

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091418\
 Data File : BF109016.D
 Acq On : 15 Sep 2018 00:57
 Operator : JU/SJ
 Sample : J4901-02
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

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

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	445	rVB	144135	153613	3.24%	0.512%
2	5.319	503	507	511	rBV	1286198	1242092	26.23%	4.144%
3	6.342	677	681	689	rBV	1017310	847900	17.91%	2.829%
4	6.484	701	705	708	rBV	2512950	2302518	48.63%	7.681%
5	6.719	741	745	748	rBV	1244068	964458	20.37%	3.218%
6	6.878	767	772	775	rBV	3576951	3116639	65.82%	10.397%
7	7.278	835	840	843	rBV	2472961	2776562	58.64%	9.263%
8	8.001	959	963	966	rBV	1385224	1216169	25.68%	4.057%
9	9.078	1141	1146	1149	rBV	4993578	4734982	100.00%	15.796%
10	9.466	1209	1212	1215	rBV	387801	298129	6.30%	0.995%
11	9.748	1256	1260	1264	rBV2	1707482	1437543	30.36%	4.796%
12	10.430	1371	1376	1379	rBV	80088	60104	1.27%	0.201%
13	10.530	1389	1393	1405	rBV	2224956	2032207	42.92%	6.780%
14	11.224	1507	1511	1514	rBV	1736685	1434711	30.30%	4.786%
15	11.766	1600	1603	1607	rBV	51118	53083	1.12%	0.177%
16	12.813	1776	1781	1784	rBV	4697528	4615528	97.48%	15.398%
17	13.718	1931	1935	1948	rBV3	32494	63224	1.34%	0.211%
18	13.848	1953	1957	1961	rBV	1214328	1054175	22.26%	3.517%
19	14.707	2099	2103	2107	rBV	264253	242442	5.12%	0.809%
20	14.954	2141	2145	2152	rVB	57434	60984	1.29%	0.203%
21	15.248	2190	2195	2201	rBV	835694	1023671	21.62%	3.415%
22	15.307	2201	2205	2213	rVB	67744	89035	1.88%	0.297%
23	15.712	2269	2274	2281	rVB	56611	81964	1.73%	0.273%
24	16.177	2348	2353	2359	rBV2	44465	73338	1.55%	0.245%

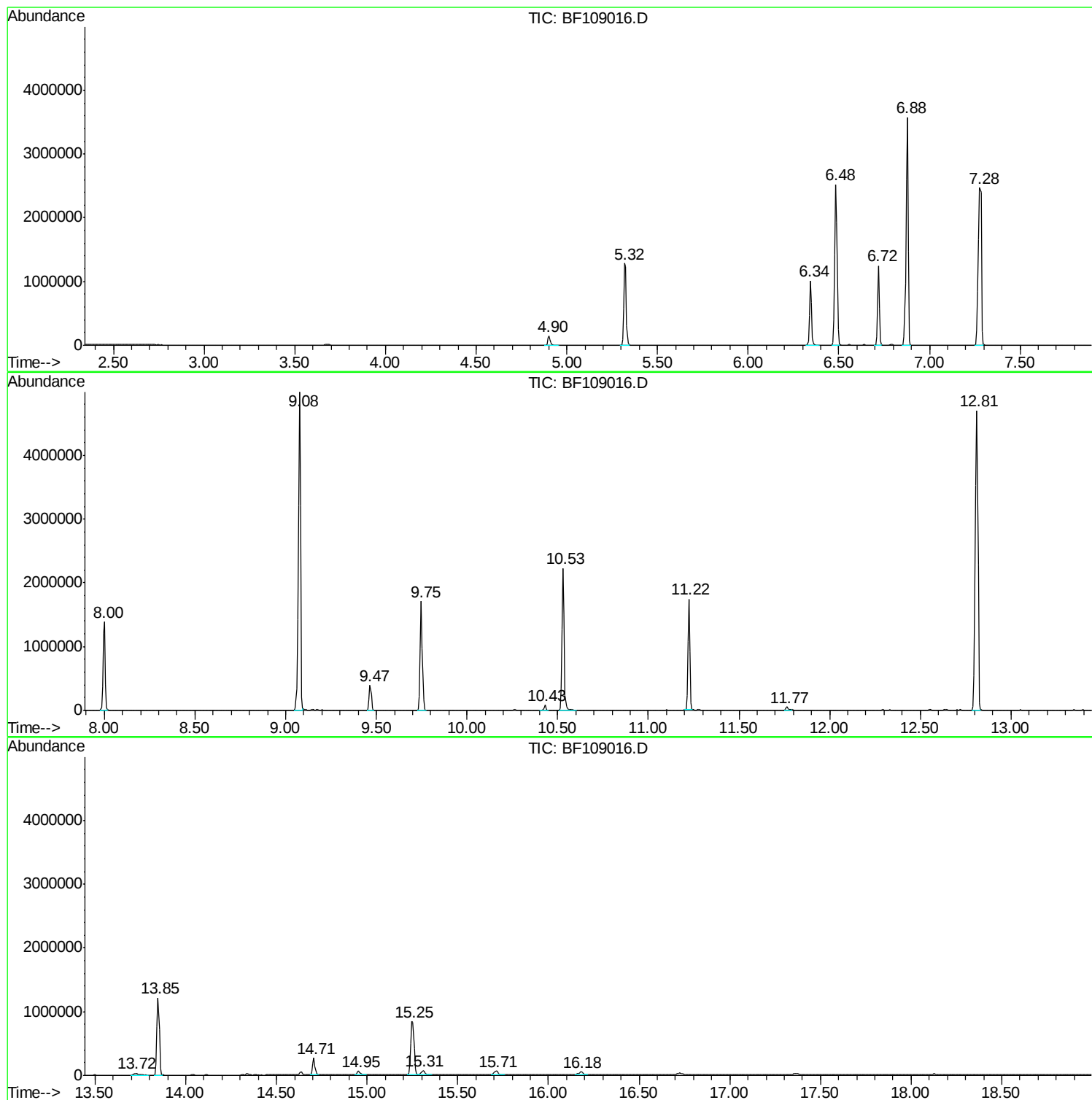
Sum of corrected areas: 29975071

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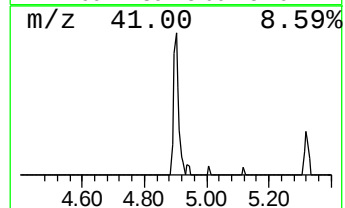
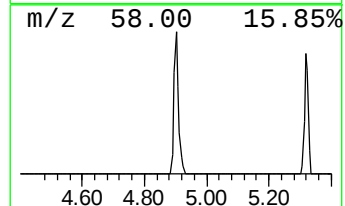
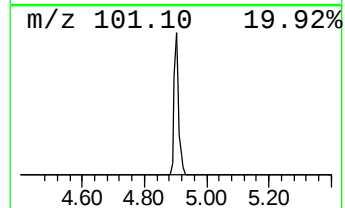
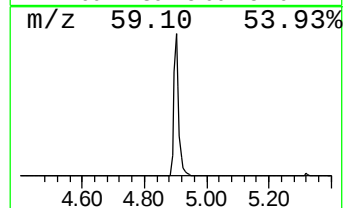
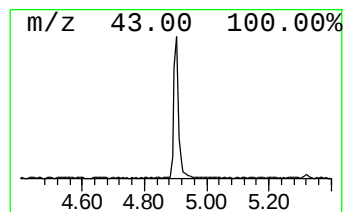
