

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
 Data File : BF117592.D
 Acq On : 29 Oct 2019 15:51
 Operator : JU
 Sample : K5540-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 156-56-(0-1.3)

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-BF101819.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	5.357	553	556	578	rBV	580741	786378	85.53%	10.893%
2	6.387	727	731	748	rBV	709016	898193	97.70%	12.442%
3	6.504	748	751	768	rVB	1002440	919382	100.00%	12.736%
4	6.728	786	789	804	rVB	261028	245267	26.68%	3.398%
5	6.881	812	815	828	rBV	642768	590949	64.28%	8.186%
6	7.292	882	885	903	rBV	413136	505720	55.01%	7.006%
7	8.010	1004	1007	1027	rBV	257561	296909	32.29%	4.113%
8	9.081	1186	1189	1202	rBV	719993	663675	72.19%	9.194%
9	9.480	1254	1257	1268	rBV	87295	91346	9.94%	1.265%
10	9.763	1301	1305	1319	rBB	304224	309361	33.65%	4.285%
11	10.557	1436	1440	1456	rBV	368332	414909	45.13%	5.748%
12	11.251	1554	1558	1567	rBV	244093	265774	28.91%	3.682%
13	11.774	1645	1647	1657	rBV	24984	32573	3.54%	0.451%
14	12.827	1822	1826	1834	rBV	565397	474198	51.58%	6.569%
15	13.739	1977	1981	1991	rVB3	44455	82656	8.99%	1.145%
16	13.892	2004	2007	2015	rBV	212147	226039	24.59%	3.131%
17	14.045	2030	2033	2036	rBV4	9518	11874	1.29%	0.164%
18	14.345	2081	2084	2086	rVB3	17301	14546	1.58%	0.202%
19	14.380	2086	2090	2092	rBV5	8618	12951	1.41%	0.179%
20	14.639	2132	2134	2140	rVB4	23322	27466	2.99%	0.380%
21	14.710	2143	2146	2149	rBV	19062	18309	1.99%	0.254%
22	14.957	2185	2188	2191	rBV2	27711	26608	2.89%	0.369%
23	15.021	2197	2199	2205	rBV7	8037	12694	1.38%	0.176%
24	15.333	2245	2252	2262	rVB	140388	221813	24.13%	3.073%
25	15.427	2264	2268	2271	rBV6	9972	12940	1.41%	0.179%
26	15.715	2313	2317	2322	rBV3	23196	34854	3.79%	0.483%
