

Skyline fault observed regularly: **Occasionally missing integration limits for peaks at random**. Report generated contains N/A values for integration. Integration limits cannot be adjusted, because they are missing for some peaks in the first place. Most transitions are shown correctly and even if integration limits are not the way they might be ideally, they can be adjusted and the report contains useful values for those.

- Molecule interface
- DIA
- Transition list with > 100 entries
- Transitions are defined by Explicit Retention Time
- Transition list is correct – automatically generated by my own code, no systematic errors

Variation of Explicit Retention Time has in some cases resolved issue, but not always. Some peaks / transitions remain without integration limits. Zooming in, reintegrating, re loading transition list and data does not help. Issue occurs both when loading transition lists manually and via windows batch files using Skyline runner.

The following 3 slides show an example file with three transitions (for simplicity). The two first shown have integration limits (all OK), the third one doesn't!

How can Skyline be forced to display integration limits so that these can be manually adjusted and a report with actual values for each transition can be generated?

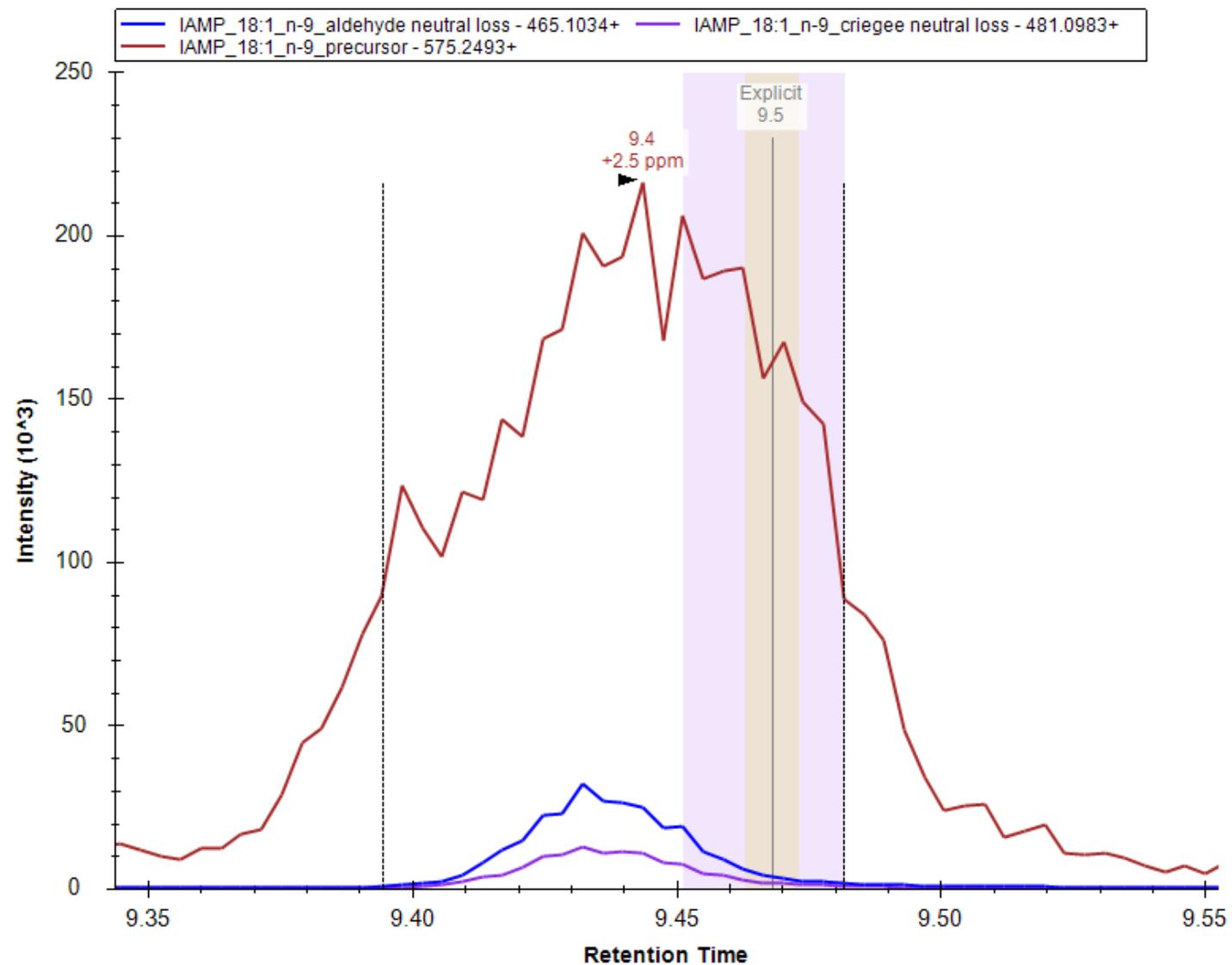
Thanks heaps for any help !!!



