

Data Path : Z:\HPCHEM1\BNA F\Data\BF040517\
 Data File : BF094191.D
 Acq On : 5 Apr 2017 16:07
 Operator : SJ/MA
 Sample : I2523-15
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CEMETERY-3(0-7)

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:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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	1.922	3	6	14	rVB	69582	84362	1.86%	0.228%
2	4.010	356	361	369	rBV	403657	532612	11.75%	1.441%
3	4.404	423	428	431	rBV	3653651	3633805	80.19%	9.829%
4	5.475	603	610	613	rBV	3090024	3783630	83.50%	10.234%
5	5.610	628	633	636	rBV	3717100	3882184	85.67%	10.501%
6	5.863	672	676	680	rBV	1157439	1012279	22.34%	2.738%
7	6.039	701	706	710	rBV	2908746	3050512	67.32%	8.251%
8	6.510	780	786	789	rBV	2121489	2468349	54.47%	6.676%
9	7.363	926	931	935	rBV	1389330	1389522	30.66%	3.758%
10	8.692	1150	1157	1160	rBV	3836891	4531458	100.00%	12.257%
11	9.180	1235	1240	1244	rBV	282573	271107	5.98%	0.733%
12	9.504	1286	1295	1299	rBV2	1519126	1571637	34.68%	4.251%
13	10.098	1391	1396	1400	rVB	93219	88487	1.95%	0.239%
14	10.474	1455	1460	1464	rBV	1868953	2012662	44.42%	5.444%
15	10.680	1492	1495	1498	rBV	103908	107937	2.38%	0.292%
16	11.233	1586	1589	1593	rBV	54945	57656	1.27%	0.156%
17	11.327	1599	1605	1609	rBV	1505964	1504190	33.19%	4.069%
18	13.309	1935	1942	1945	rBV	3559742	4209362	92.89%	11.385%
19	14.480	2136	2141	2152	rBV2	112183	218110	4.81%	0.590%
20	14.574	2152	2157	2161	rBV	1316883	1354847	29.90%	3.665%
21	15.686	2342	2346	2350	rBV	116154	114655	2.53%	0.310%
