

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101218\
 Data File : BF109865.D
 Acq On : 13 Oct 2018 6:00
 Operator : JU/SJ
 Sample : J5444-08
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 101018-DBRI-F-D-S

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	473	476	490	rBV	110496	142916	3.47%	0.663%
2	5.316	546	549	573	rBV	612573	886698	21.54%	4.112%
3	6.339	720	723	740	rBV	371231	656661	15.95%	3.045%
4	6.463	740	744	769	rVV	1727644	1916483	46.55%	8.888%
5	6.692	780	783	805	rVB	519582	675593	16.41%	3.133%
6	6.851	805	810	836	rBV	2715387	2851763	69.27%	13.226%
7	7.263	875	880	913	rBV	1804190	2413654	58.63%	11.194%
8	7.975	997	1001	1025	rBV	657913	830500	20.17%	3.852%
9	9.051	1179	1184	1212	rBV	3724989	4116936	100.00%	19.093%
10	9.445	1247	1251	1266	rVB	65393	80598	1.96%	0.374%
11	9.722	1294	1298	1318	rBV	833715	846613	20.56%	3.926%
12	10.504	1428	1431	1451	rBV	900229	1248061	30.32%	5.788%
13	11.198	1546	1549	1570	rBV	516999	683638	16.61%	3.171%
14	12.780	1814	1818	1839	rBV	2562165	2668661	64.82%	12.377%
15	13.692	1968	1973	1983	rBV7	19551	59554	1.45%	0.276%
16	13.827	1992	1996	2017	rVB	489272	602088	14.62%	2.792%
17	14.662	2133	2138	2142	rBV	354005	359564	8.73%	1.668%
18	15.227	2230	2234	2251	rVB	276545	480783	11.68%	2.230%
19	15.645	2299	2305	2310	rBV	26756	41550	1.01%	0.193%

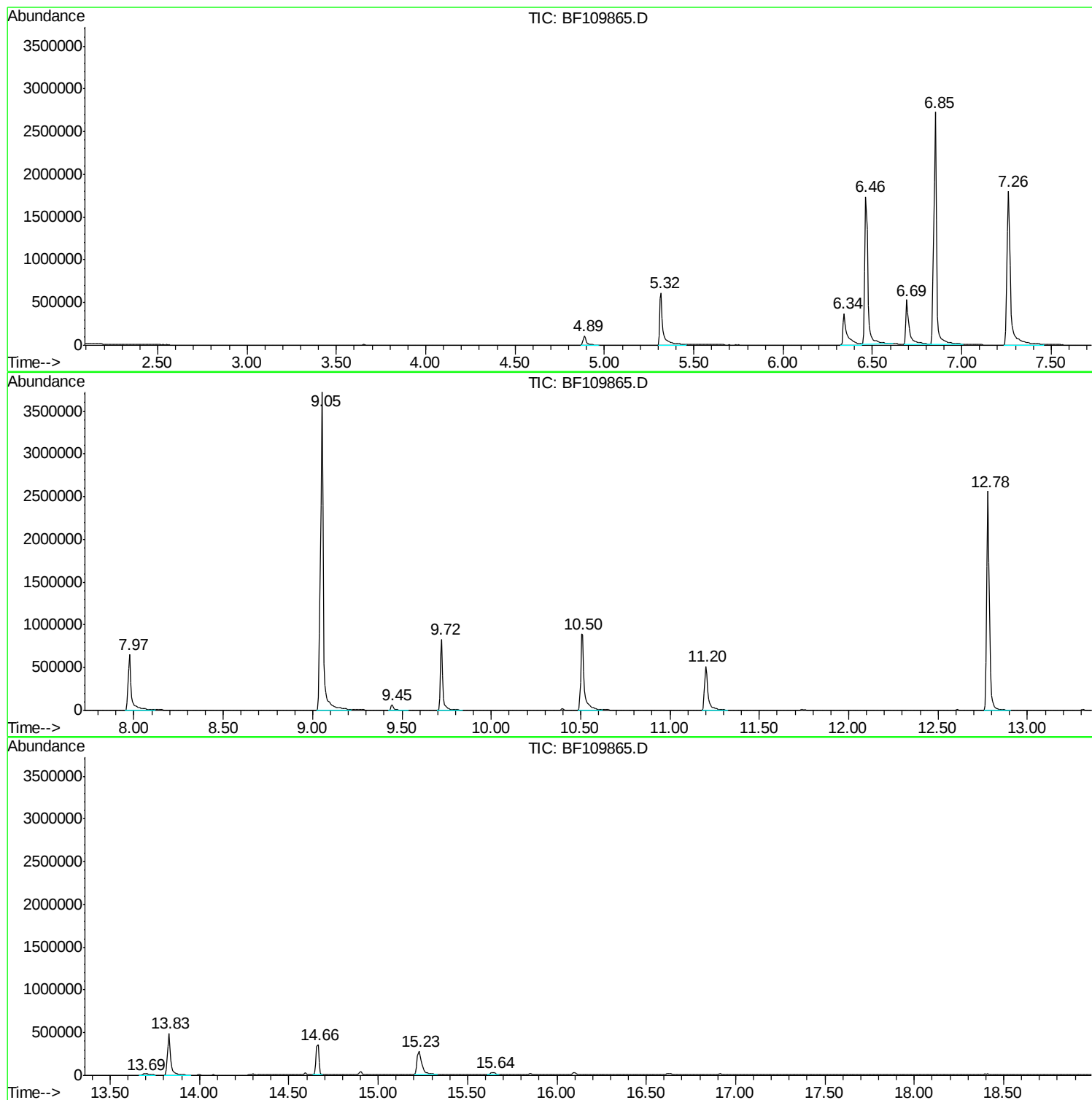
Sum of corrected areas: 21562314

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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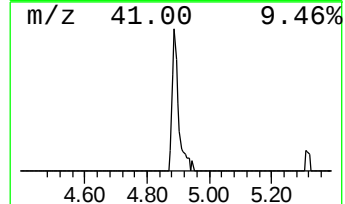