27	16.180	2393	2396	2401	rVB6	14150	21467	2.33%	0.297%

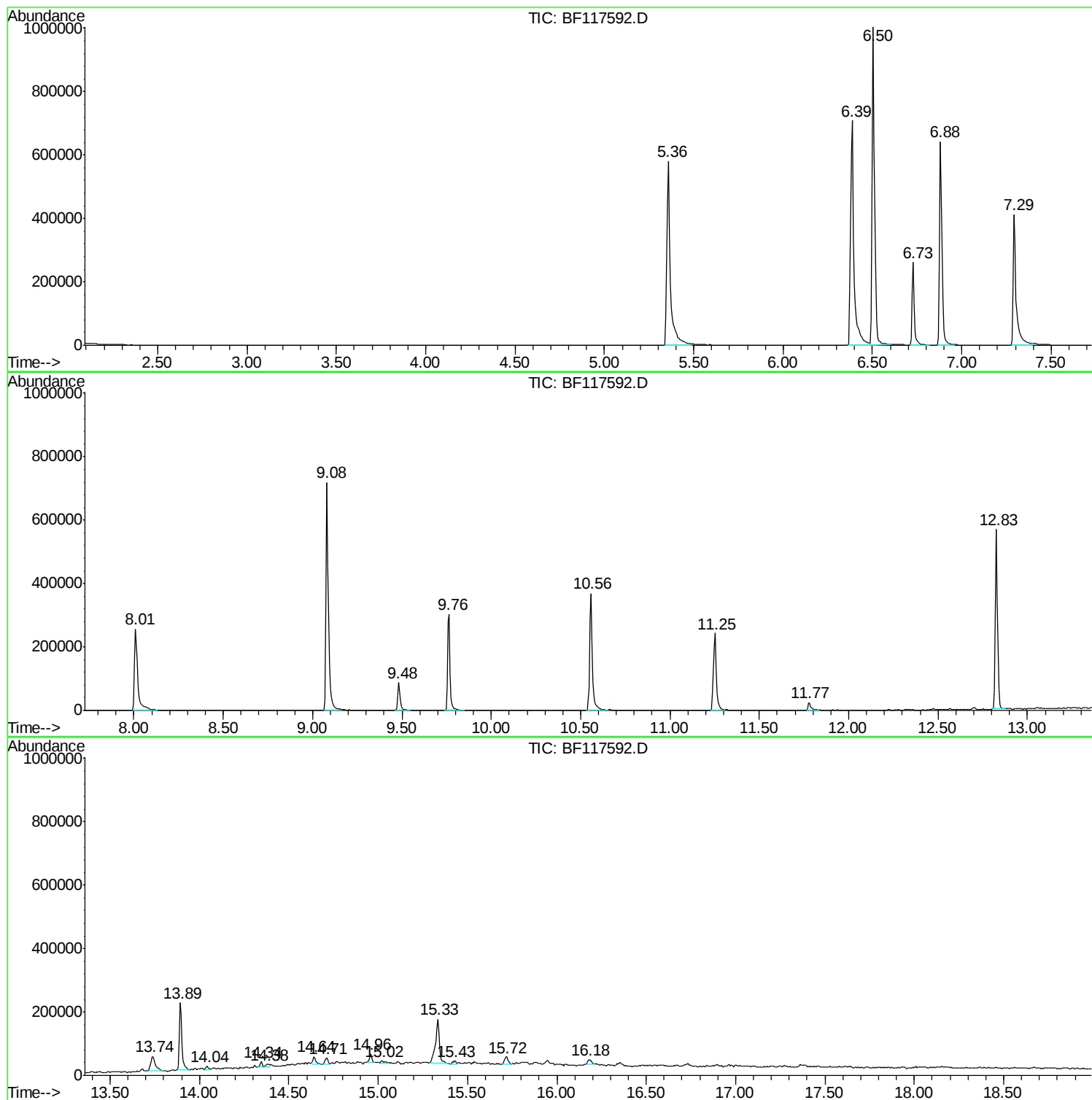
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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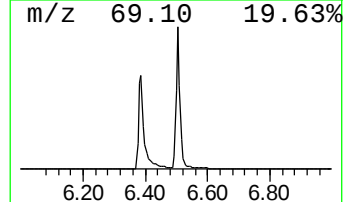
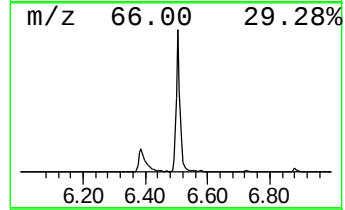
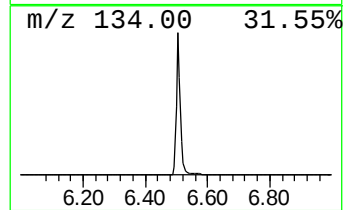
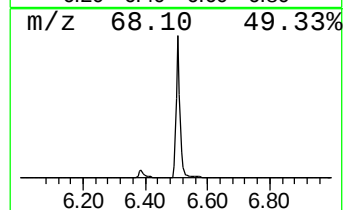
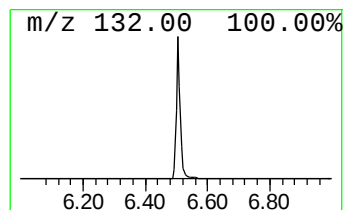
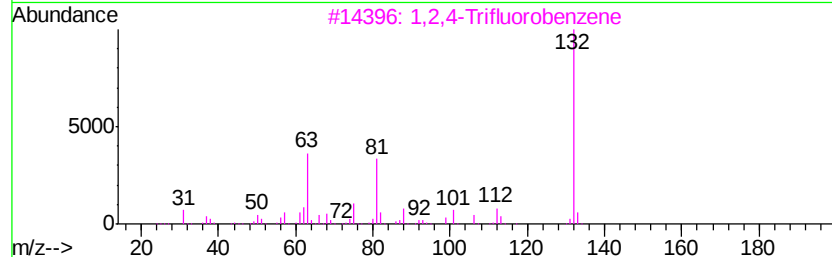
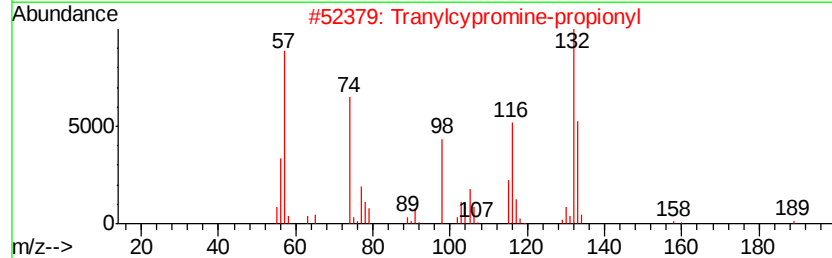
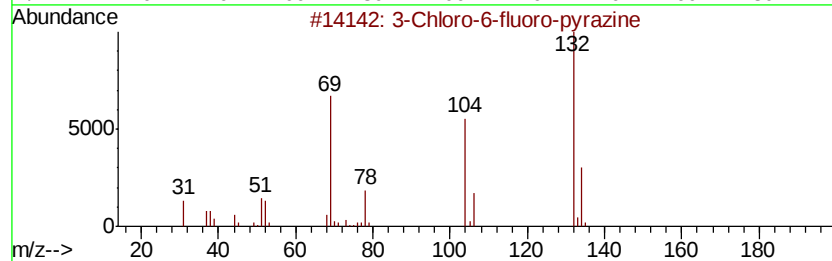
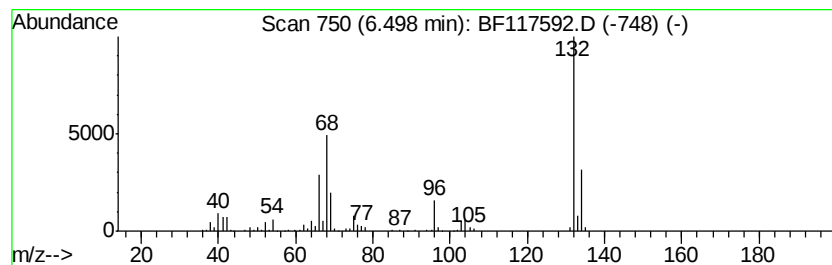
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	74.97 ng	919382	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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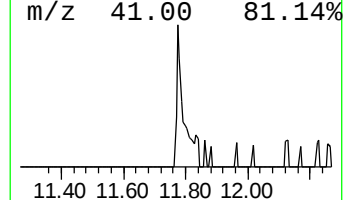
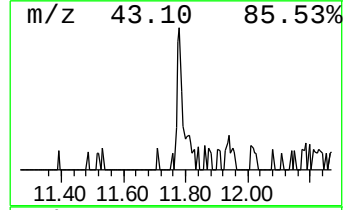
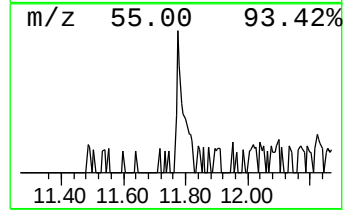