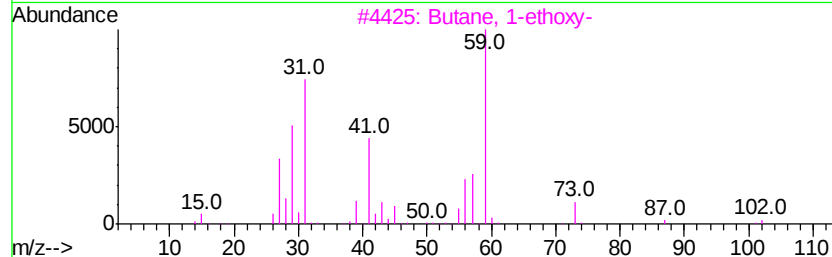
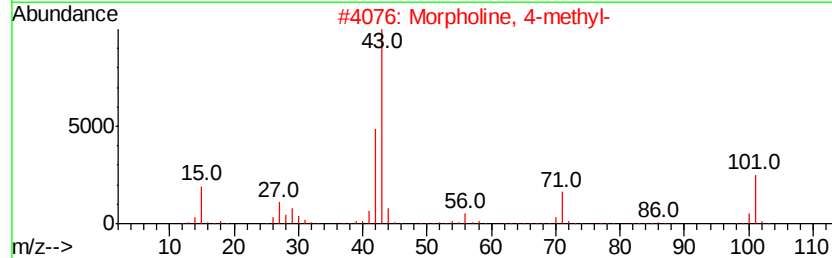
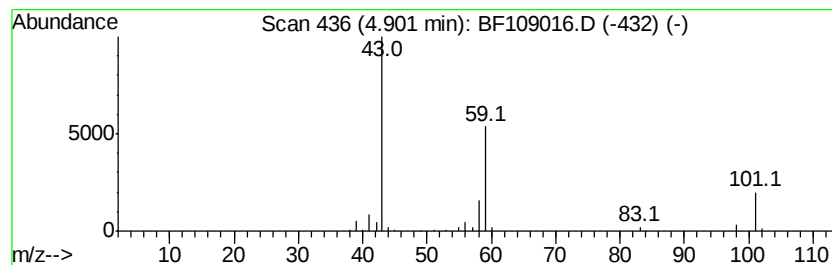
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
4.90	3.19 ng	153613	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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
4	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9	
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9	



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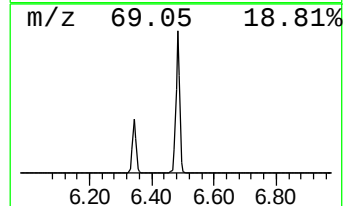
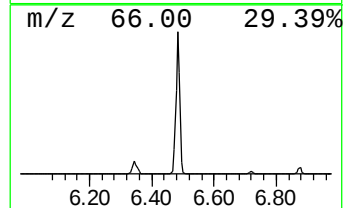
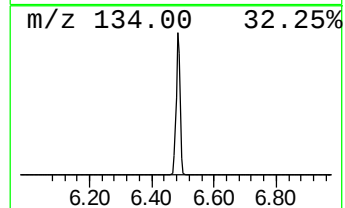
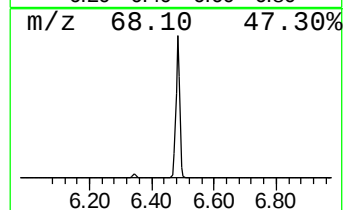
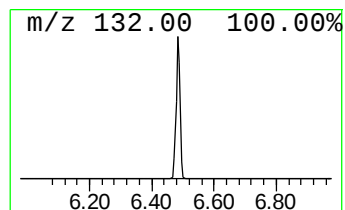
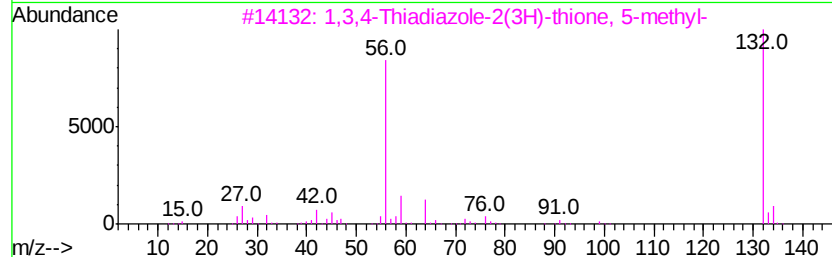
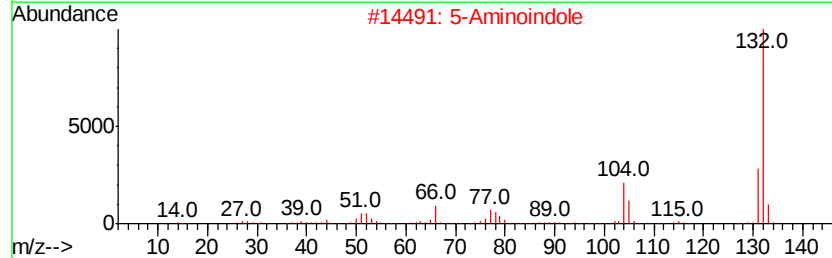
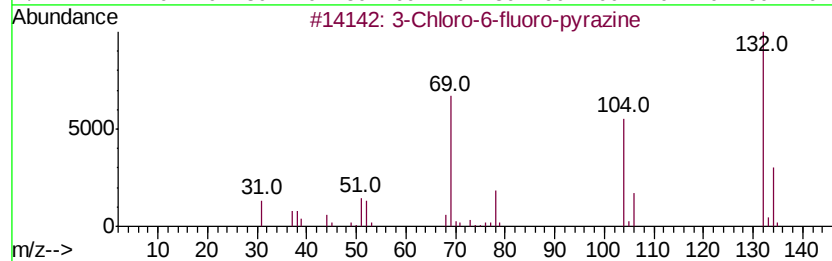
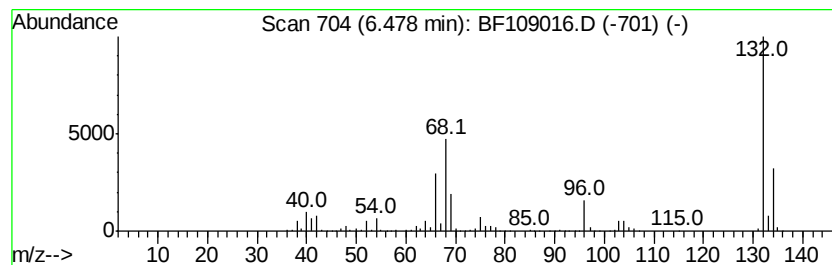
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Peak Number 2 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	47.75 ng	2302520	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		