22	16.198	2428	2433	2438	rBV	867344	1025351	22.63%	2.773%
23	17.174	2595	2599	2606	rVB5	35587	66555	1.47%	0.180%

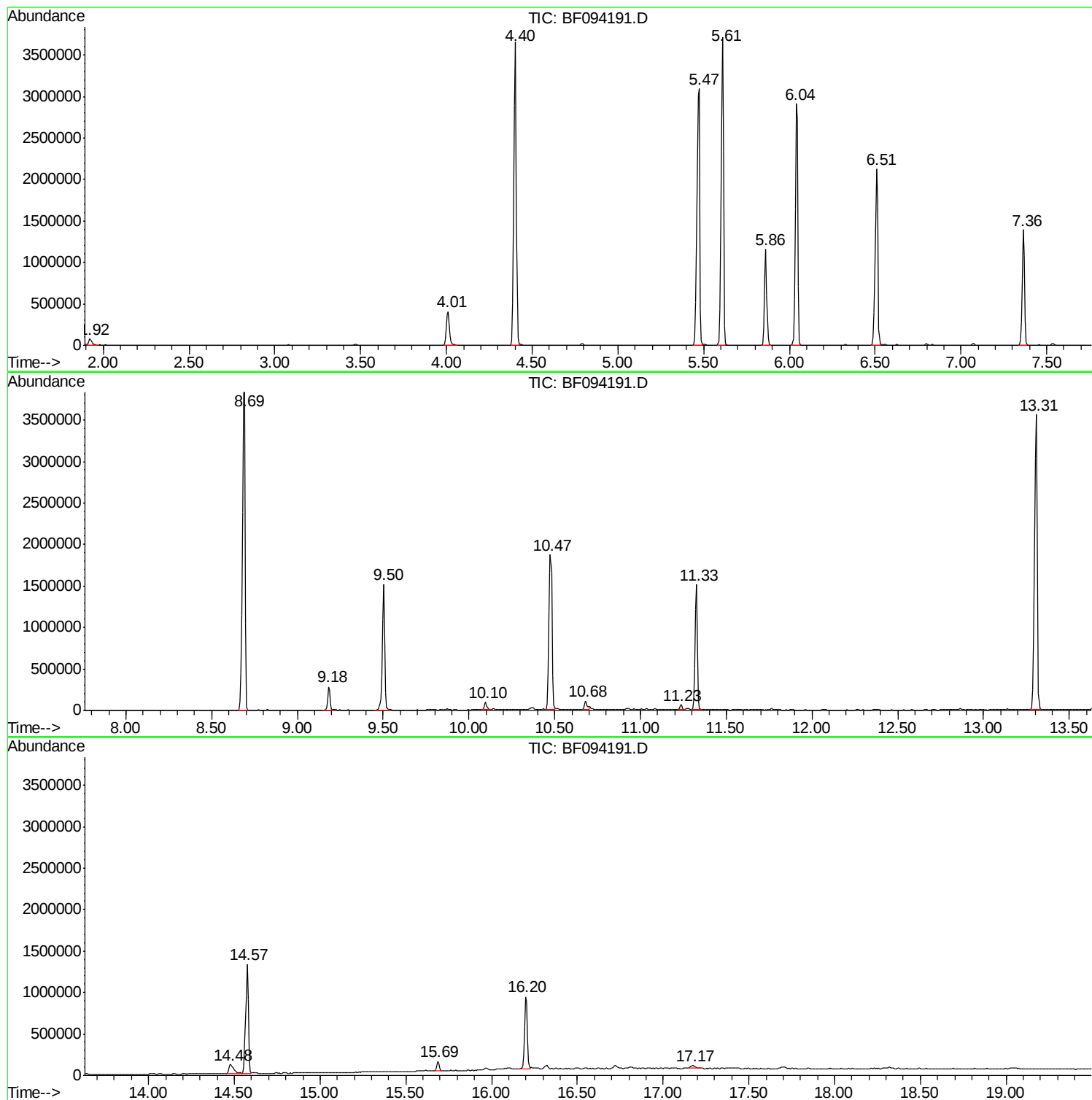
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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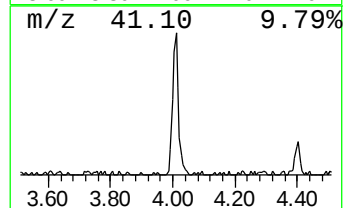
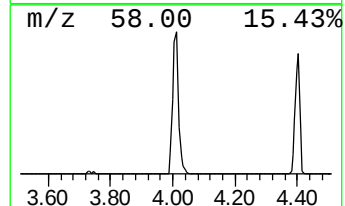
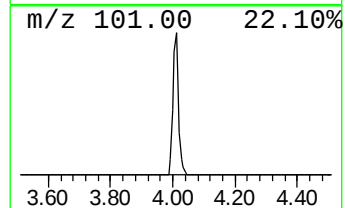
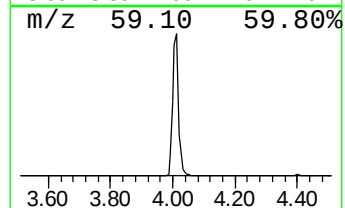
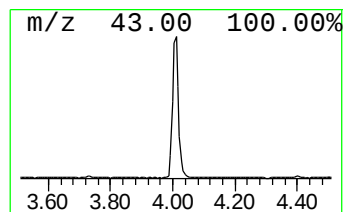
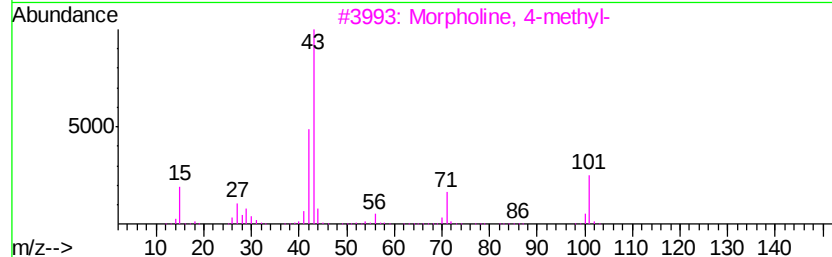
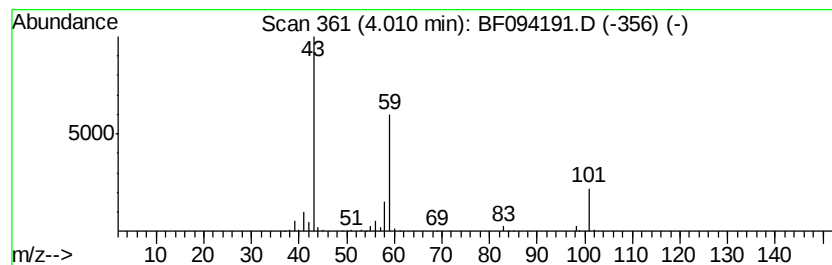
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.01	10.52 ng	532612	1,4-Dichlorobenzene-d4	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	9



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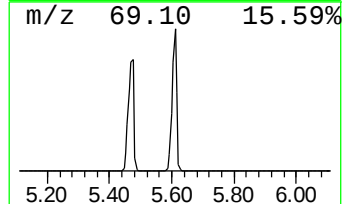
