

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091418\
 Data File : BF109015.D
 Acq On : 15 Sep 2018 00:30
 Operator : JU/SJ
 Sample : J4901-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091218-TIPC-F-D-B

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	433	436	443	rBV	129343	141635	2.74%	0.420%
2	5.319	503	507	511	rBV	1500315	1480433	28.64%	4.393%
3	6.342	677	681	691	rBV	1192927	1045054	20.22%	3.101%
4	6.484	701	705	709	rVB	2830089	2667394	51.60%	7.916%
5	6.719	741	745	754	rBV	1308183	1080529	20.90%	3.207%
6	6.878	767	772	775	rBV	3677780	3379454	65.38%	10.029%
7	7.284	835	841	844	rBV	2802101	3009457	58.22%	8.931%
8	8.001	958	963	966	rBV	1555531	1348706	26.09%	4.002%
9	9.078	1141	1146	1149	rBV	4979814	5106241	98.78%	15.154%
10	9.466	1209	1212	1216	rBV	617163	503877	9.75%	1.495%
11	9.748	1256	1260	1264	rBV2	1845676	1597363	30.90%	4.740%
12	10.430	1373	1376	1379	rBV	154351	107829	2.09%	0.320%
13	10.530	1389	1393	1397	rBV	2368913	2340840	45.29%	6.947%
14	11.224	1507	1511	1515	rBV	1902186	1607697	31.10%	4.771%
15	11.766	1600	1603	1611	rBV2	85315	85272	1.65%	0.253%
16	12.813	1776	1781	1784	rBV	4831631	5169068	100.00%	15.340%
17	13.724	1931	1936	1951	rBV	42421	80558	1.56%	0.239%
18	13.848	1953	1957	1961	rBV	1383460	1230756	23.81%	3.652%
19	14.707	2099	2103	2107	rBV	324344	294508	5.70%	0.874%
20	14.954	2141	2145	2152	rVB	63656	68978	1.33%	0.205%
21	15.254	2190	2196	2201	rBV	968430	1100178	21.28%	3.265%
22	15.307	2201	2205	2216	rVB	72605	95983	1.86%	0.285%
23	15.712	2269	2274	2283	rVB	62865	84627	1.64%	0.251%
24	16.177	2348	2353	2359	rVB2	44276	70171	1.36%	0.208%

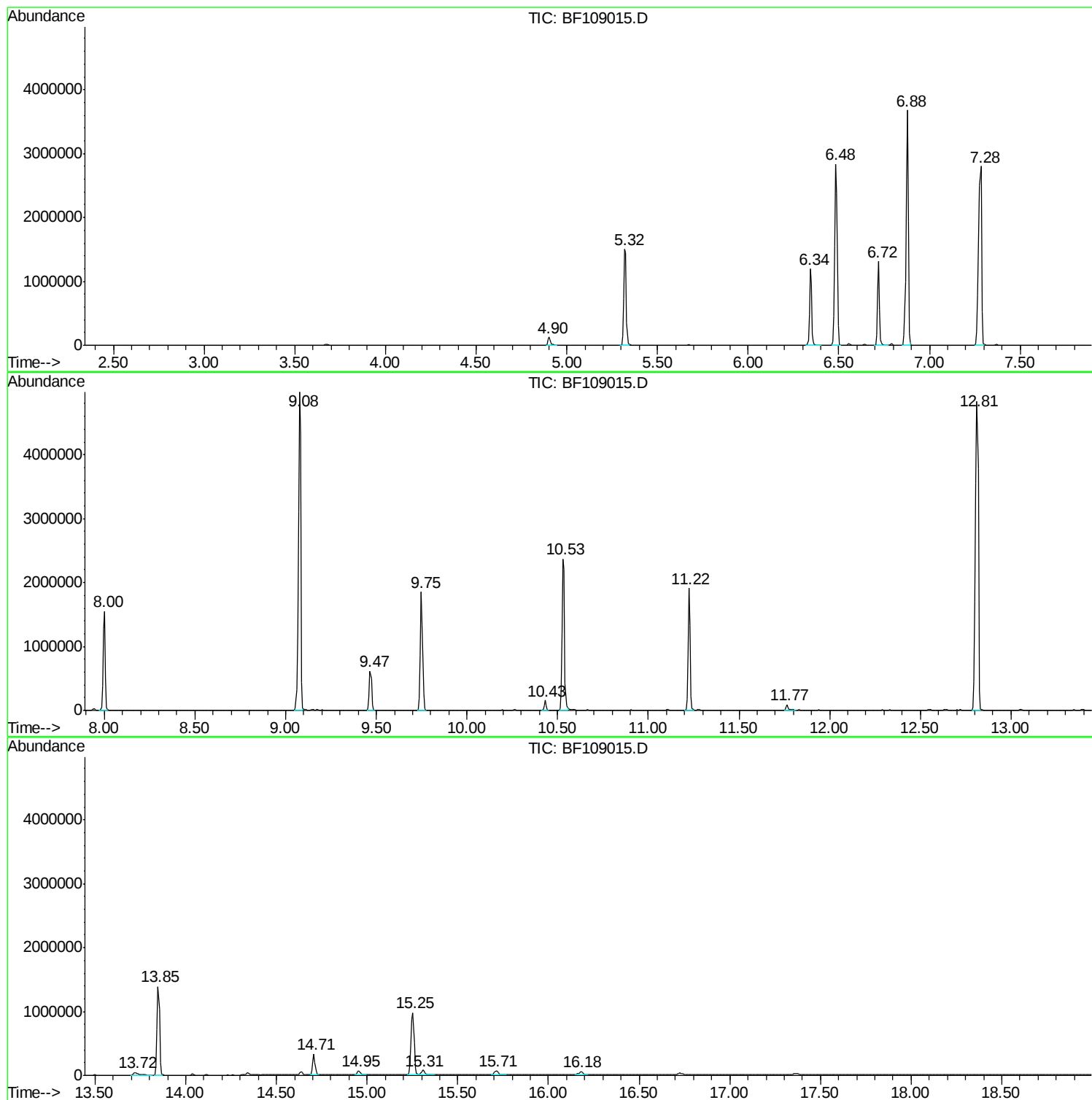
Sum of corrected areas: 33696608

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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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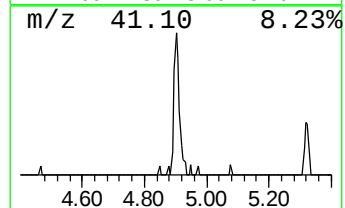