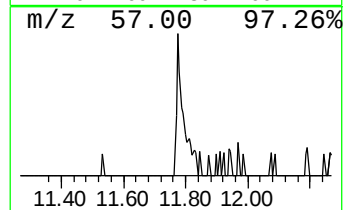
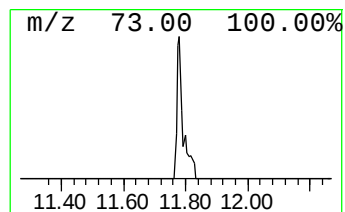
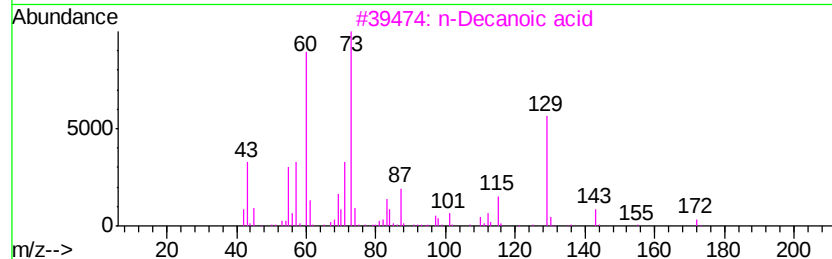
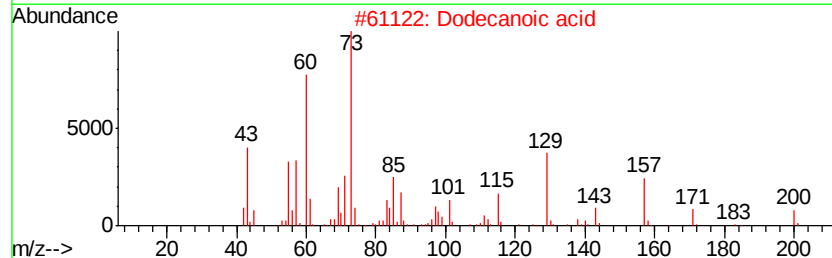
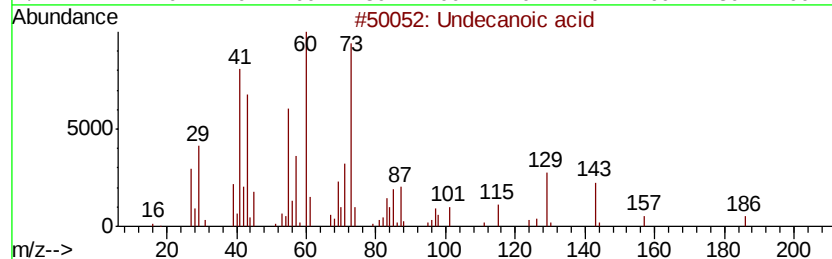
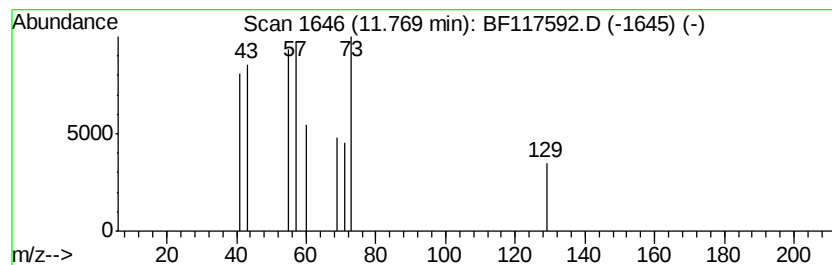
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Peak Number 3 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.77	2.45 ng	32573	Phenanthrene-d10		11.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	72
2			Dodecanoic acid	200	C12H24O2	000143-07-7	64
3			n-Decanoic acid	172	C10H20O2	000334-48-5	59
4			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	14
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	14



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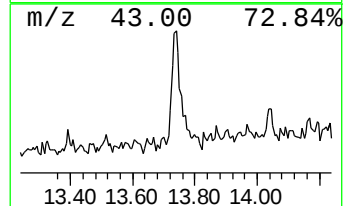
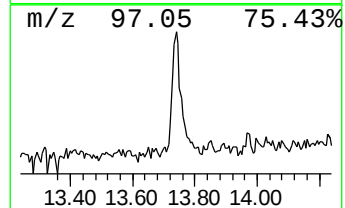
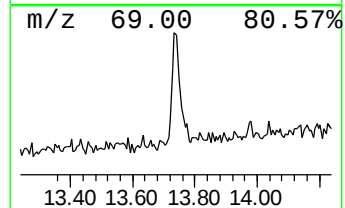
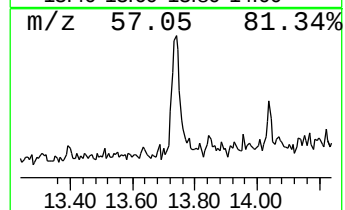