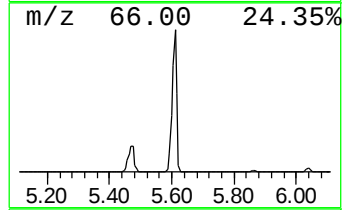
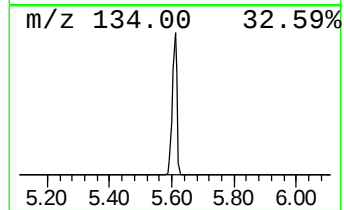
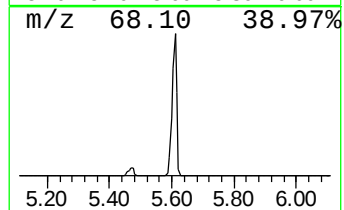
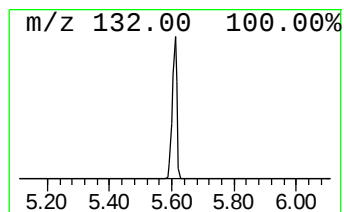
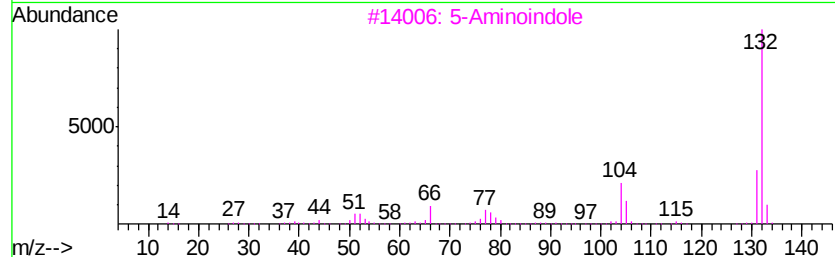
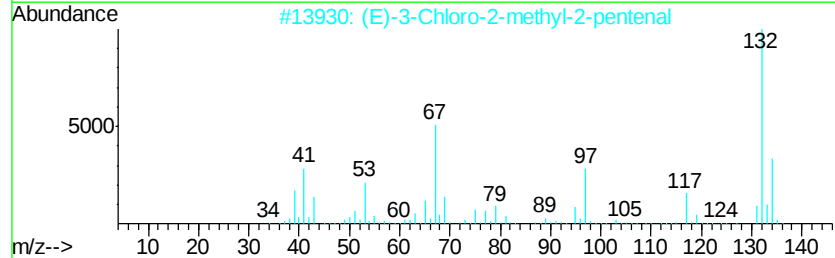
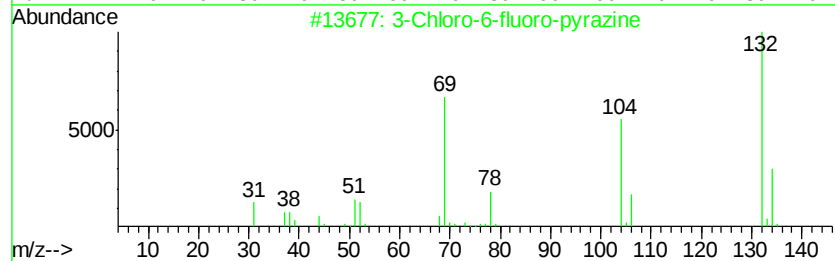
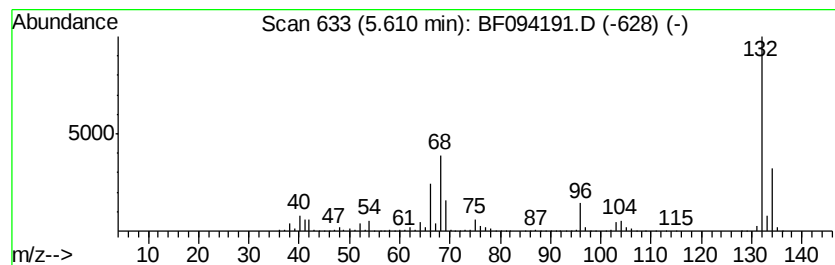
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Peak Number 2 unknown5.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.61	76.70 ng	3882180	1,4-Dichlorobenzene-d4	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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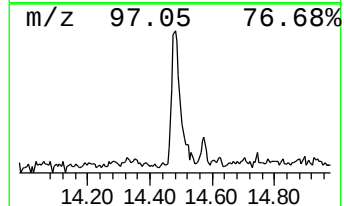
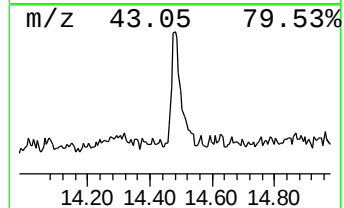
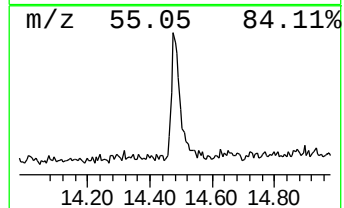
