

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112219\
 Data File : BF117932.D
 Acq On : 22 Nov 2019 21:47
 Operator : JU
 Sample : K5840-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHIPPS-BH-NE-02

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-BF111319.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	2.222	15	23	29	rVB	764994	988864	15.76%	2.269%
2	5.122	508	516	525	rBV	1078593	1368205	21.81%	3.140%
3	5.522	579	584	587	rBV	3415357	3169466	50.51%	7.273%
4	6.528	749	755	759	rBV	3444893	3741172	59.62%	8.585%
5	6.669	775	779	783	rBV	3498521	3569468	56.89%	8.191%
6	6.904	815	819	822	rBV	1173025	942520	15.02%	2.163%
7	7.063	841	846	849	rBV	3744051	3308405	52.73%	7.592%
8	7.463	909	914	917	rBV	2408119	2535556	40.41%	5.818%
9	8.192	1033	1038	1041	rBV	1210620	1211513	19.31%	2.780%
10	9.269	1216	1221	1224	rBV	4980290	4743031	75.59%	10.884%
11	9.663	1283	1288	1291	rBV	453234	411375	6.56%	0.944%
12	9.951	1332	1337	1341	rBV	1753921	1522800	24.27%	3.494%
13	10.739	1466	1471	1475	rBV	2368911	2425966	38.66%	5.567%
14	11.445	1587	1591	1595	rBV	2012352	1722637	27.45%	3.953%
15	11.963	1676	1679	1684	rBV	159364	151869	2.42%	0.348%
16	13.039	1857	1862	1865	rBV	6395863	6274583	100.00%	14.398%
17	13.927	2010	2013	2029	rBV	577011	848728	13.53%	1.948%
18	14.092	2037	2041	2045	rVB	2069683	1835218	29.25%	4.211%
19	14.251	2065	2068	2076	rBV	74482	80526	1.28%	0.185%
20	14.557	2116	2120	2133	rBV2	103199	149312	2.38%	0.343%
21	14.874	2168	2174	2180	rBV	107181	112062	1.79%	0.257%
22	14.957	2184	2188	2193	rBV	301712	327283	5.22%	0.751%
