

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
 Data File : BF109426.D
 Acq On : 28 Sep 2018 10:58
 Operator : JU/SJ
 Sample : J5133-06
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 092618-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-BF092218.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	472	476	486	rBV	90008	100872	2.87%	0.523%
2	5.310	545	548	562	rBV	924373	877890	24.96%	4.555%
3	6.340	719	723	731	rBV	665491	662018	18.83%	3.435%
4	6.475	742	746	749	rBV	1952881	1682789	47.85%	8.732%
5	6.704	782	785	789	rBV	802456	621055	17.66%	3.223%
6	6.863	808	812	815	rBV	2654430	2323161	66.06%	12.055%
7	7.269	876	881	884	rBV	1973132	1927308	54.80%	10.001%
8	7.987	999	1003	1008	rBV	966217	769183	21.87%	3.991%
9	9.063	1182	1186	1190	rBV	3530280	3516669	100.00%	18.247%
10	9.457	1250	1253	1261	rVB	76904	71959	2.05%	0.373%
11	9.733	1297	1300	1315	rVB	966088	863023	24.54%	4.478%
12	10.522	1430	1434	1450	rBV	1275651	1212698	34.48%	6.293%
13	11.210	1548	1551	1555	rBV	820495	727748	20.69%	3.776%
14	12.798	1816	1821	1824	rBV	2892641	2651847	75.41%	13.760%
15	13.839	1994	1998	2004	rVV	670492	647484	18.41%	3.360%
16	14.686	2138	2142	2146	rBV	122240	111030	3.16%	0.576%
17	15.239	2231	2236	2241	rBV	403737	505331	14.37%	2.622%

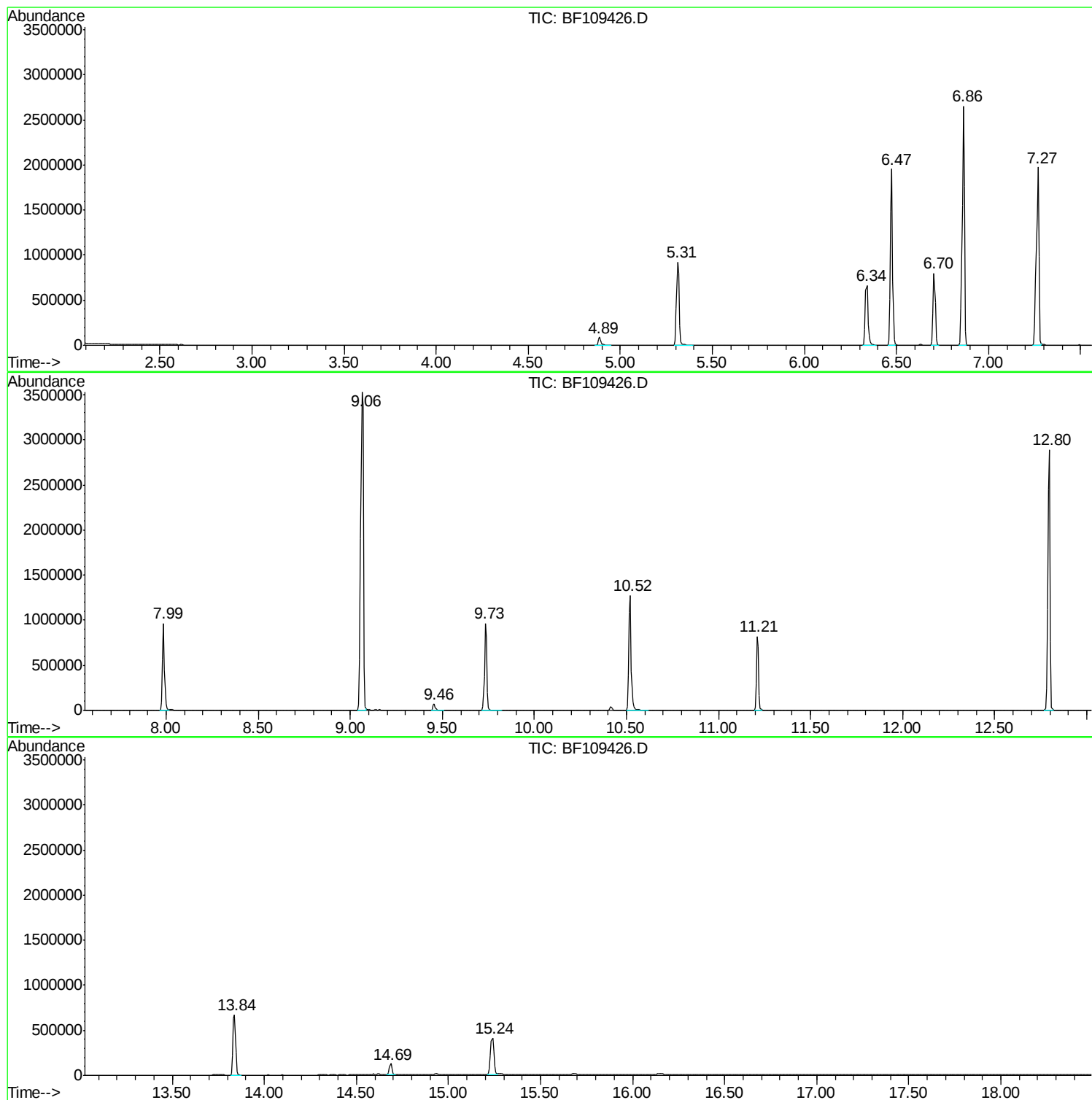
Sum of corrected areas: 19272065

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.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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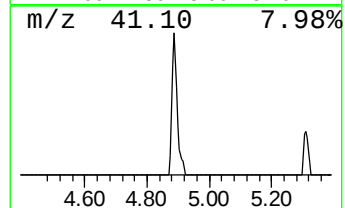
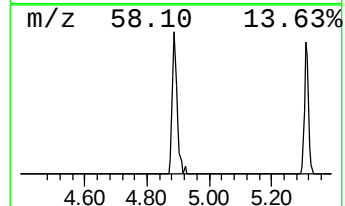
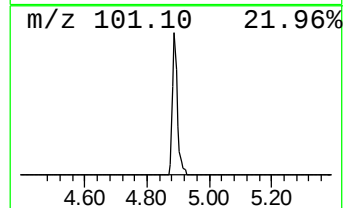
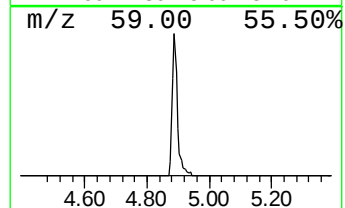
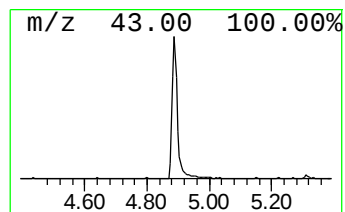