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	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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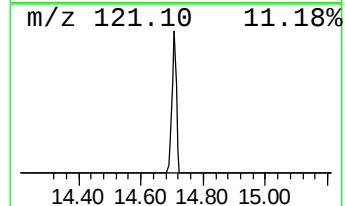
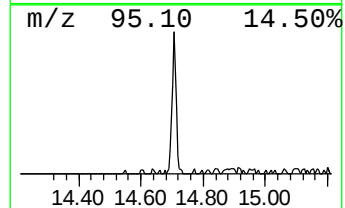
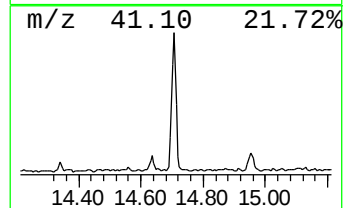
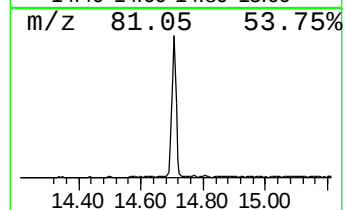
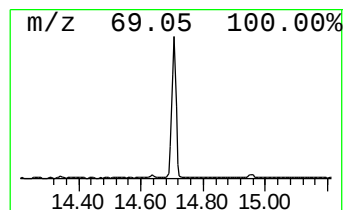
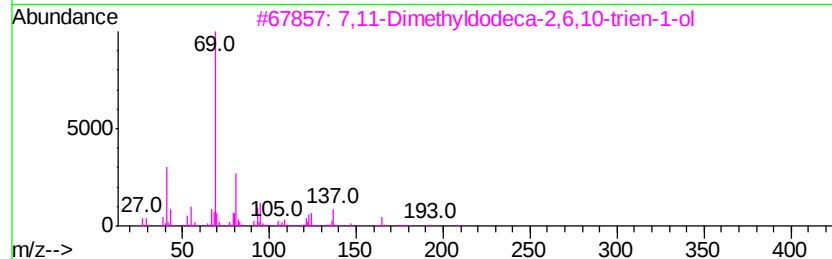
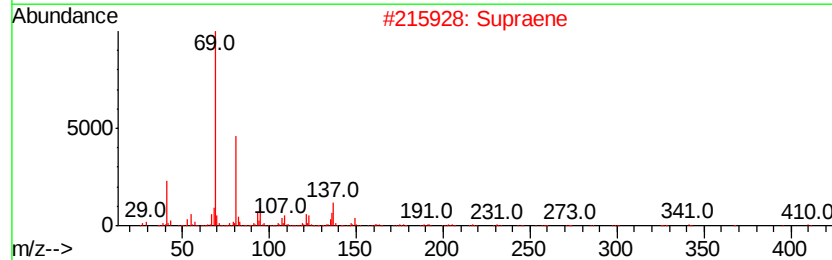
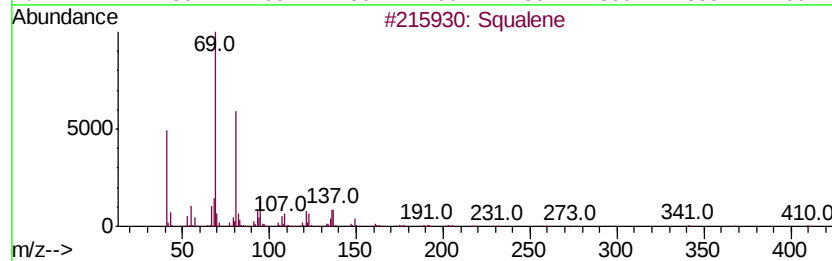
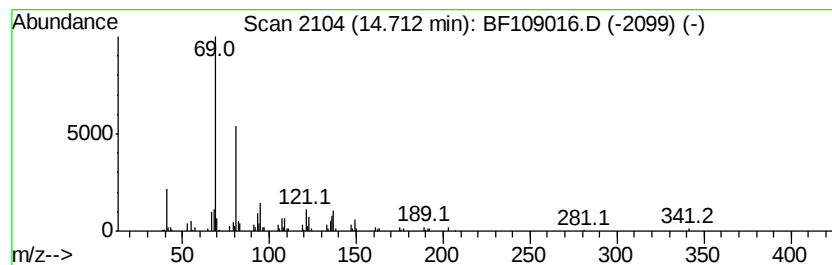
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Peak Number 4 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	4.74 ng	242442	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		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
5		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	3.2	ng	153613	1	6.72	964458	20.0
unknown6.48	6.48	47.8	ng	2302520	1	6.72	964458	20.0
Squalene	14.71	4.7	ng	242442	6	15.25	1023670	20.0