

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101218\
 Data File : BF109863.D
 Acq On : 13 Oct 2018 5:06
 Operator : JU/SJ
 Sample : J5444-06
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 101018-SIDI-F-U-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	489	rBV	86667	107533	2.88%	0.561%
2	5.316	546	549	577	rBV	493234	770502	20.63%	4.022%
3	6.339	720	723	739	rBV	303164	550824	14.75%	2.875%
4	6.463	741	744	764	rVV	1564742	1751066	46.88%	9.140%
5	6.692	780	783	805	rBV	451488	611946	16.38%	3.194%
6	6.851	805	810	839	rBV	2567403	2624411	70.25%	13.699%
7	7.263	875	880	913	rBV	1622371	2182378	58.42%	11.392%
8	7.975	997	1001	1024	rBV	577535	742987	19.89%	3.878%
9	9.051	1179	1184	1210	rBV	3473504	3735574	100.00%	19.499%
10	9.445	1248	1251	1264	rVB	47086	57355	1.54%	0.299%
11	9.722	1294	1298	1311	rBV	695917	735974	19.70%	3.842%
12	10.504	1428	1431	1450	rBV	819779	1096353	29.35%	5.723%
13	11.198	1546	1549	1571	rBV	405802	578793	15.49%	3.021%
14	12.780	1814	1818	1839	rBV	2418400	2392597	64.05%	12.489%
15	13.698	1967	1974	1983	rBV5	16179	47217	1.26%	0.246%
16	13.827	1992	1996	2011	rVB	409067	512556	13.72%	2.675%
17	14.657	2134	2137	2142	rBV	197335	194044	5.19%	1.013%
18	15.227	2229	2234	2254	rVB	235404	425602	11.39%	2.222%
19	15.645	2299	2305	2310	rBV2	26640	39903	1.07%	0.208%

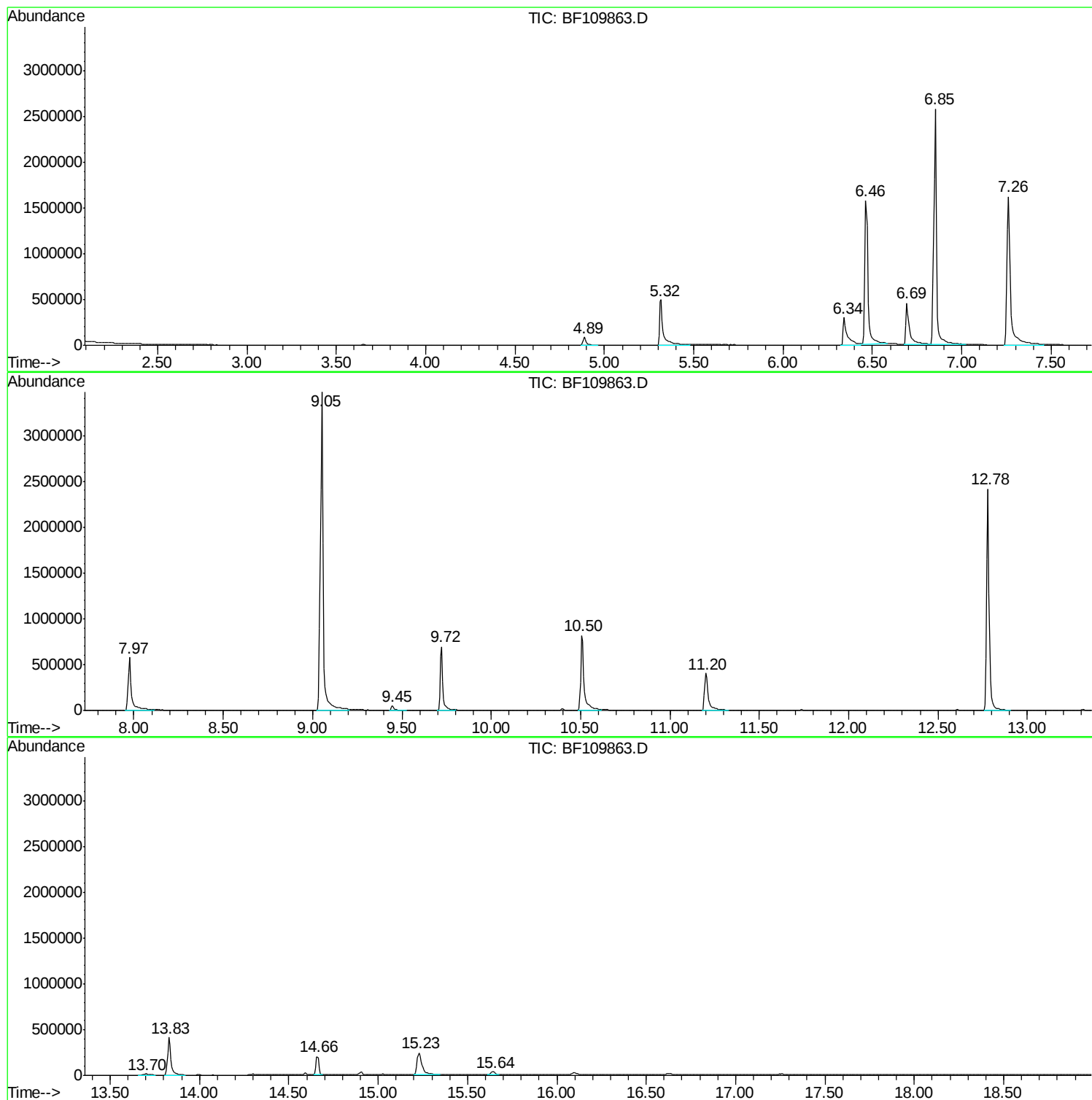
Sum of corrected areas: 19157615

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

