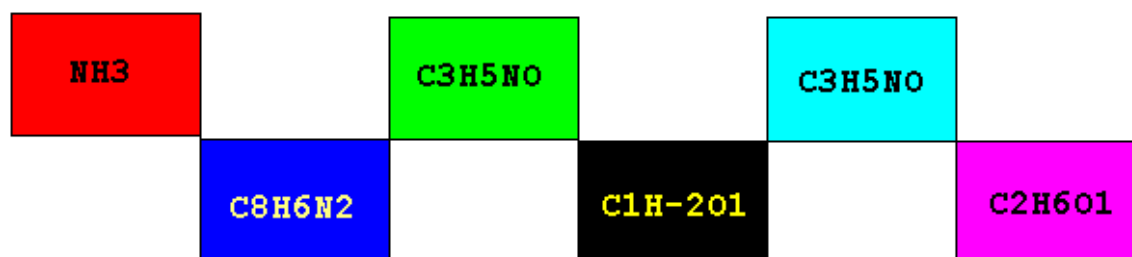
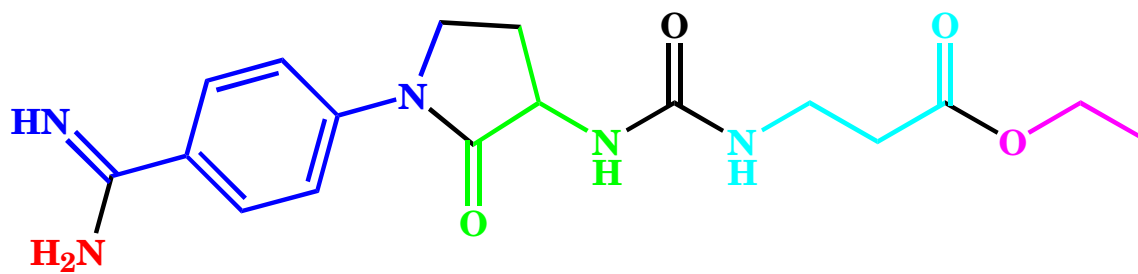
Number of partitions not fitting the elemental data: 6

Number of partitions duplicated by multisign: 1505

Number of partitions having multiple elemental compositions: 0

12. Orbofiban

The structure of orbofiban is shown above its hypothetical 6-cell modular structure. The data was analyzed using the 5-cell program.



CID-MS/MS data

245

228

0

219

202

148

0

MS/MS Spectrum

148.0886

17

191.1306

5

202.0991

6

219.1254

85

228.0783

6

245.1044

100

299.1152

2

316.1410

2

334.1518

2

362.1833

0

Elemental Composition Used: C₁₇H₂₃N₅O₄S₀Cl₀F₀ Data File: Orbo.dat

Minimum Hits Required: 6

Least Square Error per Hit: 5

Maximum Mass Error Accepted: 25

Minimum Coverage in Percent: 65

Compound's MW: 361 Total Number of Ions: 11

147.0808 147 81

190.1228 190 123

201.0913 201 91

218.1176 218 118

227.0705 227 70

244.0966 244 97

298.1074 298 107

315.1332 315 133

333.1440 333 144

333.1792 333 179

361.1755 361 175

Solution Number 1

Linear Fit 2

Coverage 69

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	11	11	3	1	0	0	0	201	910	900
Cell D:	3	2	0	1	0	0	0	54	90	105
Cell C:	2	6	0	1	0	0	0	46	410	417
Cell B:	1	1	1	1	0	0	0	43	70	58
Cell A:	0	3	1	0	0	0	0	17	270	265

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	E	201	910	900	910
2	B E	244	980	958	970
3	B DE	298	1070	1063	1070
4	A E	218	1180	1165	1180
5	AB DE	315	1340	1328	1330
6	ABCDE	361	1750	1745	1750
7		147	0	0	0
8		190	0	0	0
9		227	0	0	0
10		333	0	0	0
11		333	0	0	0

