

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100219\
 Data File : BF117300.D
 Acq On : 2 Oct 2019 15:32
 Operator : JU
 Sample : K5128-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-1A

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-BF091319.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	4.998	492	495	502	rBB	3027	3667	1.34%	0.117%
2	5.428	565	568	587	rBV	120964	165451	60.28%	5.301%
3	6.451	739	742	761	rBV	137156	196662	71.65%	6.301%
4	6.581	761	764	773	rVV	213475	202429	73.75%	6.485%
5	6.804	799	802	812	rBV	115968	117848	42.94%	3.776%
6	6.963	826	829	840	rBV	178361	160450	58.46%	5.140%
7	7.369	895	898	920	rBV	71247	111857	40.75%	3.584%
8	8.092	1017	1021	1030	rBV	131111	149156	54.34%	4.779%
9	9.163	1200	1203	1214	rBV	253344	238969	87.07%	7.656%
10	9.557	1268	1270	1277	rBB	21082	17738	6.46%	0.568%
11	9.845	1315	1319	1327	rBV	214189	196472	71.58%	6.295%
12	10.633	1450	1453	1465	rBB	118249	131164	47.79%	4.202%
13	11.333	1568	1572	1583	rBV	183961	196188	71.48%	6.285%
14	11.851	1656	1660	1664	rBV	28546	30522	11.12%	0.978%
15	12.063	1692	1696	1699	rBV3	5817	4234	1.54%	0.136%
16	12.122	1703	1706	1713	rVB3	1627	3282	1.20%	0.105%
17	12.545	1776	1778	1784	rBV2	13361	18523	6.75%	0.593%
18	12.633	1790	1793	1801	rBV4	15807	19028	6.93%	0.610%
19	12.733	1807	1810	1812	rBV2	12932	9535	3.47%	0.305%
20	12.780	1815	1818	1824	rVB	12652	14255	5.19%	0.457%
21	12.910	1836	1840	1847	rBV	332026	274468	100.00%	8.793%
22	13.139	1876	1879	1884	rBV5	6703	7677	2.80%	0.246%
23	13.386	1917	1921	1923	rBV4	3389	3788	1.38%	0.121%
24	13.445	1928	1931	1933	rBV3	5947	4507	1.64%	0.144%
25	13.480	1934	1937	1939	rBV4	8870	7052	2.57%	0.226%
26	13.598	1954	1957	1959	rBV2	9957	9821	3.58%	0.315%
27	13.669	1967	1969	1971	rBV3	4561	3714	1.35%	0.119%
28	13.816	1991	1994	2001	rBV7	22583	40842	14.88%	1.308%
29	13.939	2012	2015	2018	rBV	24241	22194	8.09%	0.711%
30	13.974	2018	2021	2029	rVB	194738	195597	71.26%	6.266%
31	14.127	2044	2047	2048	rBV2	10927	9551	3.48%	0.306%
32	14.245	2065	2067	2070	rBV3	7942	7523	2.74%	0.241%
33	14.427	2095	2098	2100	rBV3	26797	29462	10.73%	0.944%
34	14.451	2100	2102	2113	rVB9	35709	62583	22.80%	2.005%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.727	2147	2149	2152	rVB2	15003	13965	5.09%	0.447%
36	14.868	2170	2173	2177	rVB3	33805	35116	12.79%	1.125%
37	15.057	2202	2205	2209	rVB	49405	52144	19.00%	1.671%
38	15.104	2209	2213	2223	rVB	29490	78578	28.63%	2.517%
39	15.368	2256	2258	2261	rBV4	12483	14934	5.44%	0.478%
40	15.433	2265	2269	2276	rVB	131571	175761	64.04%	5.631%
41	15.621	2299	2301	2304	rVB4	12938	14853	5.41%	0.476%
42	15.851	2336	2340	2344	rVB	46536	64014	23.32%	2.051%
43	18.874	2852	2854	2856	rBV3	5840	5748	2.09%	0.184%