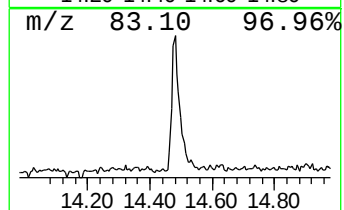
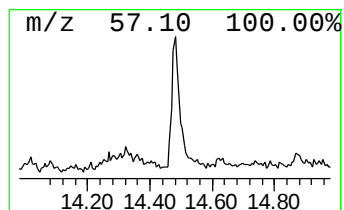
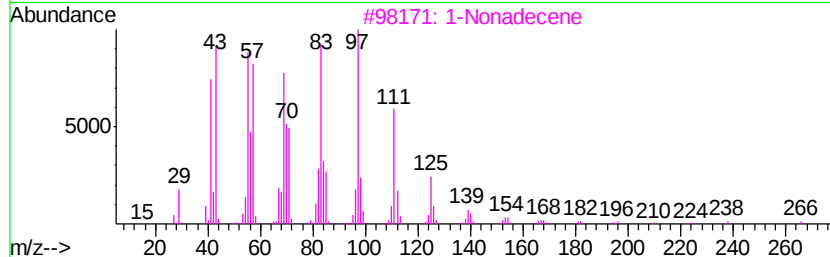
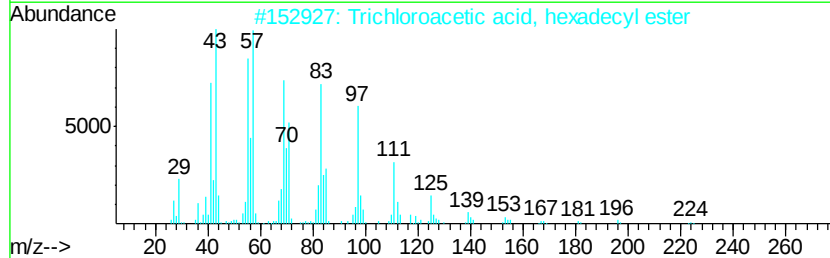
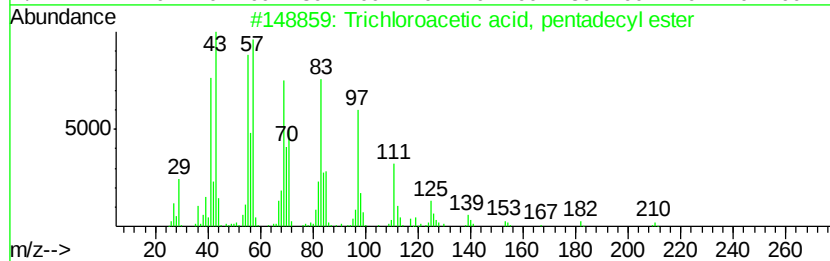
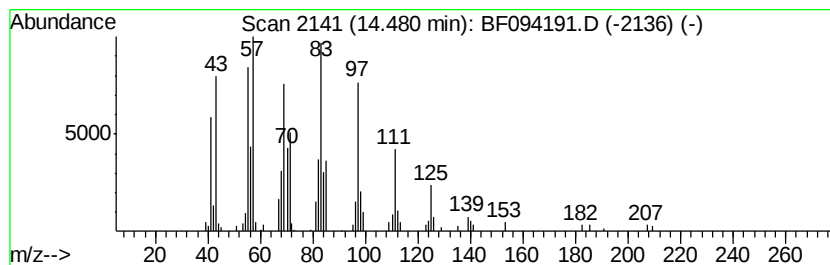
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Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	3.22 ng	218110	Chrysene-d12	14.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	91



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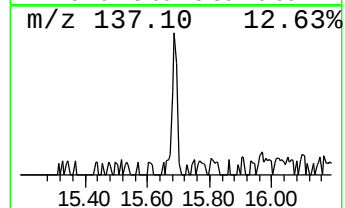
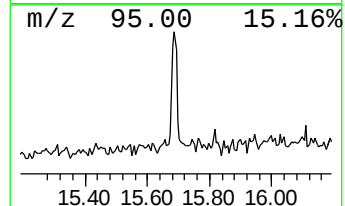
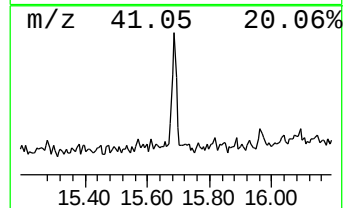
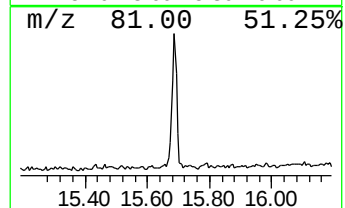
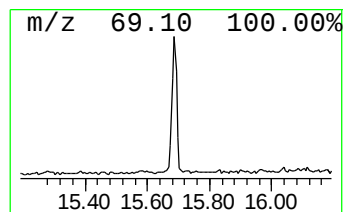
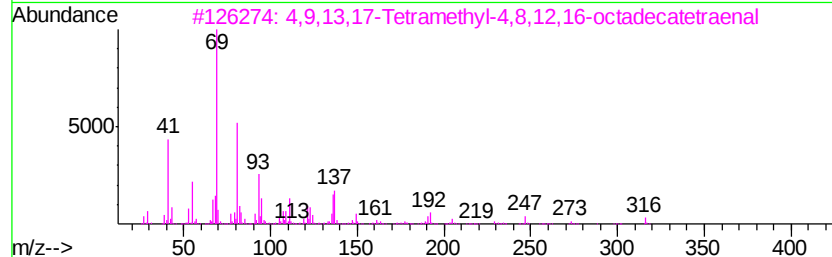
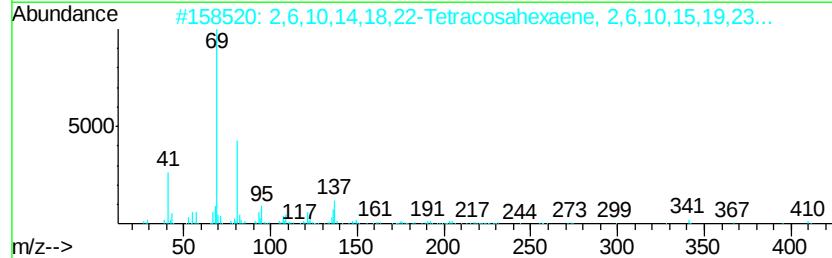