Model Used: X Best Permutation: DECBA

Model Used: X Best Permutation: DECAB

Model Used: X Best Permutation: DEBCA

Model Used: X Best Permutation: DEACB

Model Used: XY Best Permutation: DEBAC
 Model Used: XY Best Permutation: DEABC
 Model Used: X Best Permutation: CEDBA
 Model Used: X Best Permutation: CEDAB
 Model Used: X Best Permutation: BEDCA
 Model Used: X Best Permutation: AEDCB
 Model Used: XY Best Permutation: BEDAC
 Model Used: XY Best Permutation: AEDBC
 Model Used: X Best Permutation: CEBDA
 Model Used: X Best Permutation: CEADB
 Model Used: X Best Permutation: BECDA
 Model Used: X Best Permutation: AECDB
 Model Used: XY Best Permutation: BEADC
 Model Used: WXY Best Permutation: AEBDC
 Model Used: XY Best Permutation: CEBAD
 Model Used: X Best Permutation: CEABD
 Model Used: X Best Permutation: BECAD
 Model Used: X Best Permutation: AECBD
 Model Used: X Best Permutation: BEACD
 Model Used: XY Best Permutation: AEBCD
 Model Used: Y Best Permutation: DBECA
 Model Used: W Best Permutation: DBEAC
 Model Used: Y Best Permutation: CBEDA
 Model Used: W Best Permutation: CAEBD
 Model Used: W Best Permutation: CDBEA

Solution Number 2

Linear Fit 3

Coverage 69

C H N O S Cl F mass defect calcdefect

Cell E:	9	5	3	0	0	0	0	155	500	483
Cell D:	3	7	1	2	0	0	0	89	470	475
Cell C:	3	2	0	1	0	0	0	54	110	105
Cell B:	2	6	0	1	0	0	0	46	410	417
Cell A:	0	3	1	0	0	0	0	17	260	265

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	DE	244	970	958	970
2	CDE	298	1080	1063	1070
3	B E	201	910	900	910
4	A CDE	315	1340	1328	1330
5	AB E	218	1170	1165	1180
6	ABCDE	361	1750	1745	1750
7		147	0	0	0
8		190	0	0	0
9		227	0	0	0
10		333	0	0	0
11		333	0	0	0

Model Used: X Best Permutation: DECBA

Model Used: X Best Permutation: DECAB

Model Used: X Best Permutation: DEBCA

Model Used: X Best Permutation: DEACB

Model Used: X Best Permutation: DEBAC

Model Used: X Best Permutation: DEABC

Model Used: X Best Permutation: CEDBA

Model Used: X Best Permutation: CEDAB

Model Used: X Best Permutation: BEDCA

Model Used: X Best Permutation: AEDCB

Model Used: XY Best Permutation: BEDAC

Model Used: XY Best Permutation: AEDBC

Model Used: X Best Permutation: CEBDA

Model Used: X Best Permutation: CEADB

Model Used: X Best Permutation: BECDA

Model Used: X Best Permutation: AECDB

Model Used: X Best Permutation: BEADC

Model Used: X Best Permutation: AEBDC

Model Used: X Best Permutation: CEBAD

Model Used: X Best Permutation: CEABD

Model Used: X Best Permutation: BECAD

Model Used: X Best Permutation: AECBD

Model Used: X Best Permutation: BEACD

Model Used: X Best Permutation: AEBCD

Solution Number 3

Linear Fit 5

Coverage 81

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	8	9	3	0	0	0	0	147	820	795
Cell D:	4	3	1	2	0	0	0	97	160	163
Cell C:	3	2	0	1	0	0	0	54	80	105
Cell B:	2	6	0	1	0	0	0	46	420	417
Cell A:	0	3	1	0	0	0	0	17	270	265

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	E	147	820	795	810
2	DE	244	980	958	970
3	C E	201	900	900	910
4	CDE	298	1060	1063	1070