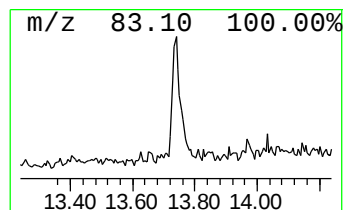
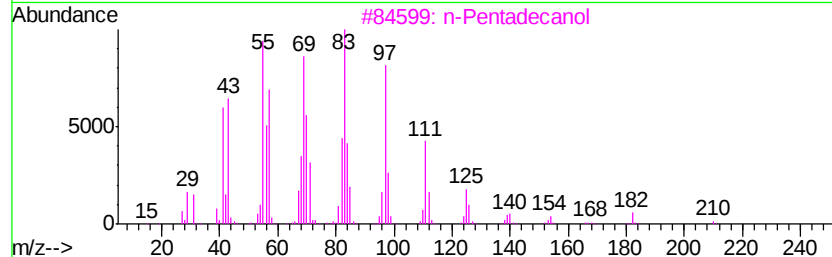
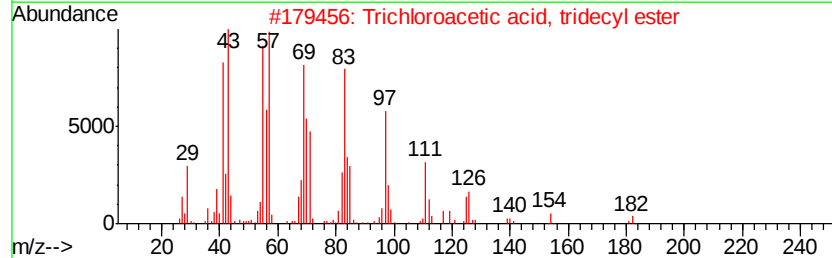
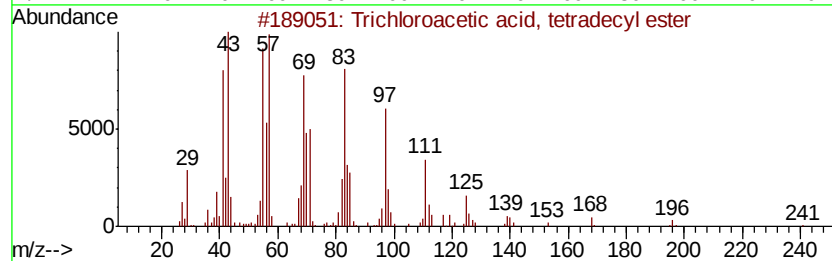
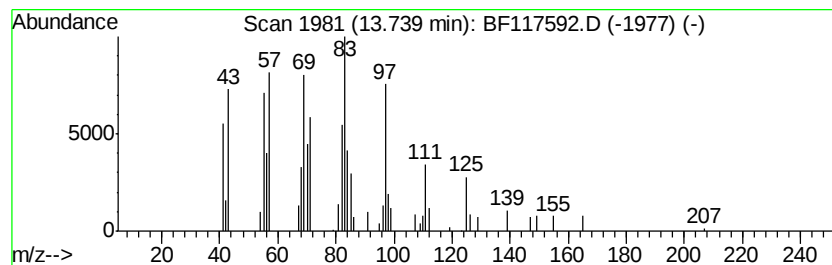
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Peak Number 4 Trichloroacetic acid, tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.74	7.31 ng	82656	Chrysene-d12		13.89		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
2			Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	87
3			n-Pentadecanol	228	C15H32O	000629-76-5	87
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87



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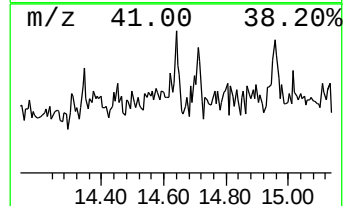
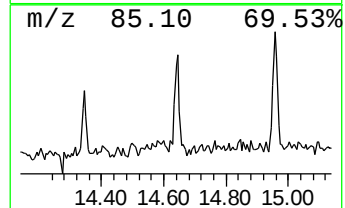
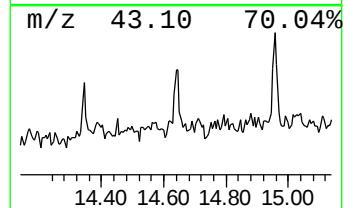
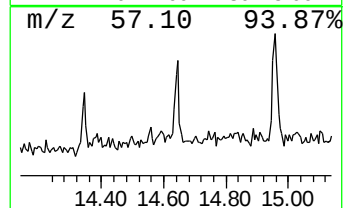
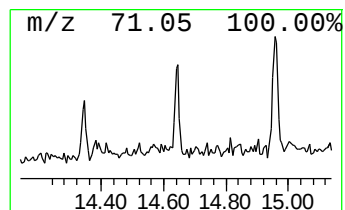
