

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091718\
 Data File : BF109080.D
 Acq On : 18 Sep 2018 6:44
 Operator : JU/SJ
 Sample : J4907-09
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CBH-140(4)

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-BF091418.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	4.901	432	436	444	rBV	208074	221650	5.47%	0.865%
2	5.325	504	508	511	rBV	1555592	1361313	33.60%	5.316%
3	6.348	678	682	690	rBV	1196581	920635	22.73%	3.595%
4	6.489	701	706	709	rBV	2620980	2320564	57.28%	9.061%
5	6.719	742	745	749	rBV	1030552	795820	19.64%	3.108%
6	6.878	768	772	775	rBV	3470531	2997544	73.99%	11.705%
7	7.283	835	841	844	rBV	2669162	2499844	61.71%	9.761%
8	8.001	959	963	966	rBV	1156732	907912	22.41%	3.545%
9	9.077	1142	1146	1149	rBV	4436825	4051106	100.00%	15.819%
10	9.466	1209	1212	1216	rBV	262673	231615	5.72%	0.904%
11	9.748	1257	1260	1264	rBV	1055692	913394	22.55%	3.567%
12	10.530	1389	1393	1406	rBV	1661381	1655012	40.85%	6.462%
13	11.224	1508	1511	1515	rBV	1039450	898549	22.18%	3.509%
14	12.813	1776	1781	1784	rBV	4159132	3914725	96.63%	15.286%
15	13.724	1931	1936	1944	rBV2	38811	65338	1.61%	0.255%
16	13.854	1954	1958	1961	rBV	1037559	906487	22.38%	3.540%
17	14.707	2099	2103	2107	rVB	242264	217868	5.38%	0.851%
18	15.254	2191	2196	2201	rBV	561761	680449	16.80%	2.657%
19	15.306	2202	2205	2211	rVB	37587	49659	1.23%	0.194%

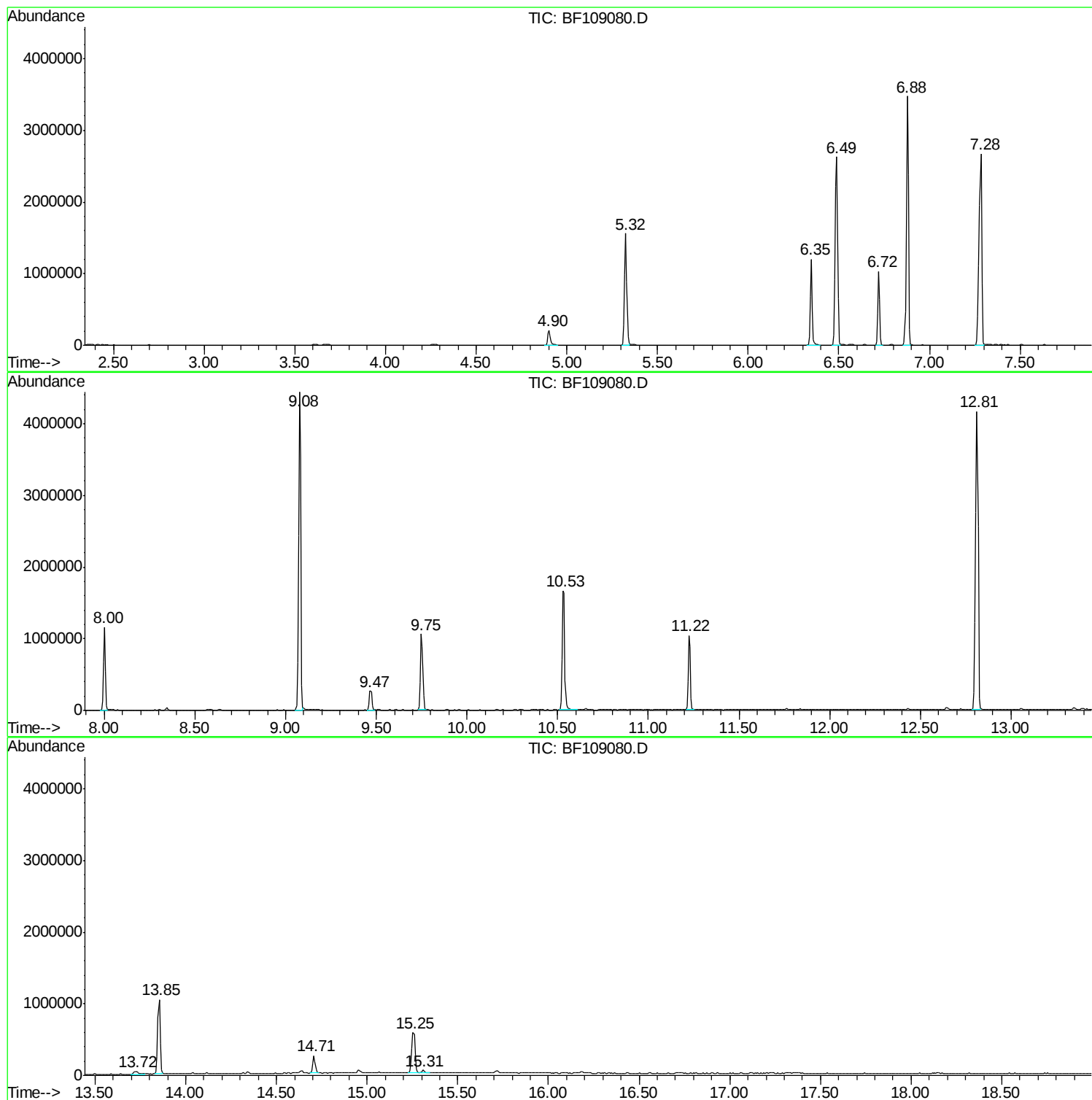