5	A C E	218	1170	1165	1180
6	A CDE	315	1330	1328	1330
7	ABCDE	361	1750	1745	1750
8		190	0	0	0
9		227	0	0	0
10		333	0	0	0
11		333	0	0	0

Model Used: XY Best Permutation: DECBA

Model Used: WXY Best Permutation: DECAB

Model Used: X Best Permutation: DEBCA

Model Used: XY Best Permutation: DEACB

Model Used: X Best Permutation: DEBAC

Model Used: X Best Permutation: DEABC

Model Used: X Best Permutation: CEDBA

Model Used: XY Best Permutation: CEDAB

Model Used: X Best Permutation: BEDCA

Model Used: XY Best Permutation: AEDCB

Model Used: X Best Permutation: BEDAC

Model Used: X Best Permutation: AEDBC

Model Used: X Best Permutation: CEBDA

Model Used: XY Best Permutation: CEADB

Model Used: XY Best Permutation: BECDA

Model Used: XY Best Permutation: AECDB

Model Used: X Best Permutation: BEADC

Model Used: X Best Permutation: AEBDC

Model Used: X Best Permutation: CEBAD

Model Used: X Best Permutation: CEABD

Model Used: X Best Permutation: BECAD

Model Used: X Best Permutation: AECBD

Model Used: X Best Permutation: BEACD

Model Used: X Best Permutation: AEBCD

Model Used: W Best Permutation: BDECA

Model Used: W Best Permutation: ACEDB

Model Used: Y Best Permutation: BCEAD

Model Used: Y Best Permutation: ACEBD

Model Used: W Best Permutation: BACED

Solution Number 4

Linear Fit 4

Coverage 75

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	9	5	3	0	0	0	0	155	490	483
Cell D:	3	4	0	2	0	0	0	72	220	210
Cell C:	3	5	1	1	0	0	0	71	360	370
Cell B:	2	6	0	1	0	0	0	46	420	417
Cell A:	0	3	1	0	0	0	0	17	270	265

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	DE	227	710	693	700
2	CDE	298	1070	1063	1070
3	B E	201	910	900	910
4	A DE	244	980	958	970
5	A CDE	315	1340	1328	1330
6	AB E	218	1180	1165	1180
7	ABCDE	361	1760	1745	1750
8		147	0	0	0
9		190	0	0	0
10		333	0	0	0
11		333	0	0	0

Model Used: X Best Permutation: DECBA
 Model Used: X Best Permutation: DECAB
 Model Used: X Best Permutation: DEBCA
 Model Used: X Best Permutation: DEACB
 Model Used: X Best Permutation: DEBAC
 Model Used: X Best Permutation: DEABC
 Model Used: X Best Permutation: CEDBA
 Model Used: X Best Permutation: CEDAB
 Model Used: X Best Permutation: BEDCA
 Model Used: X Best Permutation: AEDCB
 Model Used: XY Best Permutation: BEDAC
 Model Used: XY Best Permutation: AEDBC
 Model Used: X Best Permutation: CEBDA
 Model Used: X Best Permutation: CEADB
 Model Used: X Best Permutation: BECDA
 Model Used: X Best Permutation: AECDB
 Model Used: X Best Permutation: BEADC
 Model Used: X Best Permutation: AEBDC
 Model Used: X Best Permutation: CEBAD
 Model Used: X Best Permutation: CEABD
 Model Used: X Best Permutation: BECAD
 Model Used: X Best Permutation: AECBD
 Model Used: X Best Permutation: BEACD
 Model Used: X Best Permutation: AEBCD

Solution Number 5

Linear Fit 2	Coverage 81									
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	8	9	3	0	0	0	0	147	810	795

Cell D:	4	0	0	2	0	0	0	80	-110	-102
Cell C:	3	5	1	1	0	0	0	71	370	370
Cell B:	2	6	0	1	0	0	0	46	410	417
Cell A:	0	3	1	0	0	0	0	17	260	265