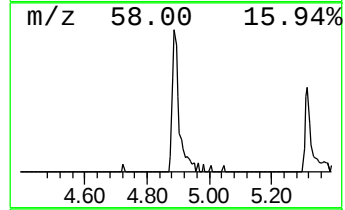
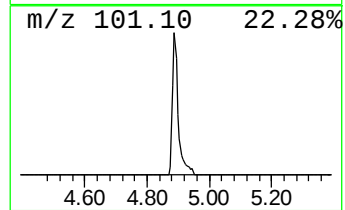
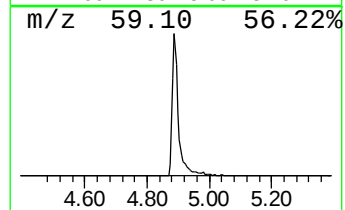
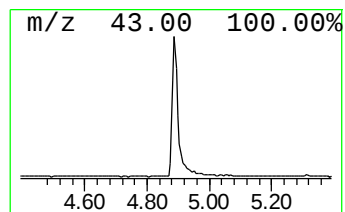
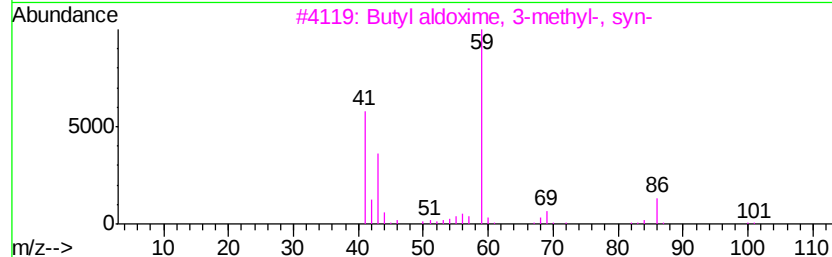
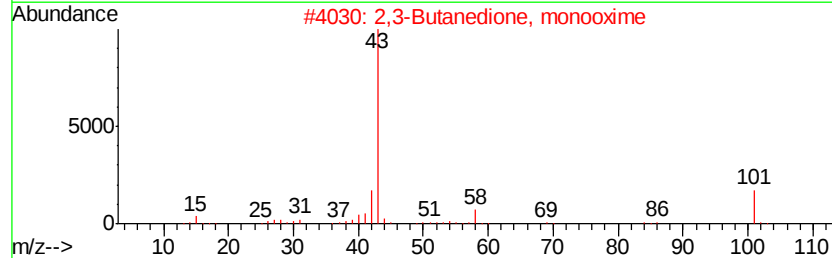
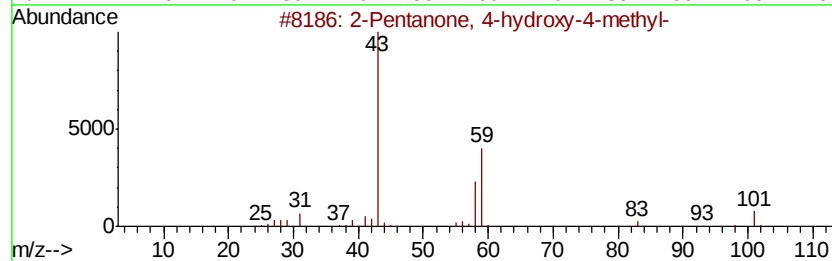
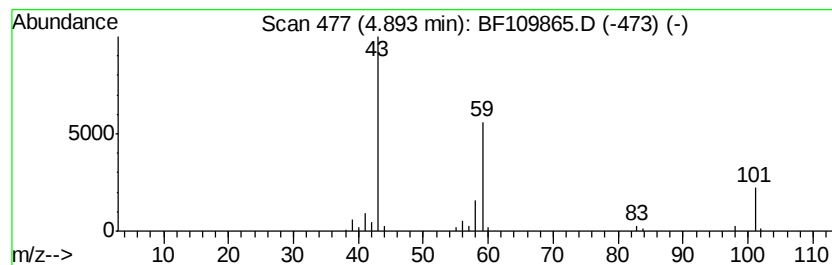
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.89	4.23 ng	142916	1,4-Dichlorobenzene-d4	6.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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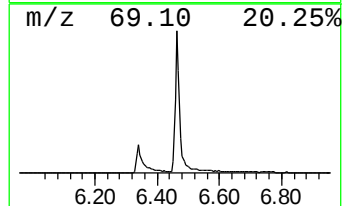
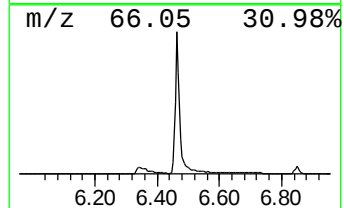
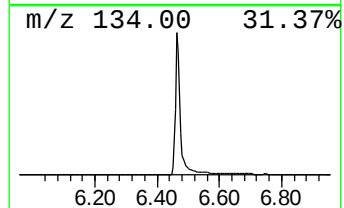
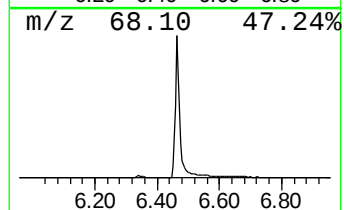
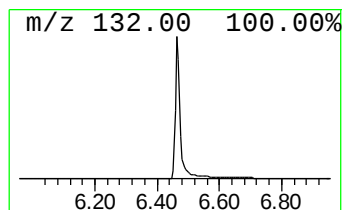