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



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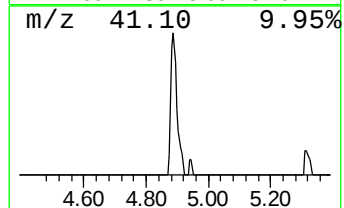
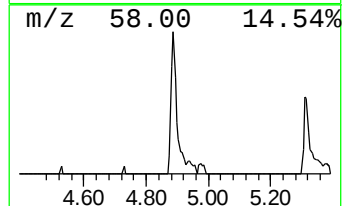
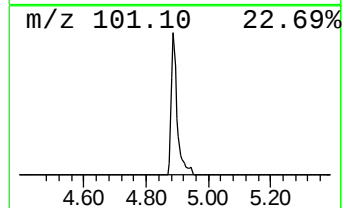
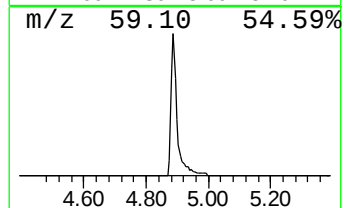
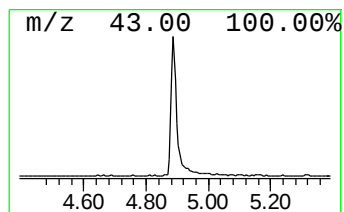
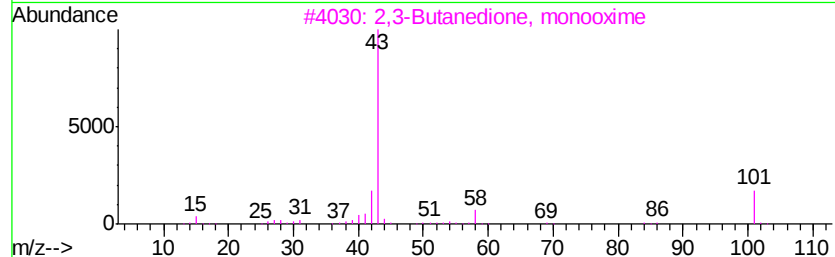
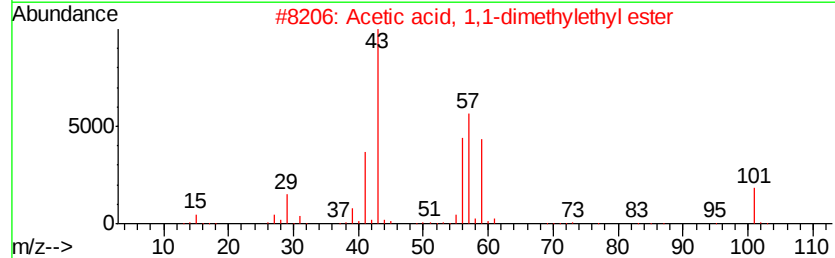
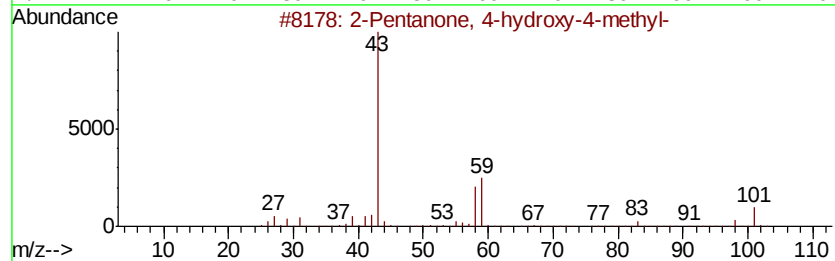
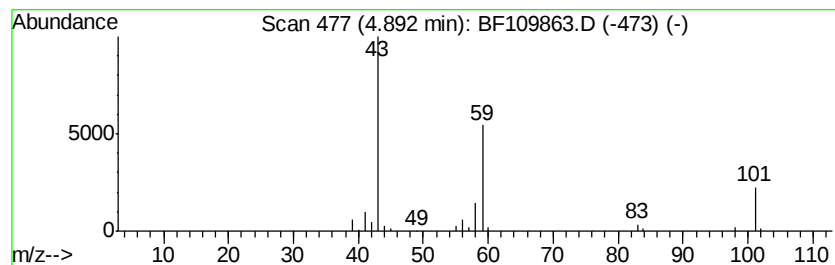
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	3.51 ng	107533	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	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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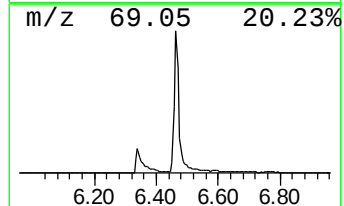