23	15.227	2230	2234	2238	rBV	113770	129117	2.06%	0.296%
24	15.598	2291	2297	2300	rBV	1237095	1611862	25.69%	3.699%
25	15.621	2300	2301	2306	rVB	95558	101888	1.62%	0.234%
26	16.086	2374	2380	2385	rBV	67119	103136	1.64%	0.237%
27	16.151	2385	2391	2399	rBV5	38075	117924	1.88%	0.271%
28	16.615	2464	2470	2476	rVB3	36419	73645	1.17%	0.169%

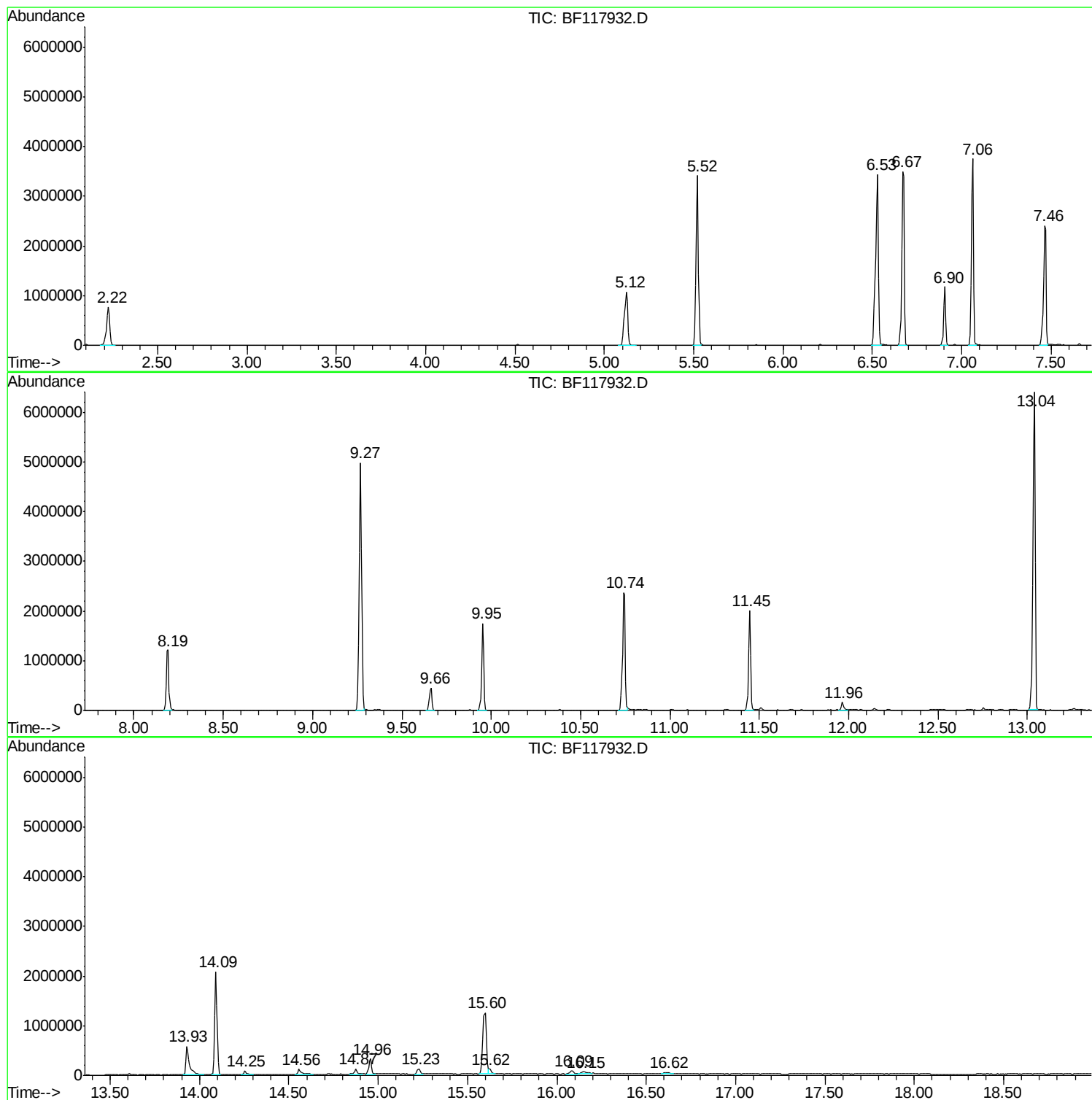
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ClientSampleId :
PHIPPS-BH-NE-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.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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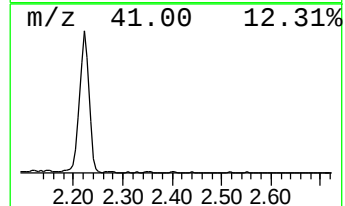
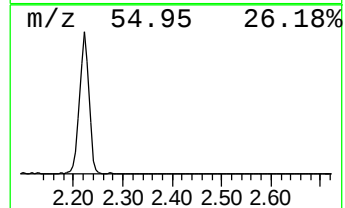
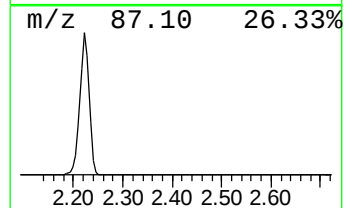
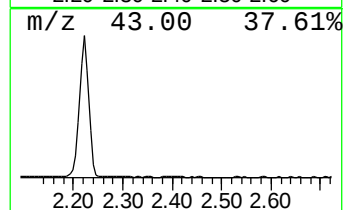
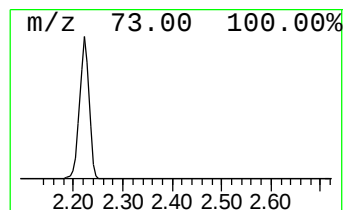