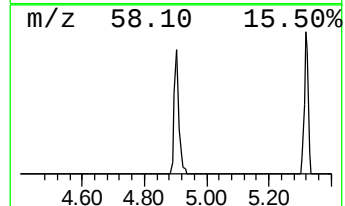
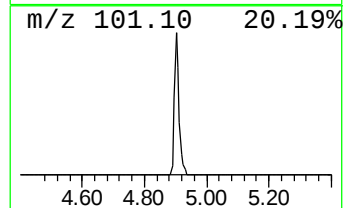
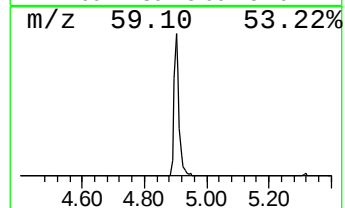
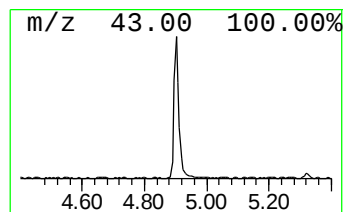
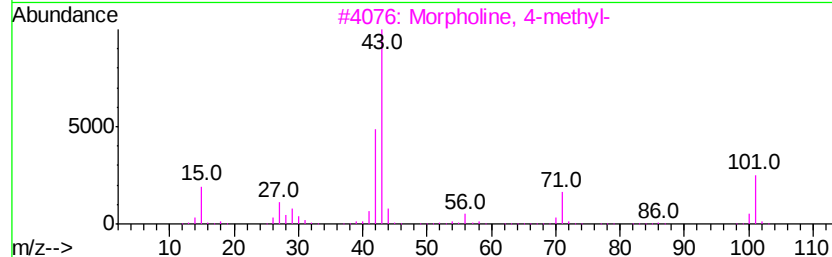
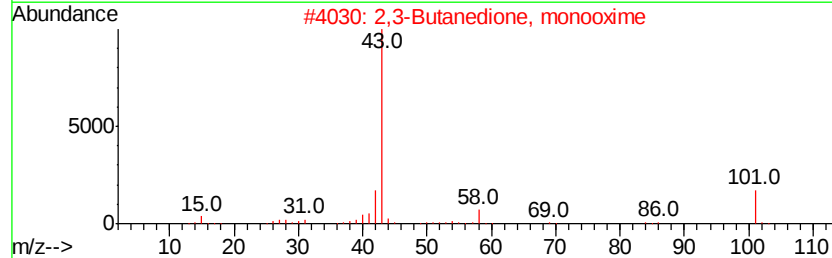
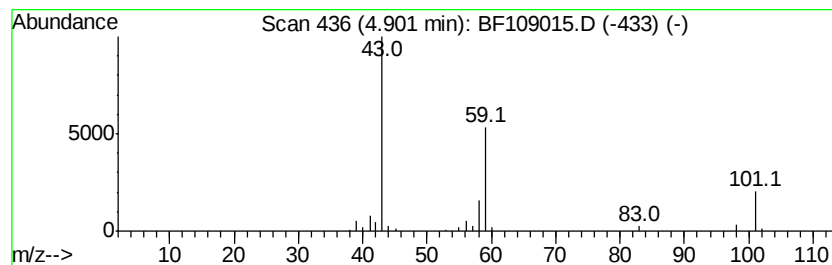
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.62 ng	141635	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	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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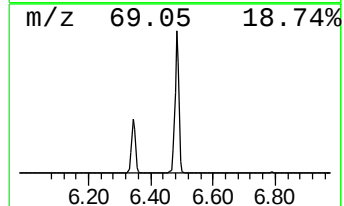
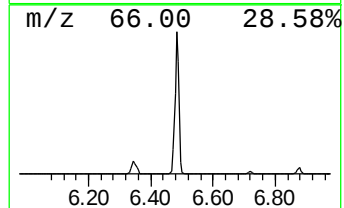
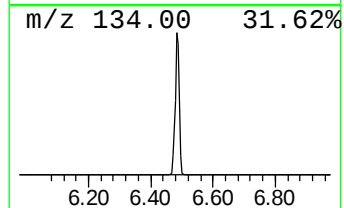
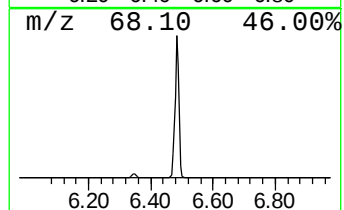
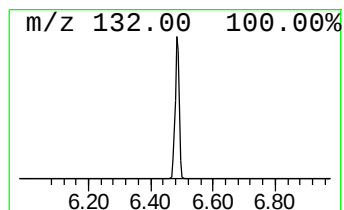
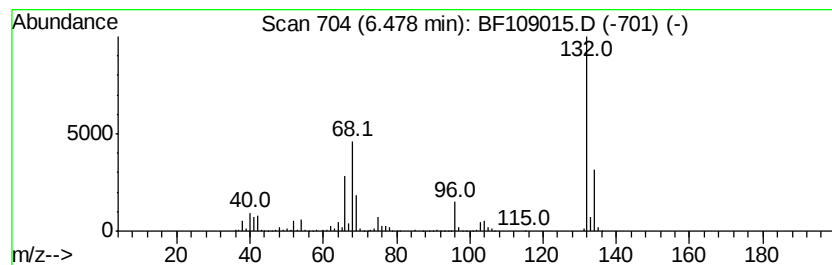
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	49.37 ng	2667390	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10	
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9	