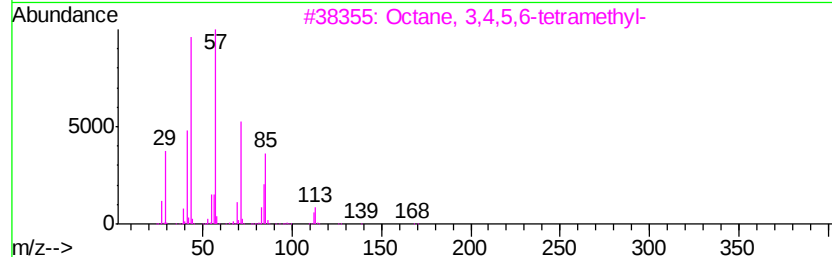
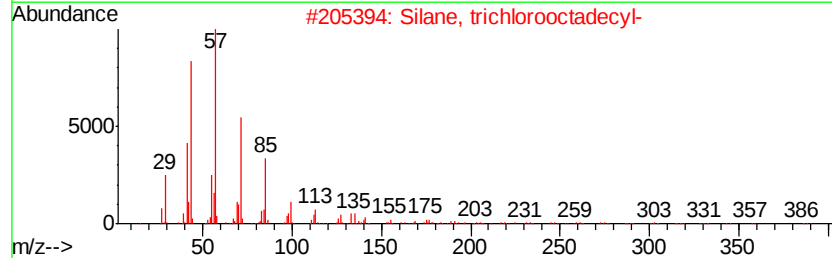
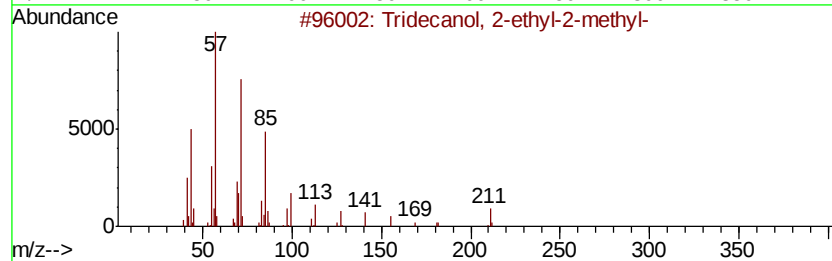
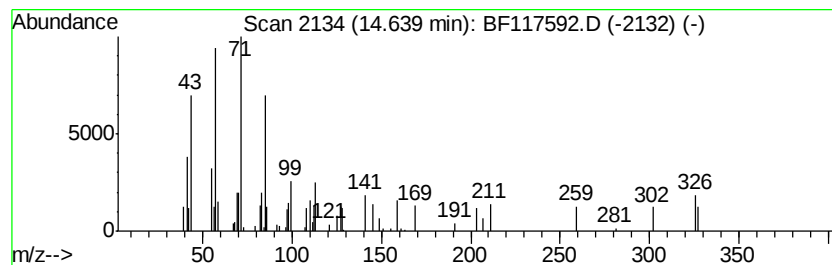
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Peak Number 5 Tridecanol, 2-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.64	2.48 ng	27466	Perylene-d12	15.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	53
2	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	50
3	Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	47
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	47
5	3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	47



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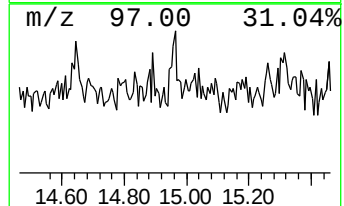
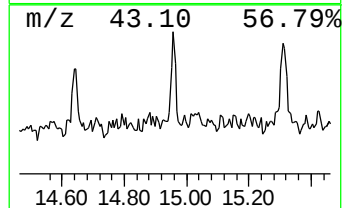
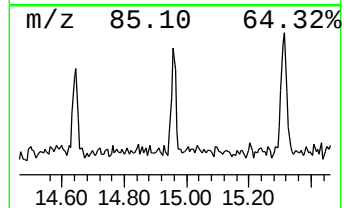
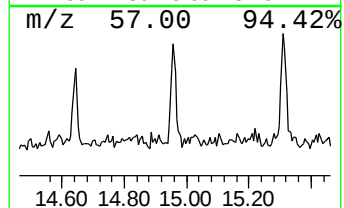
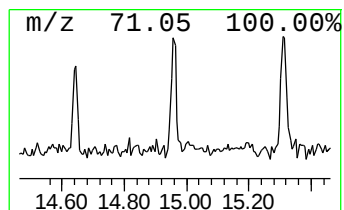