Frag	Composition	Mass	LSdefect	CalcDefect	MeasDefect
------	-------------	------	----------	------------	------------

1	E	147	810	795	810
2	DE	227	700	693	700
3	C E	218	1180	1165	1180
4	CDE	298	1070	1063	1070
5	A DE	244	960	958	970
6	A CDE	315	1330	1328	1330
7	ABCDE	361	1740	1745	1750
8		190	0	0	0
9		201	0	0	0
10		333	0	0	0
11		333	0	0	0

Model Used: X Best Permutation: DECBA

Model Used: XY Best Permutation: DECAB

Model Used: X Best Permutation: DEBCA

Model Used: XY Best Permutation: DEACB

Model Used: X Best Permutation: DEBAC

Model Used: X Best Permutation: DEABC

Model Used: XY Best Permutation: CEDBA

Model Used: WXY Best Permutation: CEDAB

Model Used: XY Best Permutation: BEDCA

Model Used: XY Best Permutation: AEDCB

Model Used: X Best Permutation: BEDAC

Model Used: X Best Permutation: AEDBC

Model Used:	X	Best Permutation:	CEBDA
Model Used:	XY	Best Permutation:	CEADB
Model Used:	X	Best Permutation:	BECDA
Model Used:	XY	Best Permutation:	AECDB
Model Used:	X	Best Permutation:	BEADC
Model Used:	X	Best Permutation:	AEBDC
Model Used:	X	Best Permutation:	CEBAD
Model Used:	X	Best Permutation:	CEABD
Model Used:	X	Best Permutation:	BECAD
Model Used:	X	Best Permutation:	AECBD
Model Used:	X	Best Permutation:	BEACD
Model Used:	X	Best Permutation:	AEBCD
Model Used:	W	Best Permutation:	ADECB
Model Used:	Y	Best Permutation:	BDEAC
Model Used:	Y	Best Permutation:	ADEBC
Model Used:	W	Best Permutation:	BCEDA
Model Used:	W	Best Permutation:	BADEC

Solution Number 6

Linear Fit 8	Coverage 87									
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	8	6	2	0	0	0	0	130	550	530
Cell D:	4	3	1	2	0	0	0	97	150	163
Cell C:	3	5	1	1	0	0	0	71	350	370
Cell B:	2	6	0	1	0	0	0	46	430	417
Cell A:	0	3	1	0	0	0	0	17	270	265

Frag Composition	Mass	LSdefect	CalcDefect	MeasDefect
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1	DE	227	700	693	700
2	C E	201	900	900	910
3	CDE	298	1050	1063	1070
4	A E	147	820	795	810
5	A DE	244	970	958	970
6	A C E	218	1170	1165	1180
7	A CDE	315	1320	1328	1330
8	ABCDE	361	1750	1745	1750
9		190	0	0	0
10		333	0	0	0
11		333	0	0	0

Model Used: X Best Permutation: DECBA

Model Used: XY Best Permutation: DECAB

Model Used: X Best Permutation: DEBCA

Model Used: XY Best Permutation: DEACB

Model Used: X Best Permutation: DEBAC

Model Used: X Best Permutation: DEABC

Model Used: X Best Permutation: CEDBA

Model Used: XY Best Permutation: CEDAB

Model Used: X Best Permutation: BEDCA

Model Used: XY Best Permutation: AEDCB

Model Used: X Best Permutation: BEDAC

Model Used: X Best Permutation: AEDBC

Model Used: X Best Permutation: CEBDA

Model Used: XY Best Permutation: CEADB

Model Used: X Best Permutation: BECDA

Model Used: XY Best Permutation: AECDB

Model Used: X Best Permutation: BEADC

Model Used: X Best Permutation: AEBDC

Model Used: X Best Permutation: CEBAD

Model Used: X Best Permutation: CEABD

Model Used: X Best Permutation: BECAD

Model Used: X Best Permutation: AECBD

Model Used: X Best Permutation: BEACD

Model Used: X Best Permutation: AEBCD

Solution Number 7

Linear Fit 1	Coverage 69									
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	8	10	4	0	0	0	0	162	910	904
Cell D:	4	2	0	2	0	0	0	82	60	54
Cell C:	2	7	1	1	0	0	0	61	510	526
Cell B:	2	4	0	0	0	0	0	28	310	312
Cell A:	1	0	0	1	0	0	0	28	-40	-51