Sum of corrected areas: 25609484

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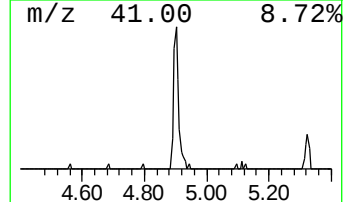
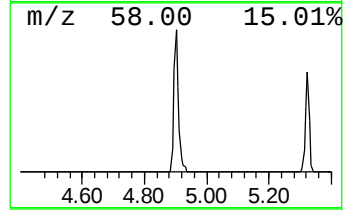
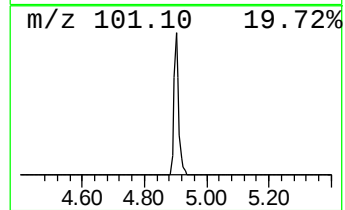
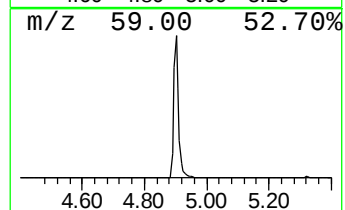
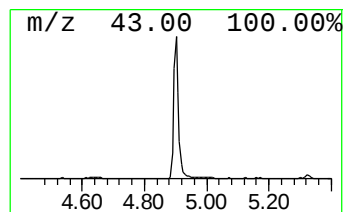
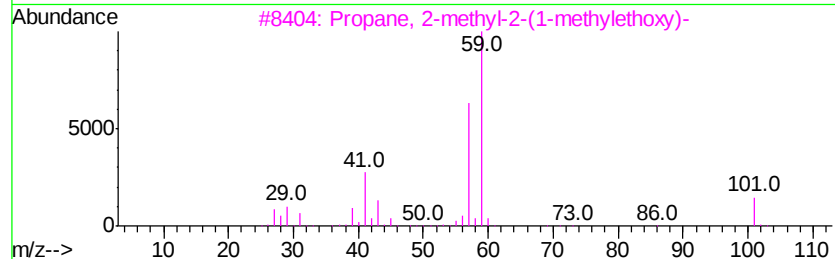
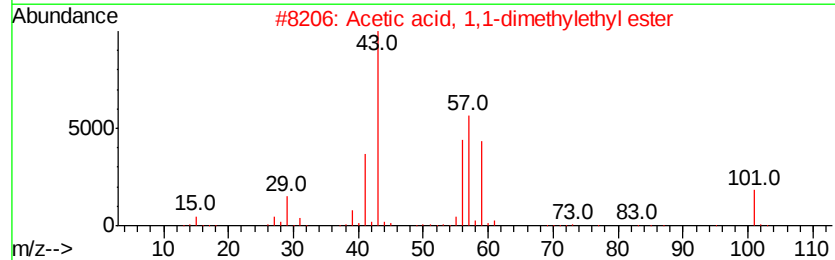
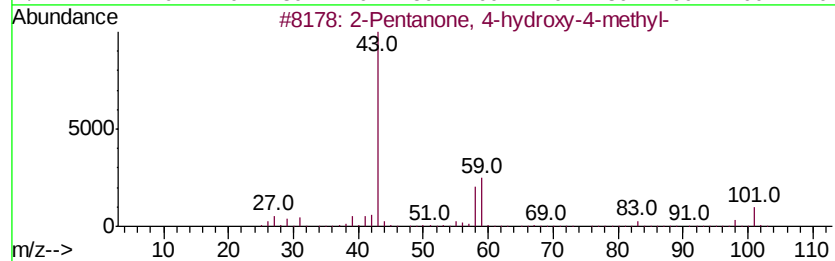
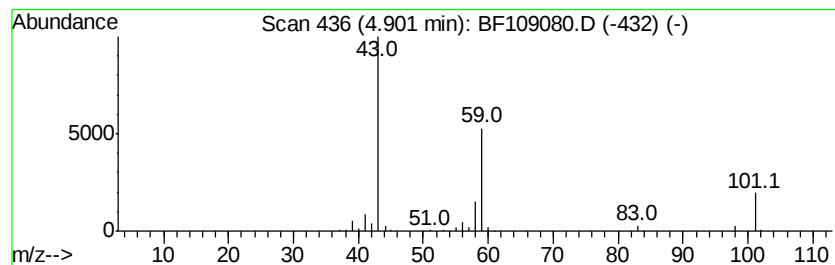
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
4.90	5.57 ng	221650	1,4-Dichlorobenzene-d4	6.72		
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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	



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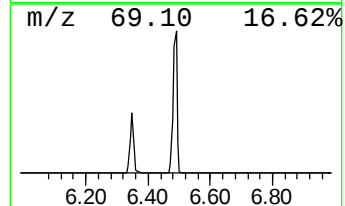