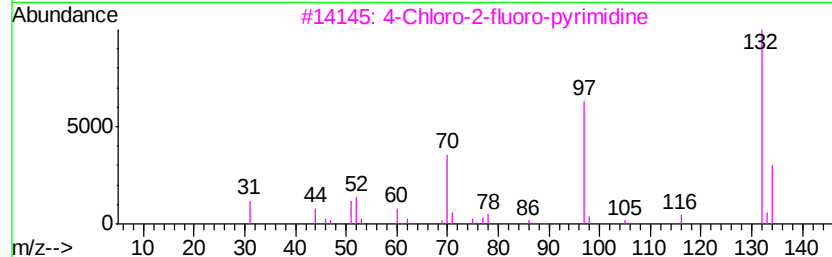
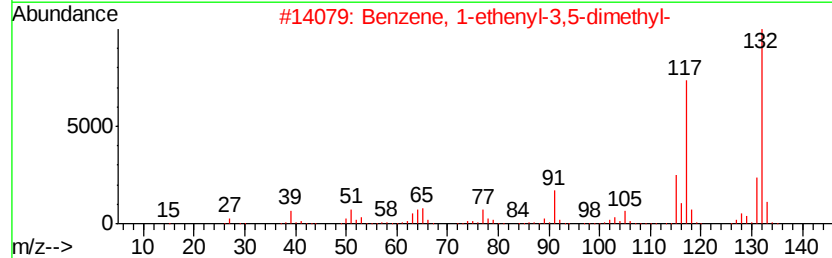
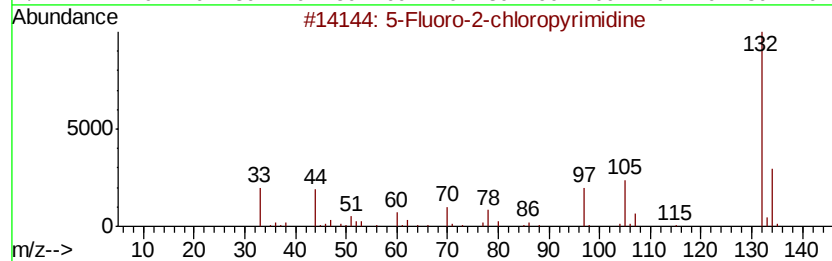
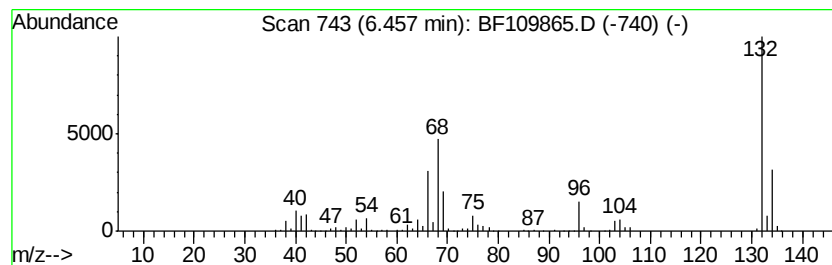
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Peak Number 2 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	56.73 ng	1916480	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
3			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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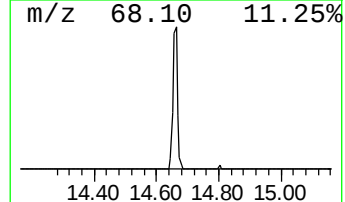
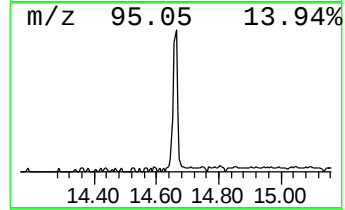
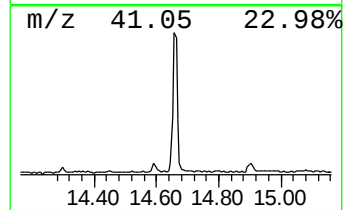
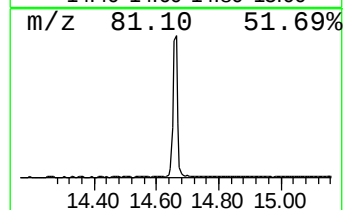
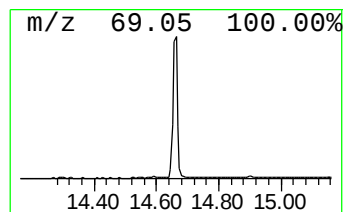
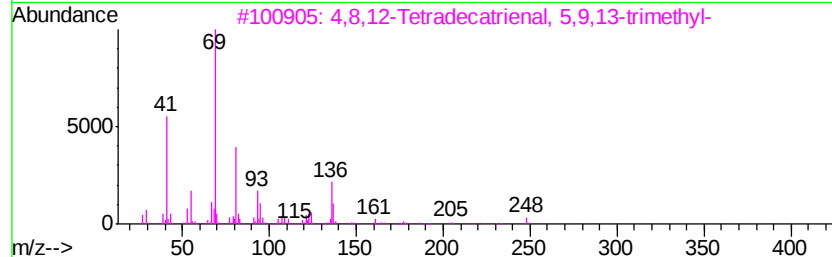
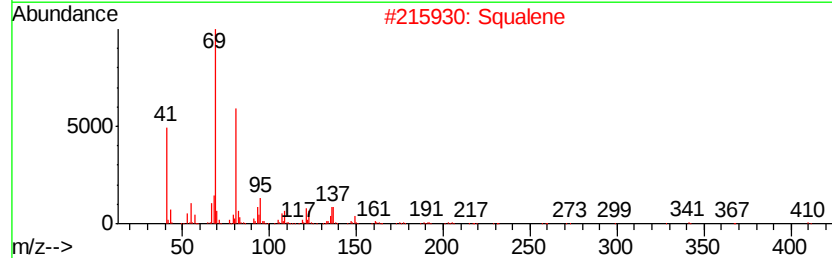