Frag Composition			Mass	LSdefect	CalcDefect	MeasDefect
1	B	E	190	1220	1216	1230
2	AB	E	218	1180	1165	1180
3	DE		244	970	958	970
4	A	CDE	333	1440	1433	1440
5	BCDE		333	1790	1796	1790
6	ABCDE		361	1750	1745	1750
7			147	0	0	0
8			201	0	0	0
9			227	0	0	0
10			298	0	0	0
11			315	0	0	0

Model Used: X Best Permutation: DECBA

Model Used: X Best Permutation: DECAB
Model Used: X Best Permutation: DEBCA
Model Used: X Best Permutation: DEACB
Model Used: X Best Permutation: DEBAC
Model Used: X Best Permutation: DEABC
Model Used: X Best Permutation: CEDBA
Model Used: X Best Permutation: CEDAB
Model Used: X Best Permutation: BEDCA
Model Used: X Best Permutation: AEDCB
Model Used: XY Best Permutation: BEDAC
Model Used: XY Best Permutation: AEDBC
Model Used: X Best Permutation: CEBDA
Model Used: X Best Permutation: CEADB
Model Used: X Best Permutation: BECDA
Model Used: X Best Permutation: AECDB
Model Used: X Best Permutation: BEADC
Model Used: X Best Permutation: AEBDC
Model Used: X Best Permutation: CEBAD
Model Used: X Best Permutation: CEABD
Model Used: X Best Permutation: BECAD
Model Used: X Best Permutation: AECBD
Model Used: X Best Permutation: BEACD
Model Used: X Best Permutation: AEBDCD

Total partitions of 5 cells: 1578197

Partitions accounting for less than 6 fragments: 1573768

Number of partitions with required number of fragments: 4429

Number of linked cells rejected: 260

Number of partitions failing least squares criterion: 526

Number of partitions not matching any model: 48

Number of partitions with contradictory CID-MSMS data: 82

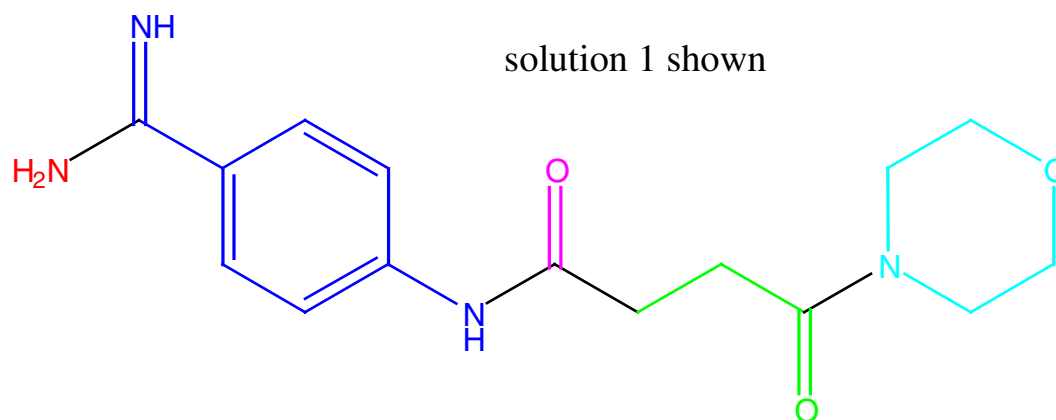
Number of partitions failing MinimumCoverage test: 3525