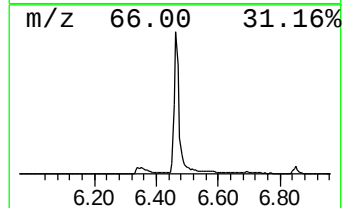
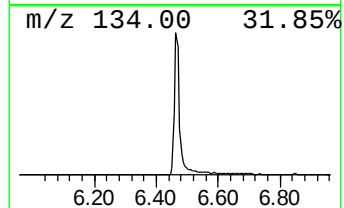
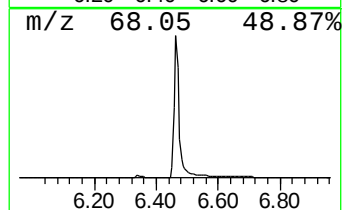
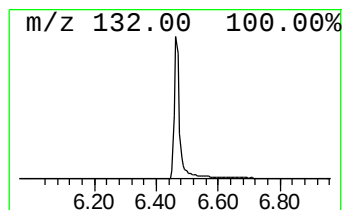
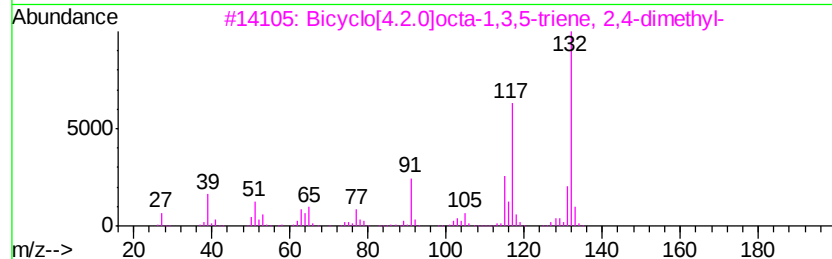
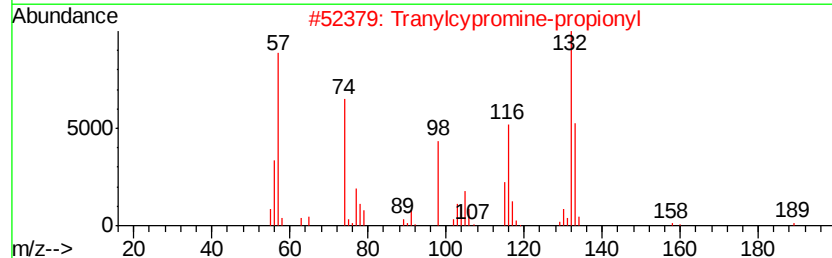
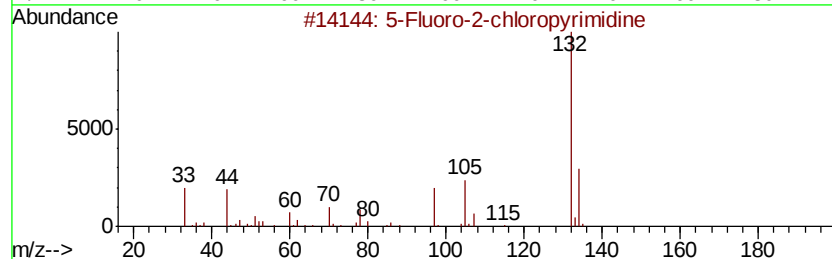
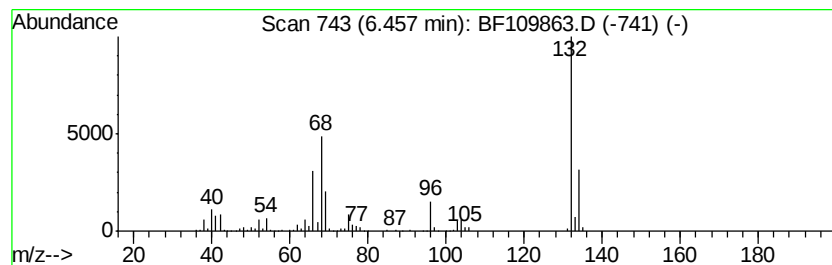
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Peak Number 2 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	57.23 ng	1751070	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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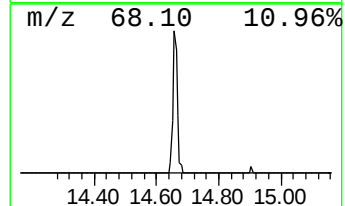
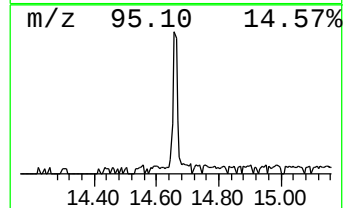
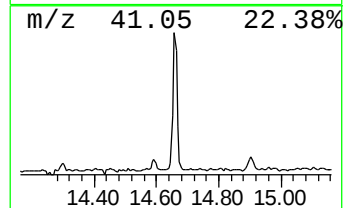