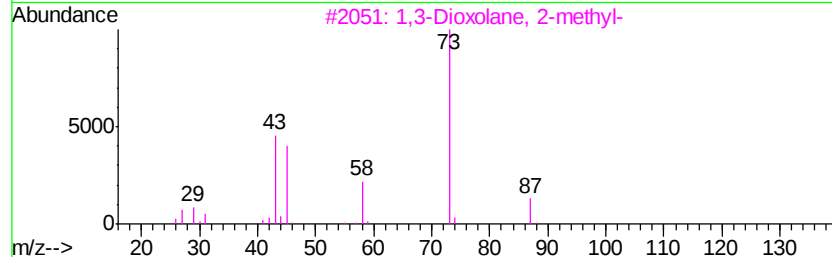
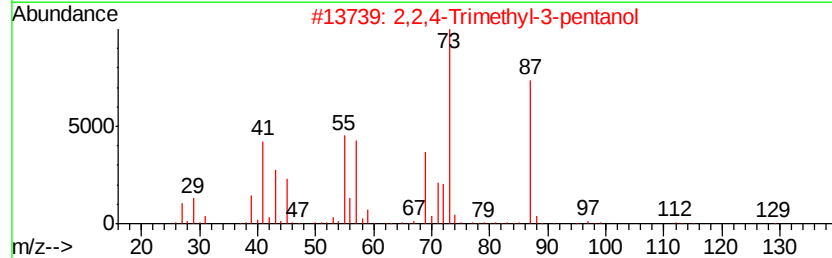
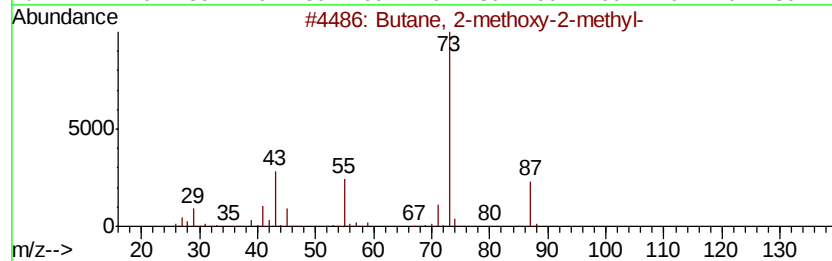
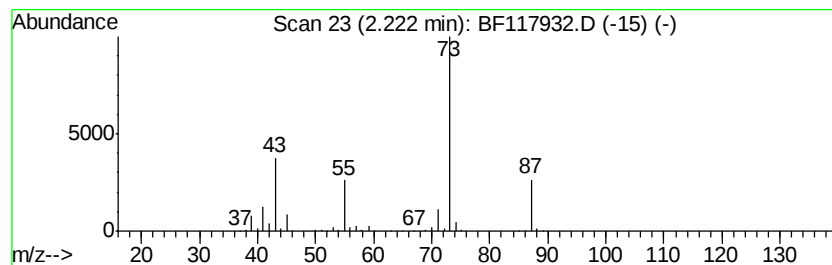
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	20.98 ng	988864	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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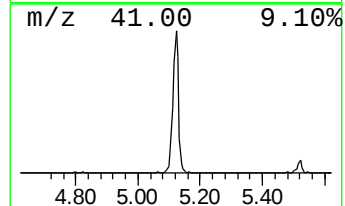
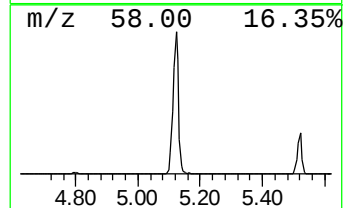
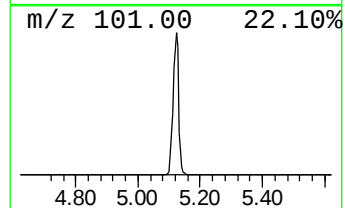
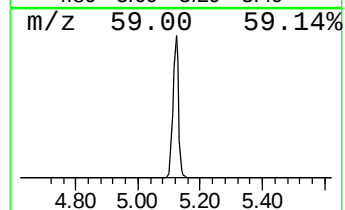
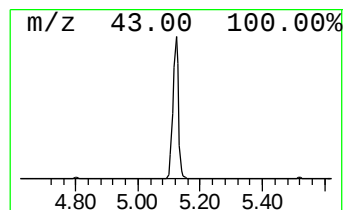
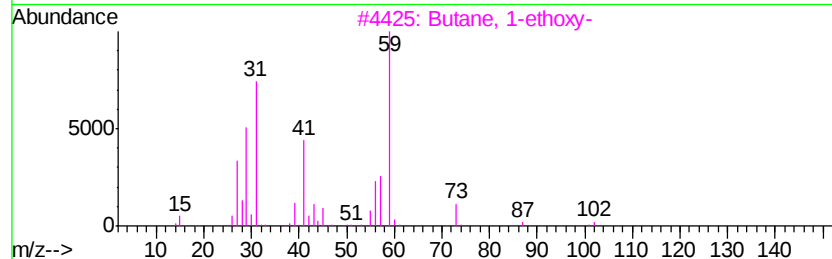
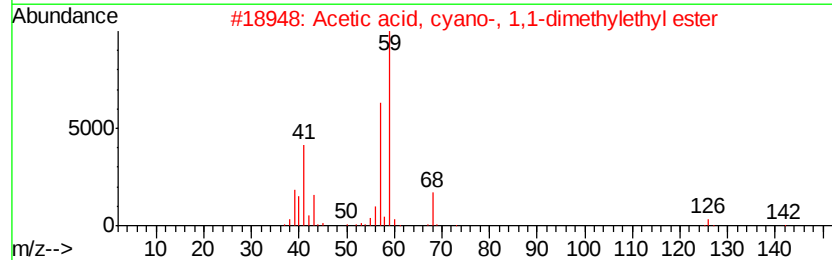
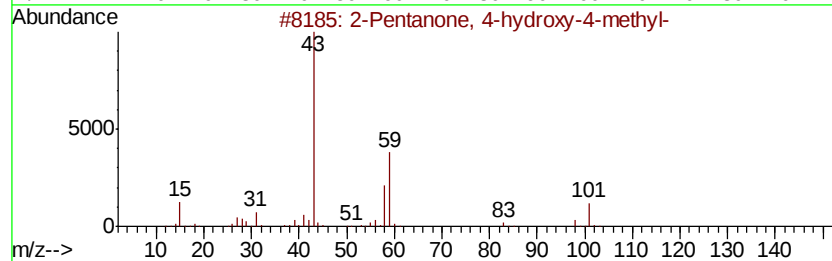
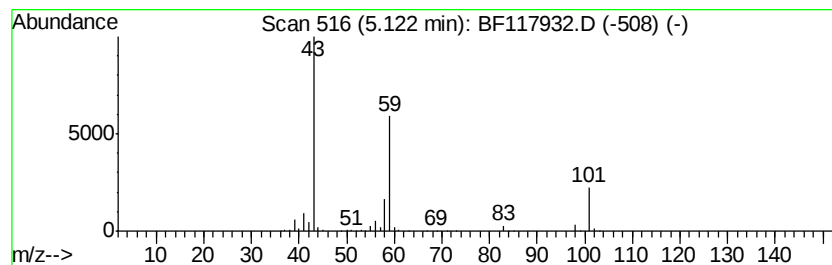