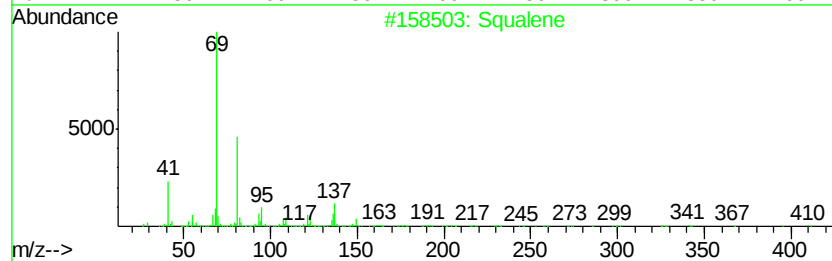
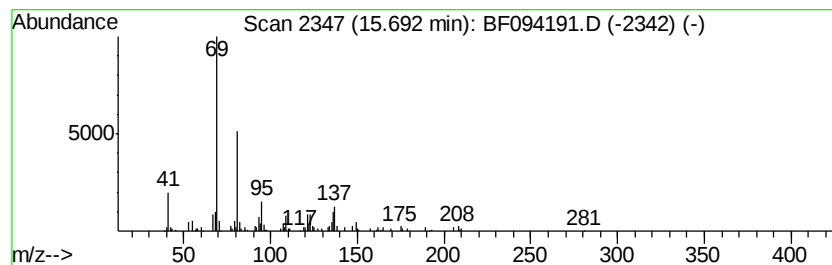
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	2.24 ng	114655	Perylene-d12	16.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	007683-64-9 91
2	2,6,10,14,18,22-Tetracosahexaene...		410 C30H50	000111-02-4 91
3	4,9,13,17-Tetramethyl-4,8,12,16-...		316 C22H360	056882-09-8 83
4	Propanoic acid, 2,2-dimethyl-, [...		306 C20H3402	1000164-38-8 72
5	7,11-Dimethyldodeca-2,6,10-trien...		208 C14H240	125529-10-4 64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.01	10.5	ng	532612	1	5.86	1012280	20.0
unknown5.61	5.61	76.7	ng	3882180	1	5.86	1012280	20.0
Trichloroacetic a...	14.48	3.2	ng	218110	5	14.57	1354850	20.0
Squalene	15.69	2.2	ng	114655	6	16.20	1025350	20.0