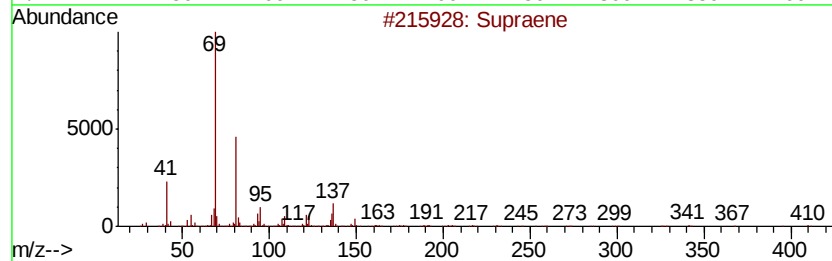
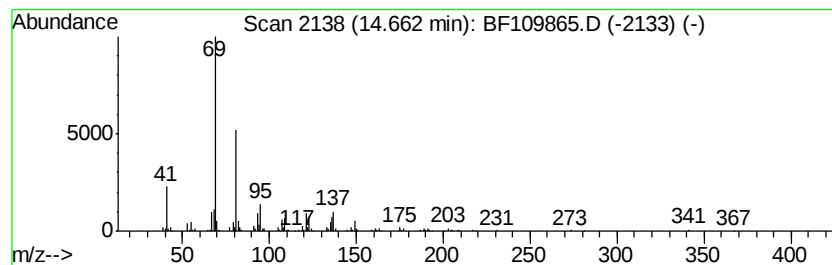
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Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	14.96 ng	359564	Perylene-d12	15.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Supraene	410 C30H50	007683-64-9	91
2	Squalene	410 C30H50	000111-02-4	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248 C17H28O	066408-55-7	80
4	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	72
5	(.+/-)-Lavandulol, pentafluorop...	300 C13H17F5O2	1000352-63-1	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	4.2	ng	142916	1	6.69	675593	20.0
unknown6.46	6.46	56.7	ng	1916480	1	6.69	675593	20.0
Supraene	14.66	15.0	ng	359564	6	15.23	480783	20.0