Targets

- IAMP_FA
 - IAMP_18:1_n-9_9.45
 - IAMP_18:2_n-6_n-9_8.66
 - IAMP_20:4_n-6_n-9_n-12_n-15_8.69

20211119_DIA_VNX19_JPM_10uL

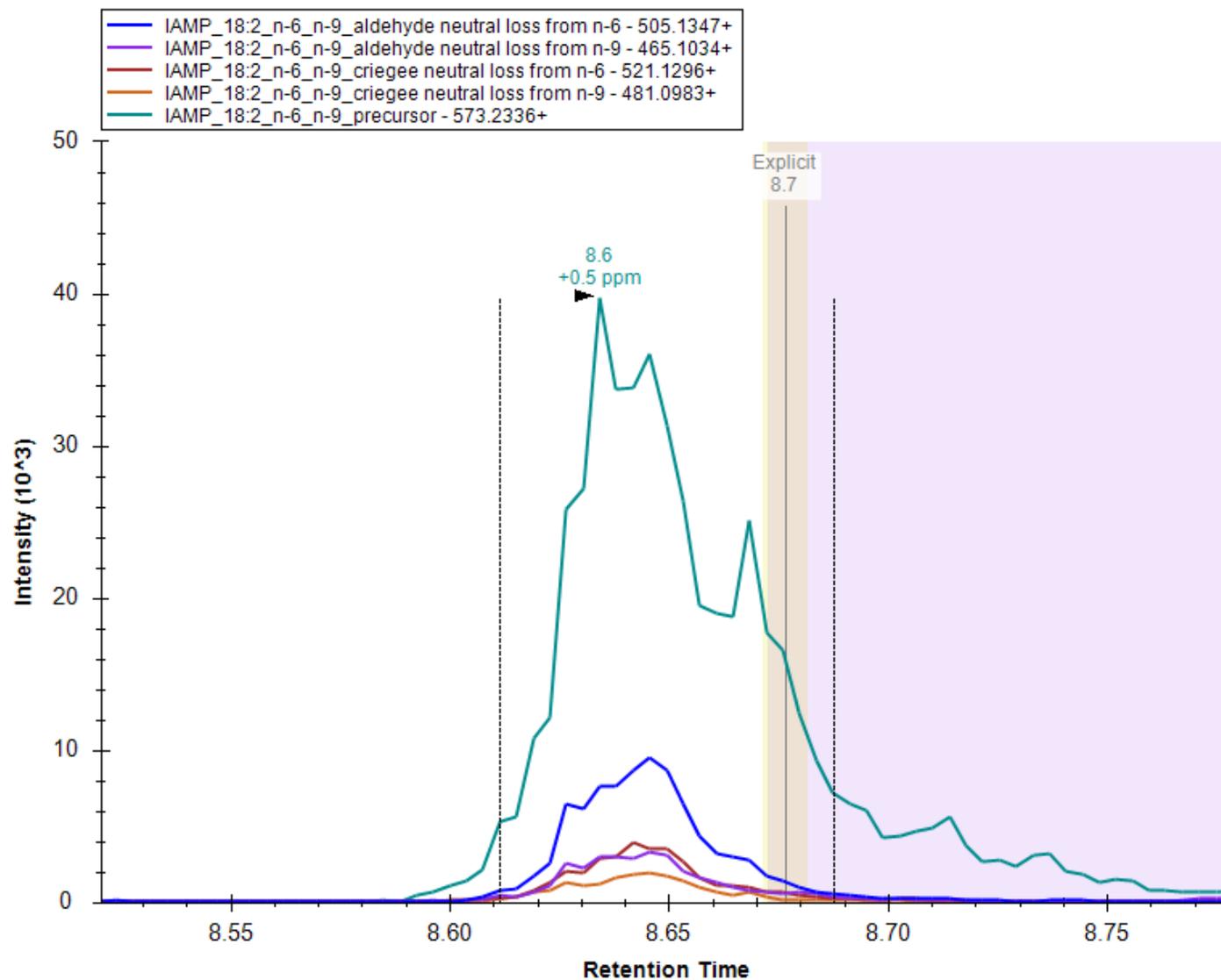




Targets

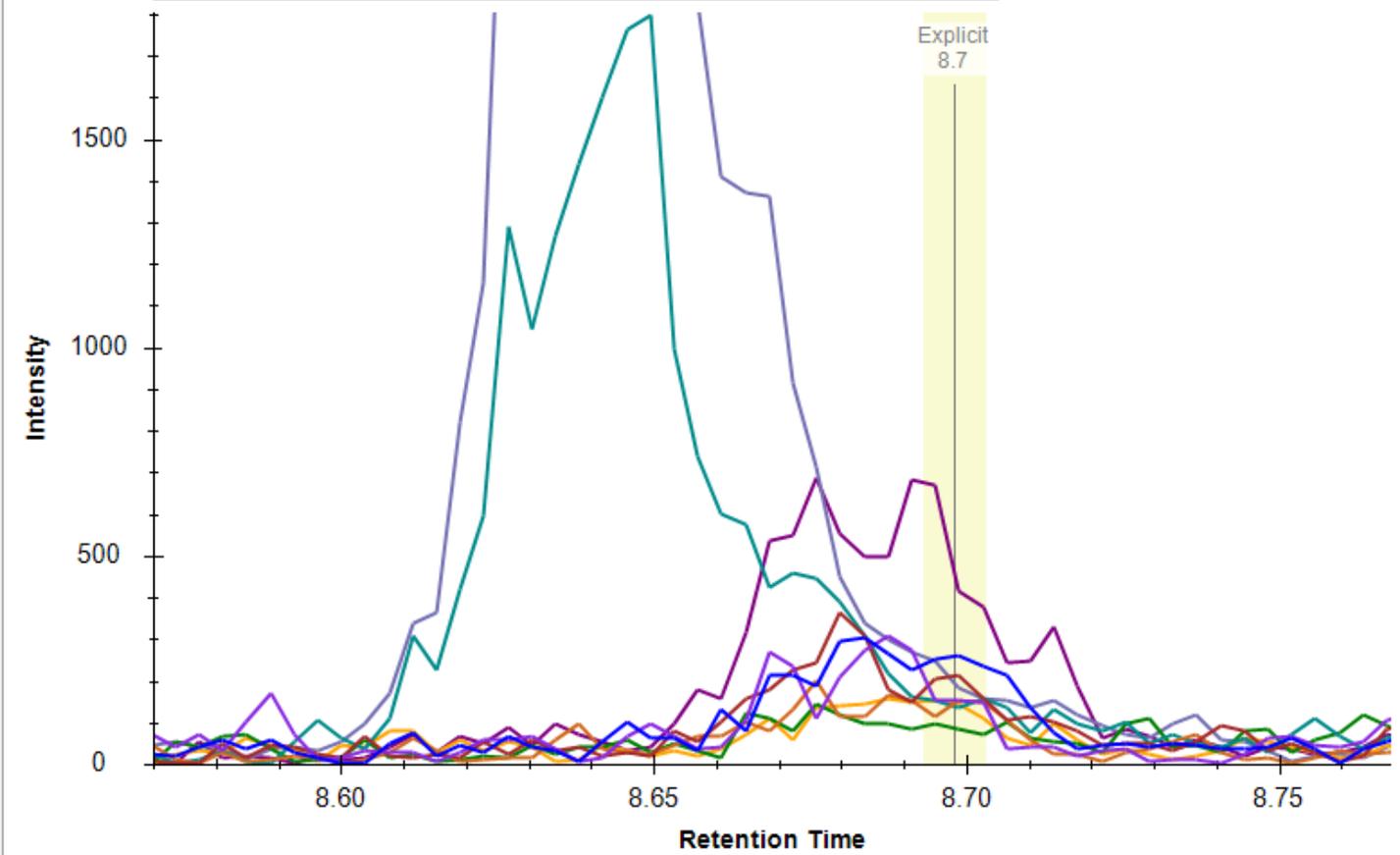
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- IAMP_20:4_n-6_n-9_n-12_n-15_aldehyde neutral loss from n-12 - 449.0721+
- IAMP_20:4_n-6_n-9_n-12_n-15_aldehyde neutral loss from n-15 - 409.0408+
- IAMP_20:4_n-6_n-9_n-12_n-15_aldehyde neutral loss from n-6 - 529.1347+
- IAMP_20:4_n-6_n-9_n-12_n-15_aldehyde neutral loss from n-9 - 489.1034+
- IAMP_20:4_n-6_n-9_n-12_n-15_criegee neutral loss from n-12 - 465.0670+
- IAMP_20:4_n-6_n-9_n-12_n-15_criegee neutral loss from n-15 - 425.0357+
- IAMP_20:4_n-6_n-9_n-12_n-15_criegee neutral loss from n-6 - 545.1296+
- IAMP_20:4_n-6_n-9_n-12_n-15_criegee neutral loss from n-9 - 505.0983+
- IAMP_20:4_n-6_n-9_n-12_n-15_precursor - 597.2336+



Why are there no integration borders?

Technically I don't care why, but a way to make sure this cannot occur in general or a way to insert integration limits or restore them would be great!

The problem also is that no integration results (problematic fields highlighted) can be found in the report for this species...