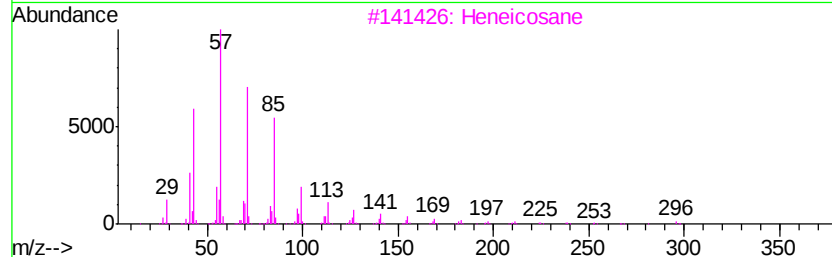
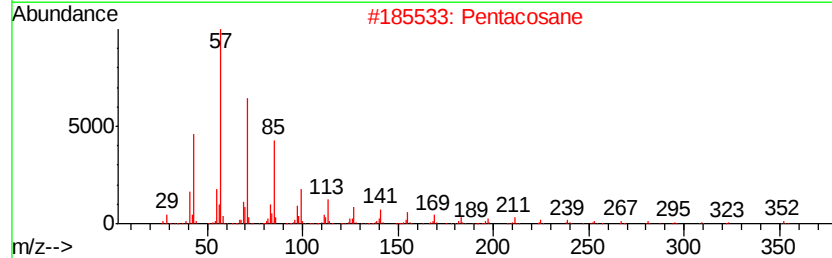
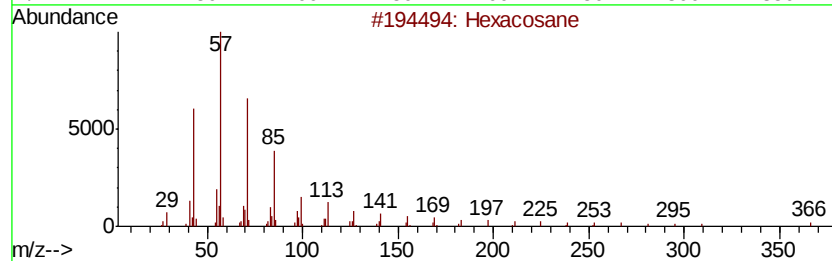
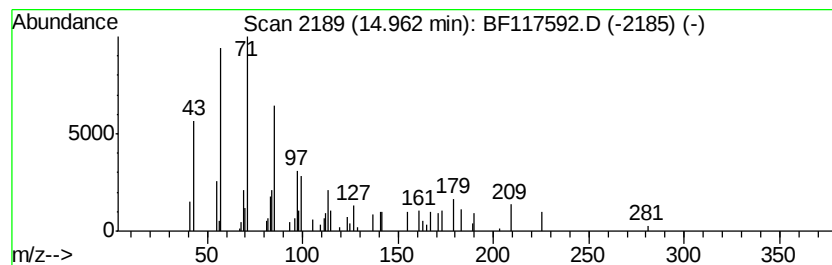
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.40 ng	26608	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	68
2	Pentacosane		352	C25H52	000629-99-2	64
3	Heneicosane		296	C21H44	000629-94-7	64
4	Hentriacontane		437	C31H64	000630-04-6	64
5	Hexatriacontane		507	C36H74	000630-06-8	64



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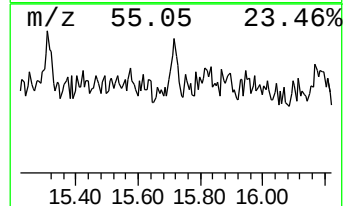
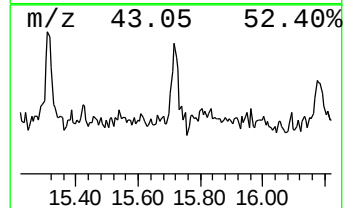
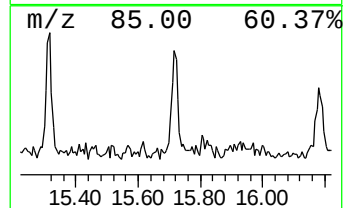
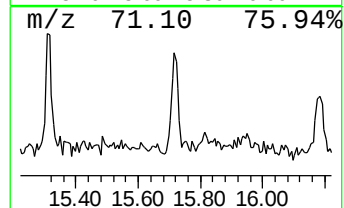
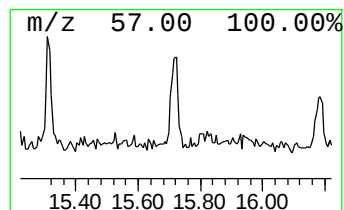
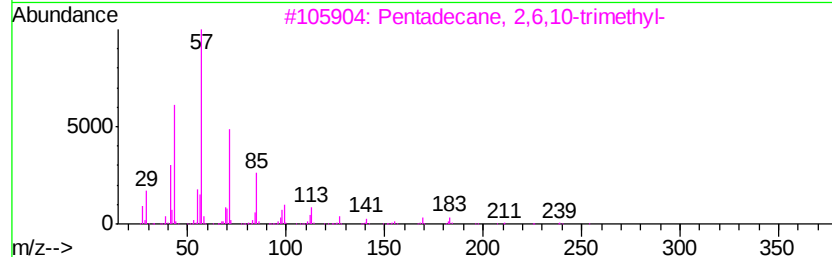
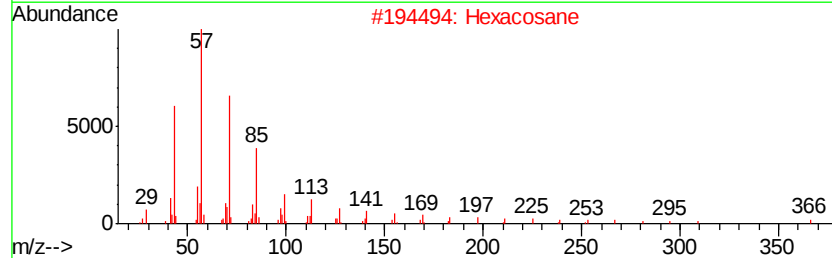
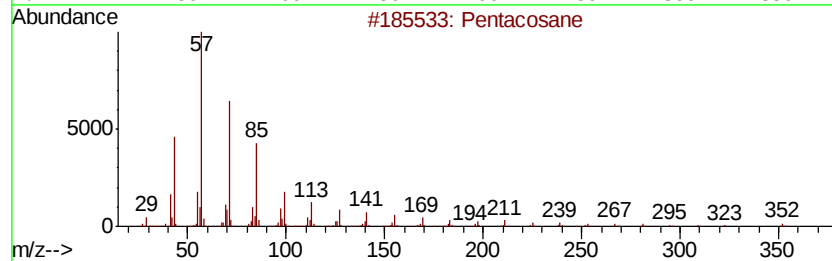