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	29.03 ng	1368210	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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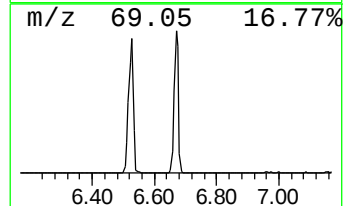
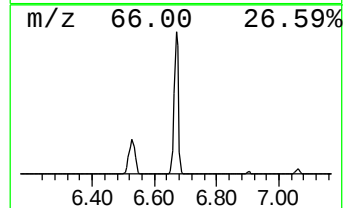
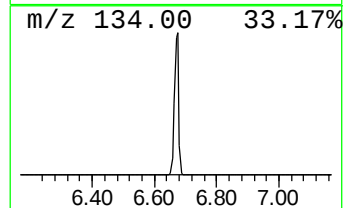
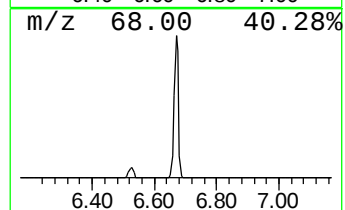
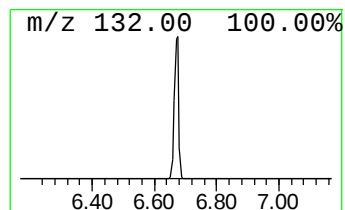
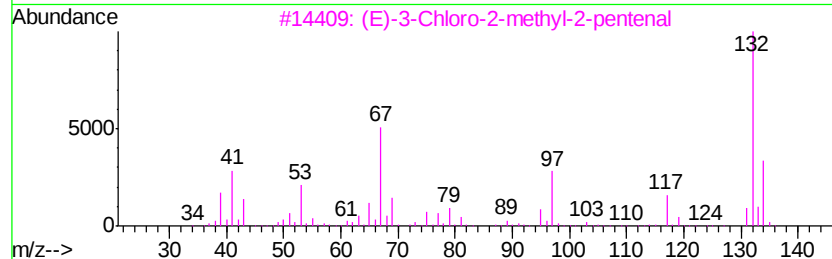
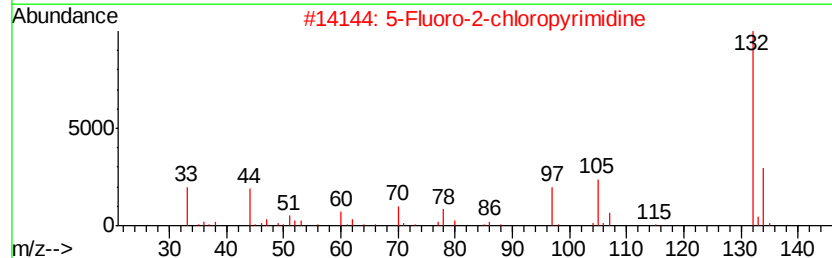
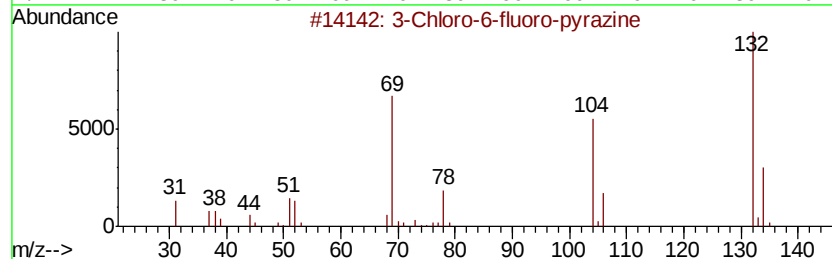
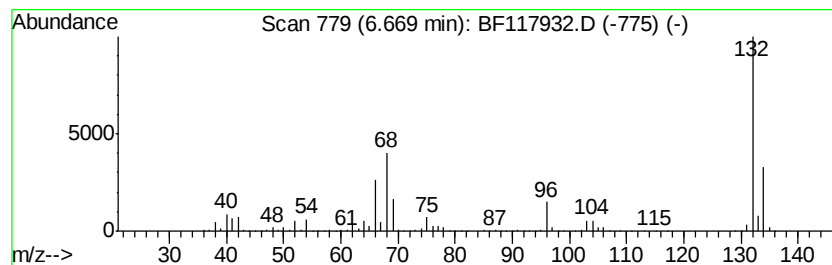
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	75.74 ng	3569470	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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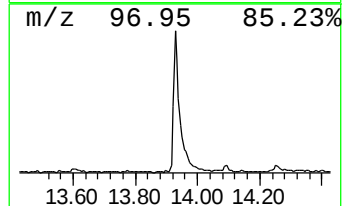
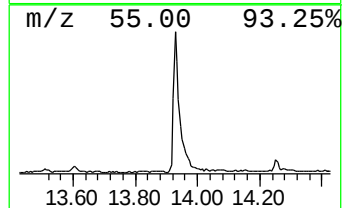
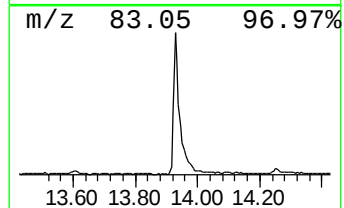