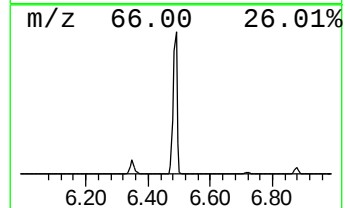
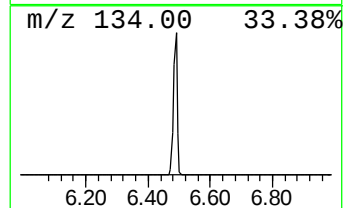
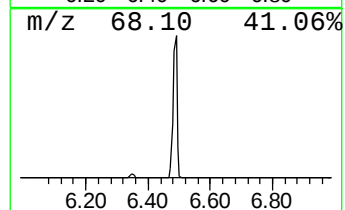
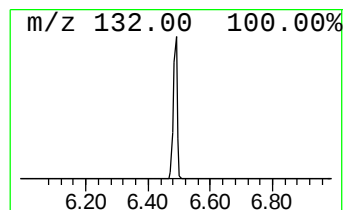
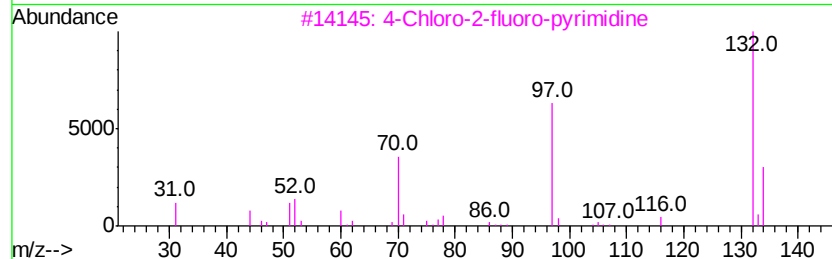
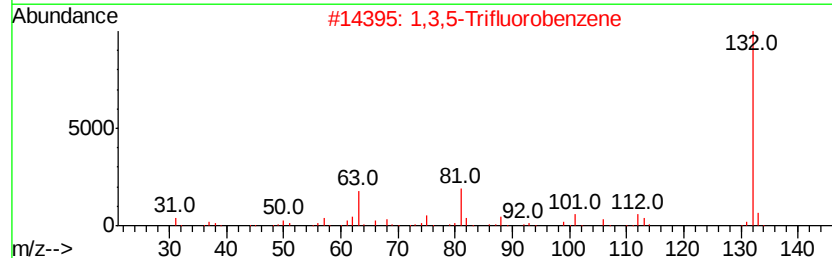
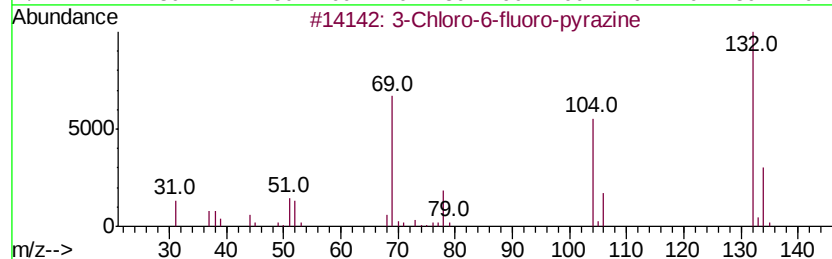
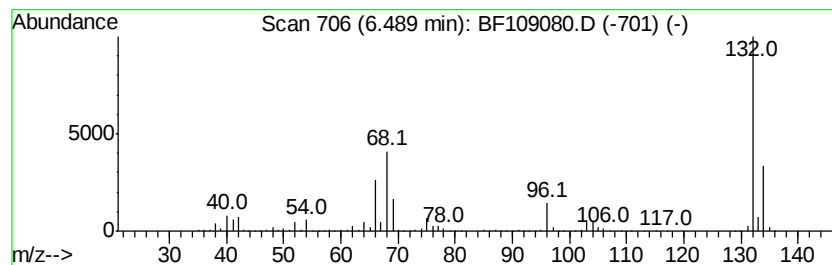
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Peak Number 2 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	58.32 ng	2320560	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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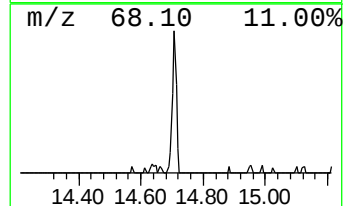
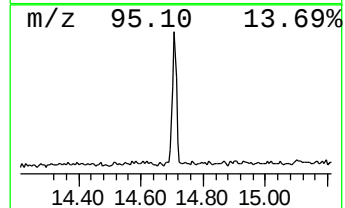
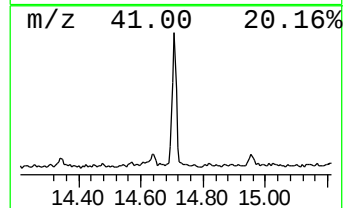