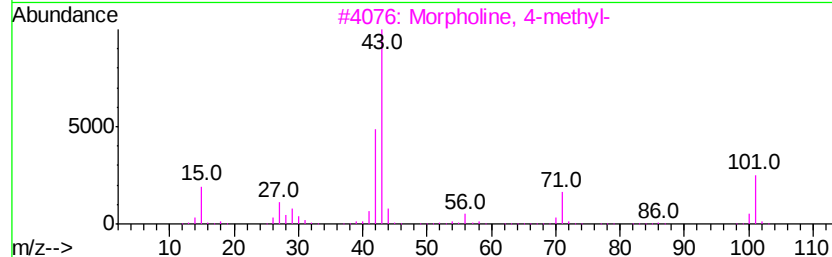
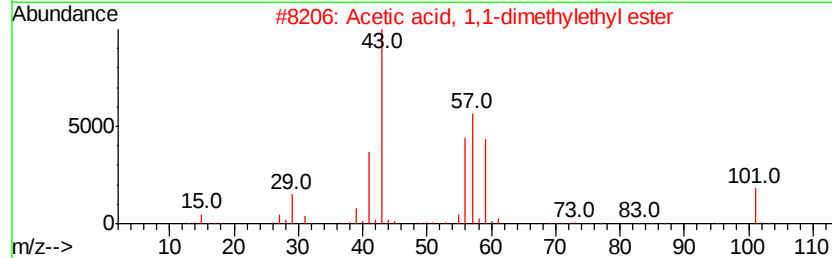
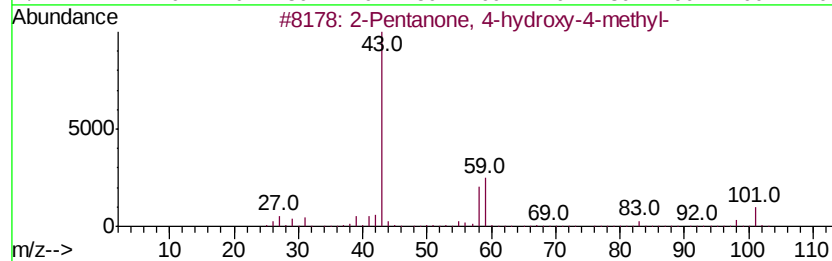
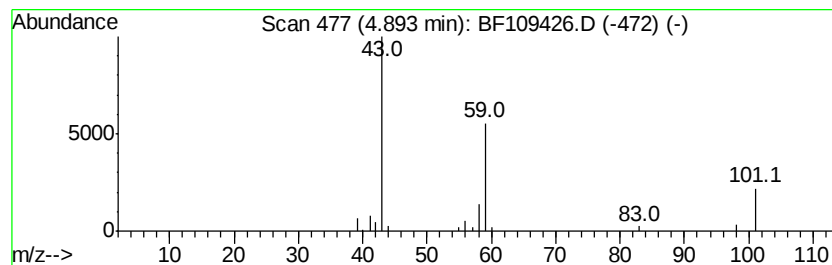
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	3.25 ng	100872	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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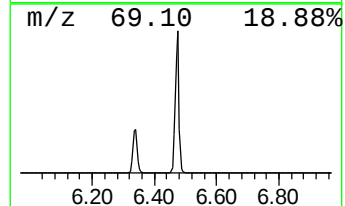
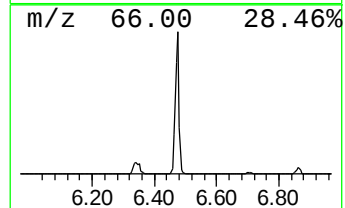
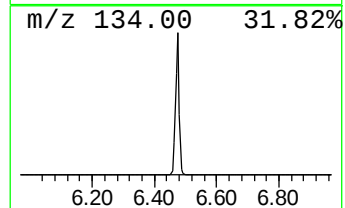
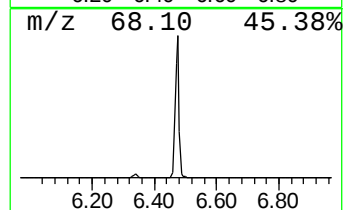
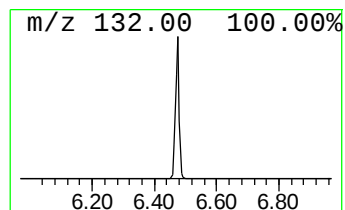
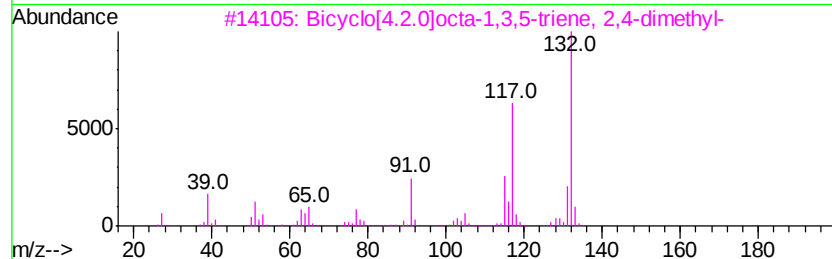
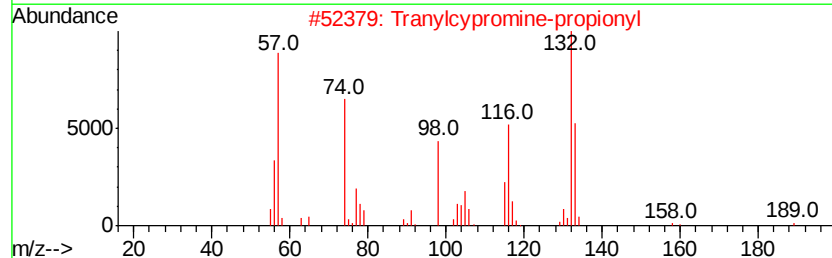
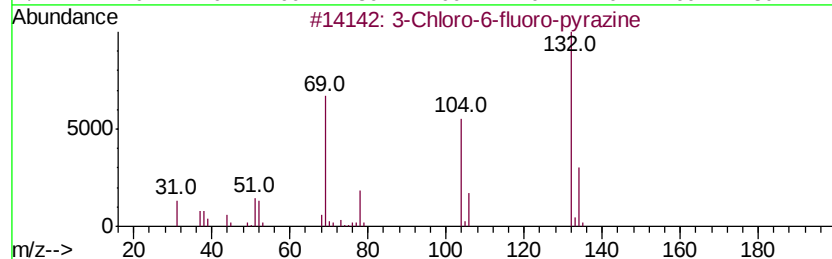
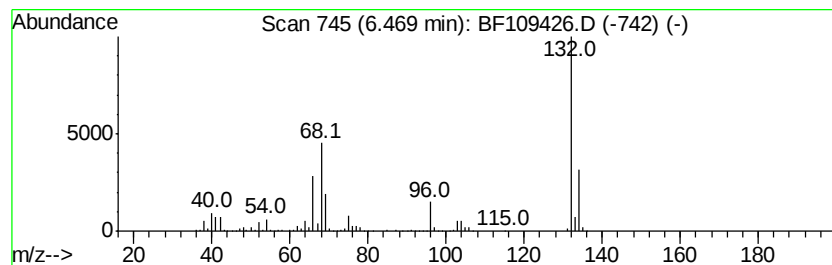
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Peak Number 2 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	54.19 ng	1682790	