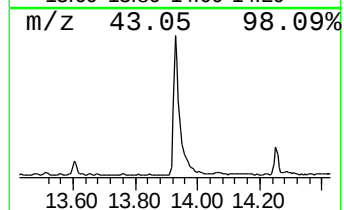
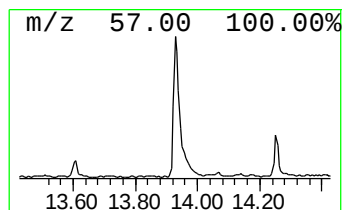
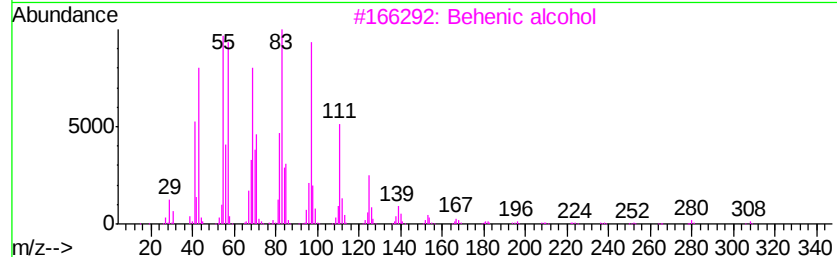
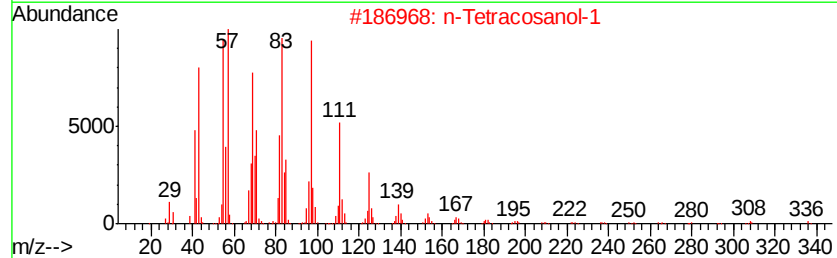
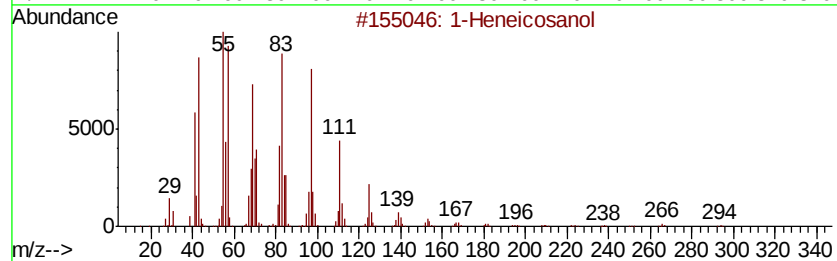
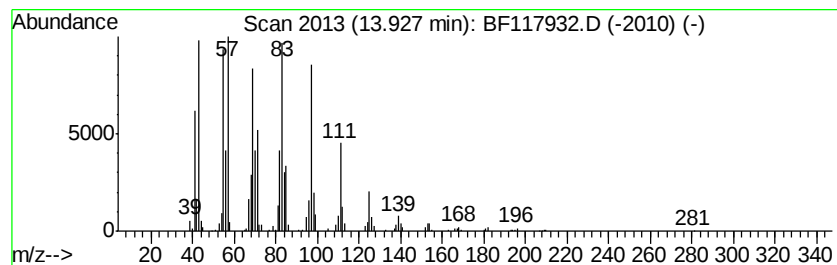
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	9.25 ng	848728	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		Behenic alcohol	326	C22H46O	000661-19-8	95
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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ClientSampleId :
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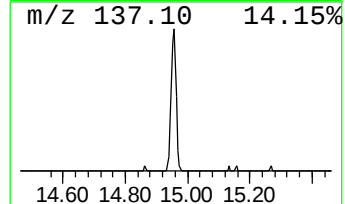
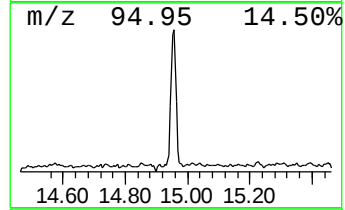
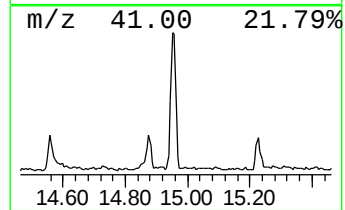
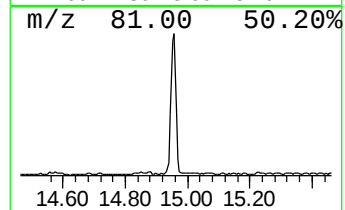
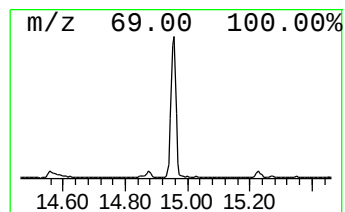