The entries for the other species is fine and usable.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	Mol	Molecule Name	Precur	Precur	Prec	Precur	Fragment Ion	Proc	Produc	Product Mz	Produ	Mass Error PPM	Retention Time	Area	Area Normalized	Background	Fwhm	Explicit Retention Time	Start Time	End Time
2	IAM	IAMP_18:1_n-9_9.45	C30H [M+]	707	1	IAMP_18:1_n-	C21H [M+]	465.103351	1	1.7	9.43	58796	â~ž	4180	0.03	9.47	9.39	9.48		
3	IAM	IAMP_18:1_n-9_9.45	C30H [M+]	707	1	IAMP_18:1_n-	C21H [M+]	481.098266	1	3	9.43	24975	â~ž	1695	0.03	9.47	9.39	9.48		
4	IAM	IAMP_18:1_n-9_9.45	C30H [M+]	707	1	IAMP_18:1_n-	C30H [M+]	575.249287	1	2.5	9.44	366645	â~ž	463743	0.05	9.47	9.39	9.48		
5	IAM	IAMP_18:2_n-6_n-9_8.66	C30H [M+]	705	1	IAMP_18:2_n-	C24H [M+]	505.134652	1	2.3	8.65	16916	â~ž	2502	0.03	8.68	8.61	8.69		
6	IAM	IAMP_18:2_n-6_n-9_8.66	C30H [M+]	705	1	IAMP_18:2_n-	C21H [M+]	465.103351	1	0.2	8.65	5858	â~ž	1472	0.03	8.68	8.61	8.69		
7	IAM	IAMP_18:2_n-6_n-9_8.66	C30H [M+]	705	1	IAMP_18:2_n-	C24H [M+]	521.129566	1	-2.2	8.64	6288	â~ž	1331	0.02	8.68	8.61	8.69		
8	IAM	IAMP_18:2_n-6_n-9_8.66	C30H [M+]	705	1	IAMP_18:2_n-	C21H [M+]	481.098266	1	4	8.65	3335	â~ž	758	0.03	8.68	8.61	8.69		
9	IAM	IAMP_18:2_n-6_n-9_8.66	C30H [M+]	705	1	IAMP_18:2_n-	C30H [M+]	573.233637	1	0.5	8.63	73152	â~ž	24233	0.03	8.68	8.61	8.69		
10	IAM	IAMP_20:4_n-6_n-9_n-12_n-15_8.69	C32H [M+]	729	1	IAMP_20:4_n-	C20H [M+]	449.072051	1	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	8.7	#N/A	#N/A	
11	IAM	IAMP_20:4_n-6_n-9_n-12_n-15_8.69	C32H [M+]	729	1	IAMP_20:4_n-	C17H [M+]	409.040751	1	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	8.7	#N/A	#N/A	
12	IAM	IAMP_20:4_n-6_n-9_n-12_n-15_8.69	C32H [M+]	729	1	IAMP_20:4_n-	C26H [M+]	529.134652	1	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	8.7	#N/A	#N/A	
13	IAM	IAMP_20:4_n-6_n-9_n-12_n-15_8.69	C32H [M+]	729	1	IAMP_20:4_n-	C23H [M+]	489.103351	1	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	8.7	#N/A	#N/A	
14	IAM	IAMP_20:4_n-6_n-9_n-12_n-15_8.69	C32H [M+]	729	1	IAMP_20:4_n-	C20H [M+]	465.066966	1	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	8.7	#N/A	#N/A	
15	IAM	IAMP_20:4_n-6_n-9_n-12_n-15_8.69	C32H [M+]	729	1	IAMP_20:4_n-	C17H [M+]	425.035666	1	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	8.7	#N/A	#N/A	
16	IAM	IAMP_20:4_n-6_n-9_n-12_n-15_8.69	C32H [M+]	729	1	IAMP_20:4_n-	C26H [M+]	545.129566	1	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	8.7	#N/A	#N/A	
17	IAM	IAMP_20:4_n-6_n-9_n-12_n-15_8.69	C32H [M+]	729	1	IAMP_20:4_n-	C23H [M+]	505.098266	1	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	8.7	#N/A	#N/A	
18	IAM	IAMP_20:4_n-6_n-9_n-12_n-15_8.69	C32H [M+]	729	1	IAMP_20:4_n-	C32H [M+]	597.233637	1	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	8.7	#N/A	#N/A	

The problem shown here is a general one, it occurs multiple times in a file with a few hundred transitions (or on more occasions in a file with more transitions).

It has also occurred with many different datasets and respectively different transition lists.

Please help, if you can

Kind regards,

Philipp

(Dr. Jan Philipp Menzel, Queensland University of Technology, Brisbane, Australia; j.p.menzel@gmail.com or j3.menzel@qut.edu.au)