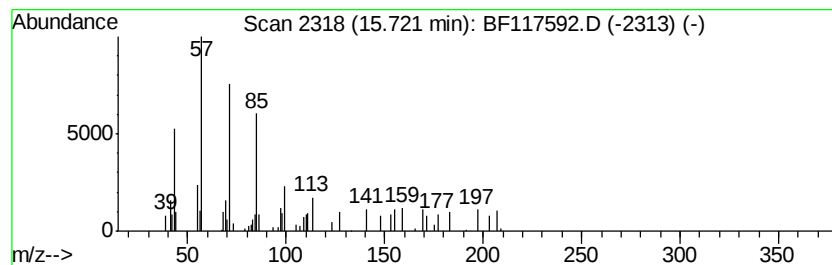
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.14 ng	34854	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	72
2	Hexacosane		366	C26H54	000630-01-3	72
3	Pentadecane, 2,6,10-trimethyl-		254	C18H38	003892-00-0	64
4	2-Bromo dodecane		248	C12H25Br	013187-99-0	59
5	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102919\
Data File : BF117592.D
Acq On : 29 Oct 2019 15:51
Operator : JU
Sample : K5540-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
156-56-(0-1.3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.50	6.50	75.0	ng	919382	1	6.73	245267	20.0
Undecanoic acid	11.77	2.5	ng	32573	4	11.25	265774	20.0
Trichloroacetic a...	13.74	7.3	ng	82656	5	13.89	226039	20.0
Tridecanol, 2-eth...	14.64	2.5	ng	27466	6	15.33	221813	20.0
Hexacosane	14.96	2.4	ng	26608	6	15.33	221813	20.0
Pentacosane	15.72	3.1	ng	34854	6	15.33	221813	20.0