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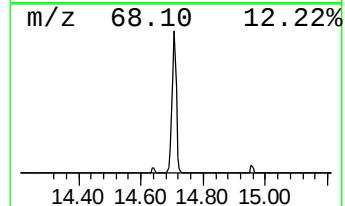
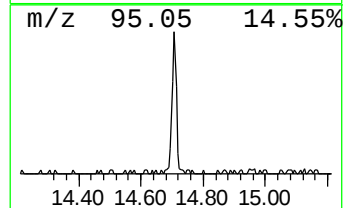
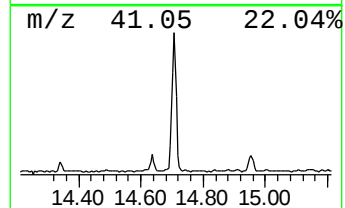
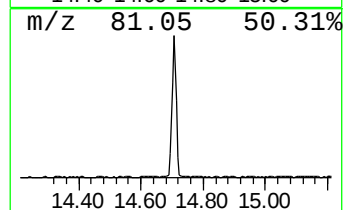
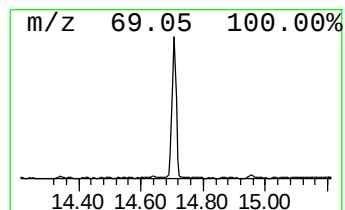
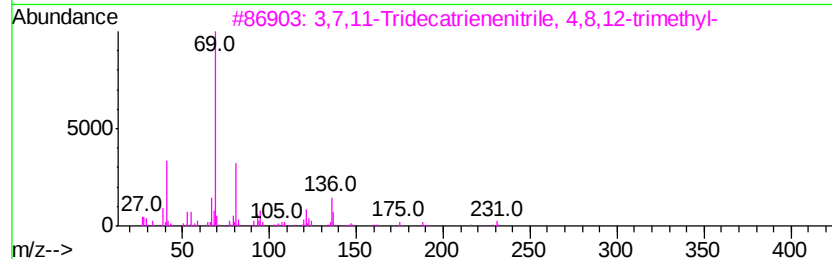
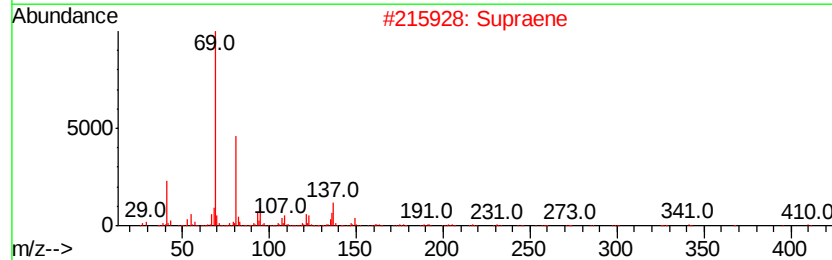
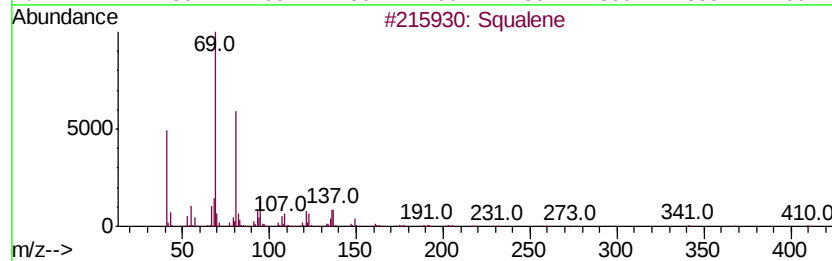
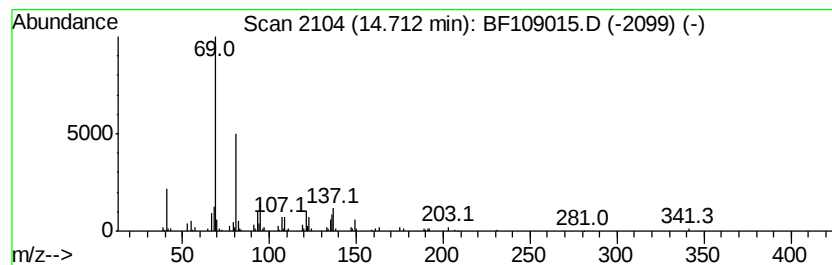
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Peak Number 4 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	5.35 ng	294508	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		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	78
4		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
5		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	2.6	ng	141635	1	6.72	1080530	20.0
unknown6.48	6.48	49.4	ng	2667390	1	6.72	1080530	20.0
Squalene	14.71	5.3	ng	294508	6	15.25	1100180	20.0