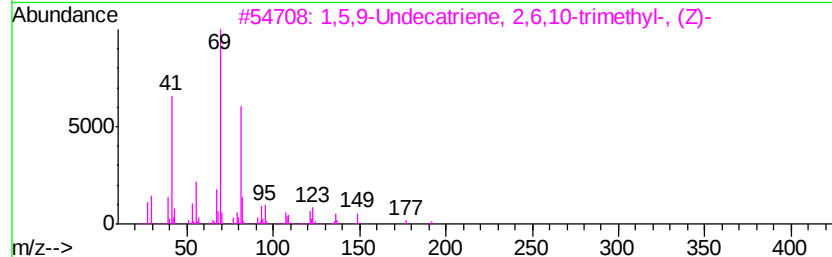
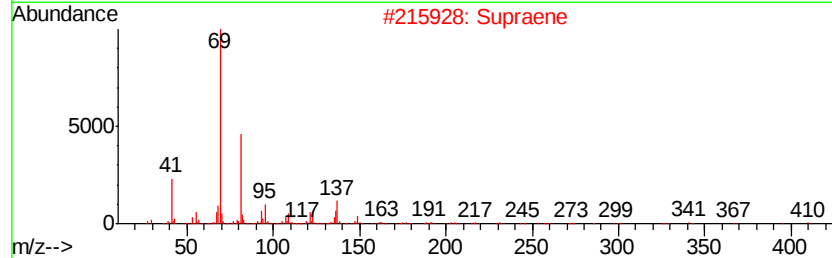
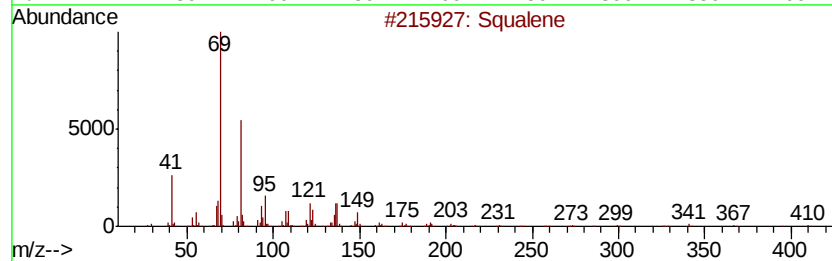
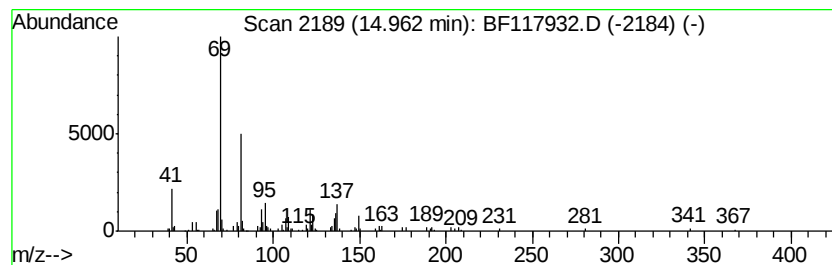
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	4.06 ng	327283	Perylene-d12	15.60

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	90
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59
5		Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	47



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Misc :
ALS Vial : 9 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	21.0	ng	988864	1	6.90	942520	20.0
2-Pentanone, 4-hy...	5.12	29.0	ng	1368210	1	6.90	942520	20.0
unknown6.67	6.67	75.7	ng	3569470	1	6.90	942520	20.0
1-Heneicosanol	13.93	9.3	ng	848728	5	14.09	1835220	20.0
Squalene	14.96	4.1	ng	327283	6	15.60	1611860	20.0