Number of partitions not fitting the elemental data: 58

Number of partitions duplicated by multisign: 77

Number of partitions having multiple elemental compositions: 0

13. Compound E



CID-MS/MS data

218

201

0

170

142

0

136

119

0

MS/MS spectrum

136.0874

20

142.0867

6

170.0816

100

201.0664

11

218.0927

47

305.1608

0

Elemental Composition Used: C15H20N4O3S0Cl0F0 Data File: CompoundE.dat

Minimum Hits Required: 6

Least Square Error per Hit: 5

Maximum Mass Error Accepted: 25

Minimum Coverage in Percent: 65

Compound's MW: 304 Total Number of Ions: 6

135.0796 135 80

141.0789 141 79

169.0738 169 74

200.0586 200 59

217.0849 217 85

304.1530 304 153

Solution Number 1

Linear Fit 3

Coverage 100

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	6	2	0	0	0	0	118	520	530
Cell D:	4	9	1	1	0	0	0	87	670	682
Cell C:	3	2	0	1	0	0	0	54	120	105
Cell B:	1	0	0	1	0	0	0	28	-60	-51
Cell A:	0	3	1	0	0	0	0	17	280	265

Frag Composition Mass

LSdefect CalcDefect MeasDefect

1	CD	141	790	787	790
2	BC E	200	580	584	590
3	BCD	169	730	736	740
4	A E	135	800	795	800
5	ABC E	217	860	849	850
6	ABCDE	304	1530	1531	1530

Model Used: W Best Permutation: AEBCD

Model Used: Y Best Permutation: DCEBA

Model Used: Y Best Permutation: BCEDA

Model Used: W Best Permutation: DCBEA

Solution Number 2

Linear Fit 3

Coverage 100

	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	8	0	2	0	0	0	124	530	522
Cell D:	4	0	2	0	0	0	0	76	70	62
Cell C:	3	9	1	0	0	0	0	59	730	733
Cell B:	1	0	0	1	0	0	0	28	-50	-51
Cell A:	0	3	1	0	0	0	0	17	250	265

Frag Composition

Mass

LSdefect

CalcDefect

MeasDefect

1	CD	135	800	795	800
2	A E	141	780	787	790
3	AB E	169	730	736	740
4	DE	200	600	584	590
5	A DE	217	850	849	850
6	ABCDE	304	1530	1531	1530

Model Used: Y Best Permutation: BEDAC

Model Used: Y Best Permutation: AEDBC

Model Used: W Best Permutation: CDEAB

Model Used: W Best Permutation: BAEDC

Solution Number 3

	Linear Fit 2							Coverage 100		
	C	H	N	O	S	Cl	F	mass	defect	calcdefect
Cell E:	7	6	2	0	0	0	0	118	540	530
Cell D:	4	2	0	2	0	0	0	82	50	54
Cell C:	3	9	1	0	0	0	0	59	750	733
Cell B:	1	0	0	1	0	0	0	28	-60	-51
Cell A:	0	3	1	0	0	0	0	17	260	265

Frag Composition		Mass	LSdefect	CalcDefect	MeasDefect	
1	DE	200		590	584	590
2	CD	141		800	787	790
3	BCD	169		740	736	740
4	A E	135		800	795	800
5	A DE	217		850	849	850
6	ABCDE	304		1540	1531	1530

Model Used: W Best Permutation: AEDCB

Model Used: Y Best Permutation: CDEBA

Model Used: Y Best Permutation: BDECA

Model Used: W Best Permutation: BCDEA

Total partitions of 5 cells: 589400

Partitions accounting for less than 6 fragments: 589239
Number of partitions with required number of fragments: 161
Number of linked cells rejected: 60
Number of partitions failing least squares criterion: 44
Number of partitions not matching any model: 75
Number of partitions with contradictory CID-MSMS data: 32
Number of partitions failing MinimumCoverage test: 0
Number of partitions not fitting the elemental data: 6
Number of partitions duplicated by multisign: 59
Monte In: 160 Monte Out: 160
Number of partitions having multiple elemental compositions: 0