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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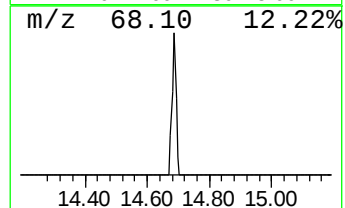
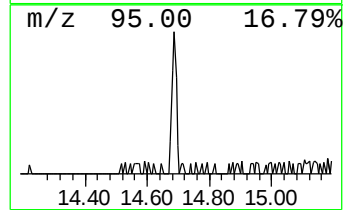
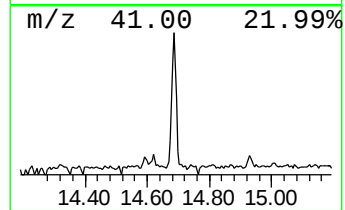
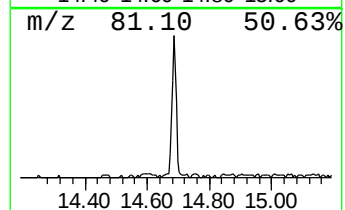
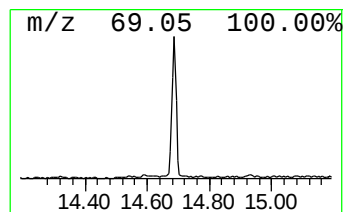
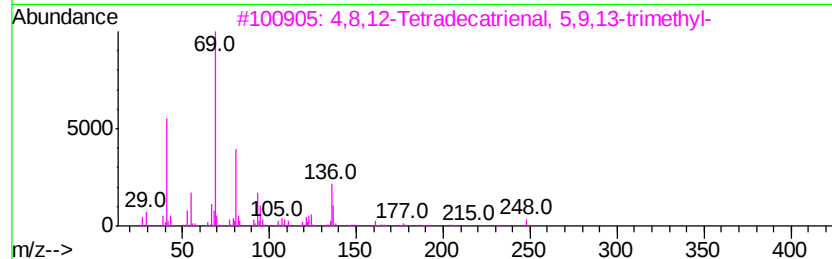
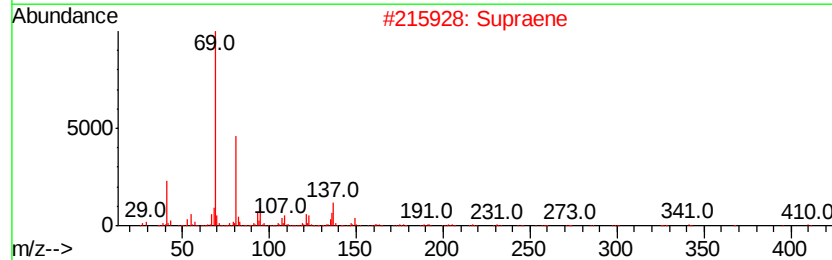
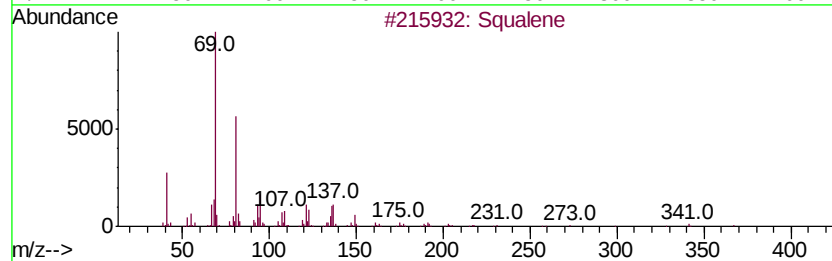
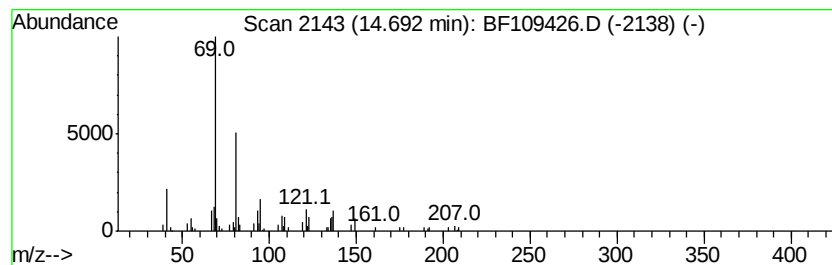
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Peak Number 4 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	4.39 ng	111030	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	86
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	3.3	ng	100872	1	6.70	621055	20.0
unknown6.47	6.47	54.2	ng	1682790	1	6.70	621055	20.0
Squalene	14.69	4.4	ng	111030	6	15.24	505331	20.0