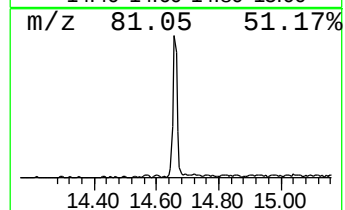
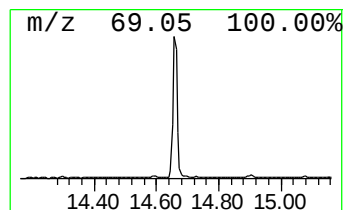
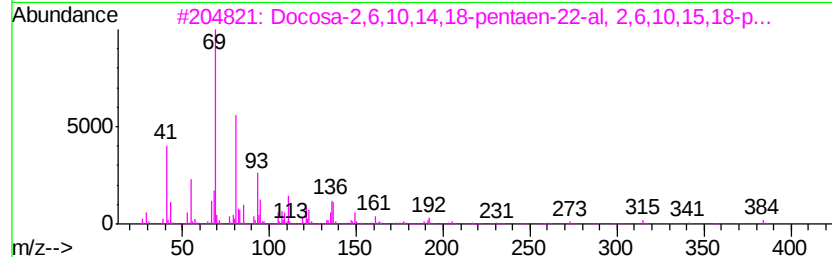
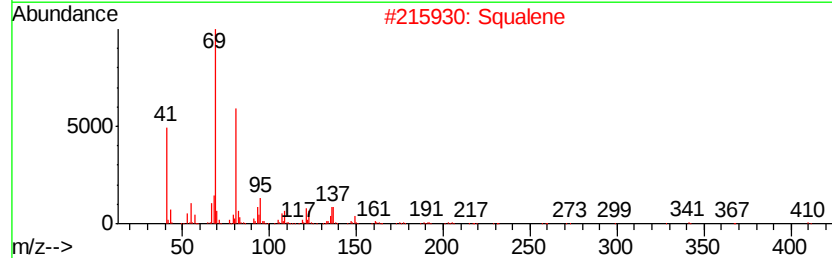
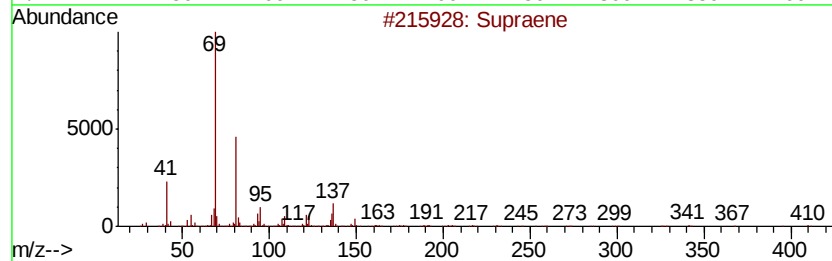
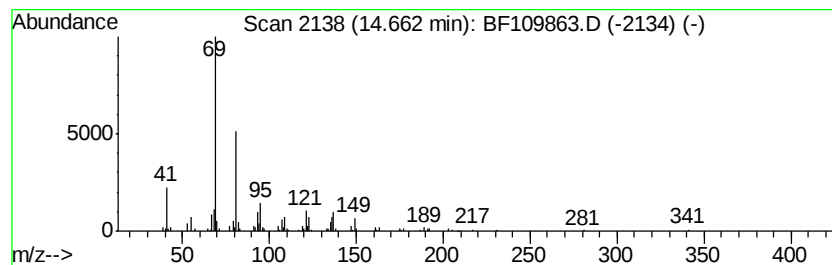
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Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	9.12 ng	194044	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	Docosa-2,6,10,14,18-pentaen-22-a...		384	C27H44O	1000163-04-7	90
4	.psi.,.psi.-Carotene, 7,7',8,8',...		547	C40H66	000502-62-5	83
5	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	3.5	ng	107533	1	6.69	611946	20.0
unknown6.46	6.46	57.2	ng	1751070	1	6.69	611946	20.0
Supraene	14.66	9.1	ng	194044	6	15.23	425602	20.0