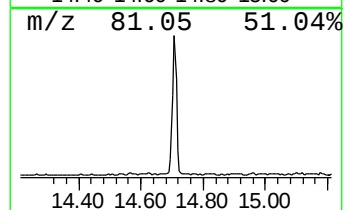
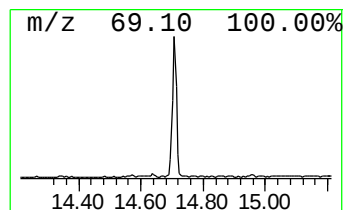
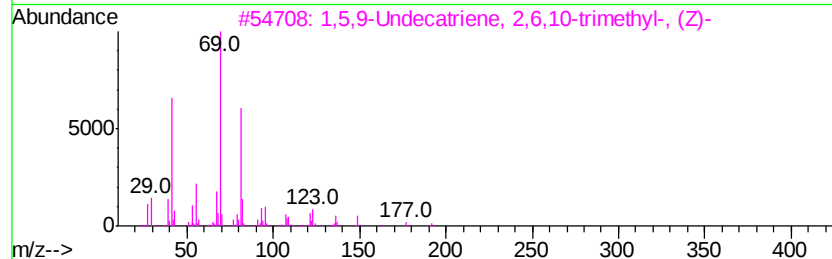
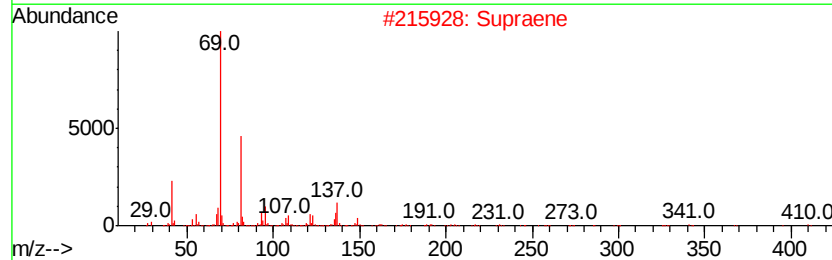
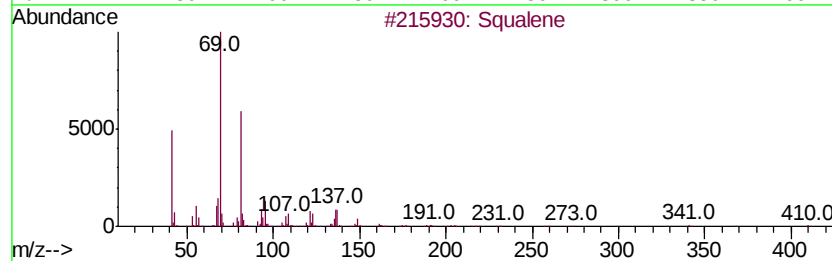
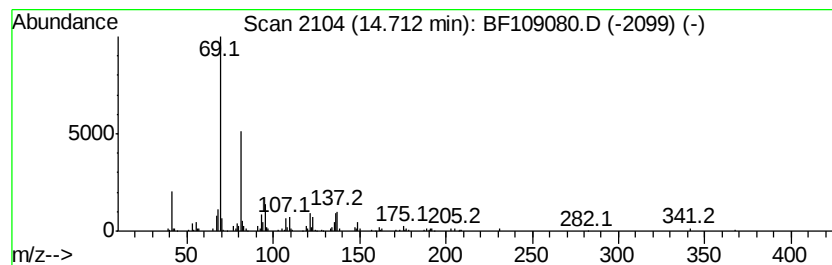
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 Peak Number 4 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	6.40 ng	217868	Perylene-d12	15.25

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		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
4		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	5.6	ng	221650	1	6.72	795820	20.0
unknown6.49	6.49	58.3	ng	2320560	1	6.72	795820	20.0
Squalene	14.71	6.4	ng	217868	6	15.25	680449	20.0