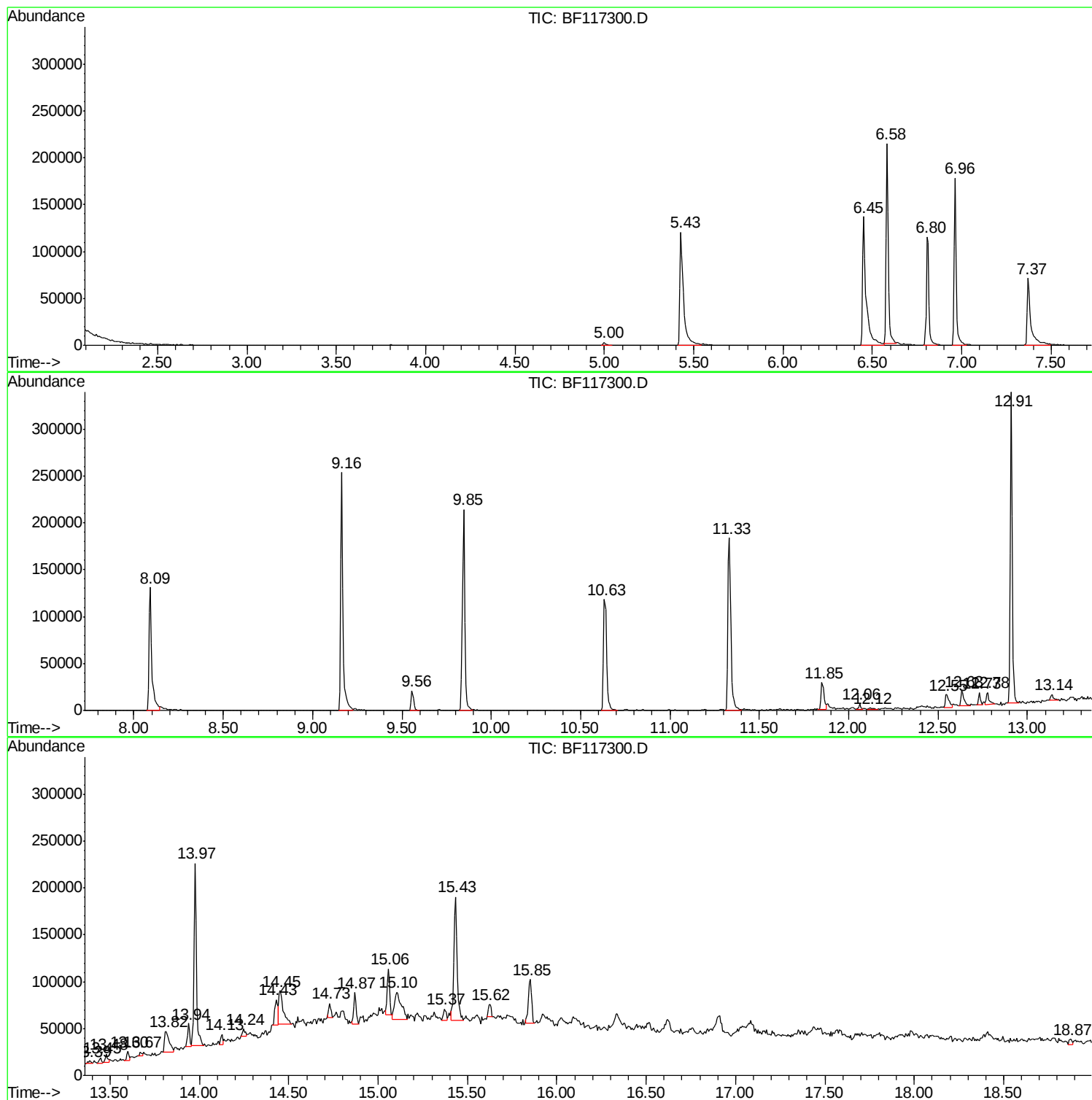
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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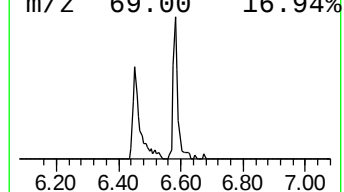
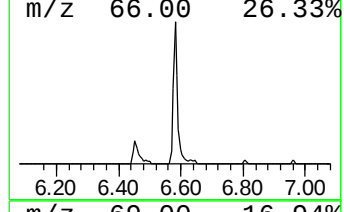
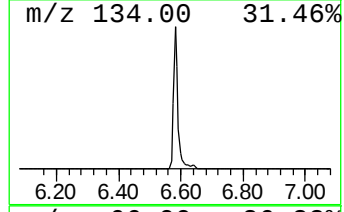
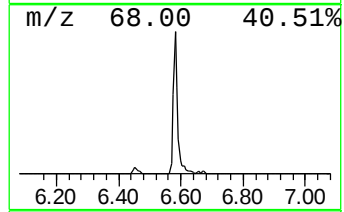
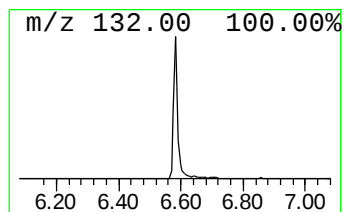
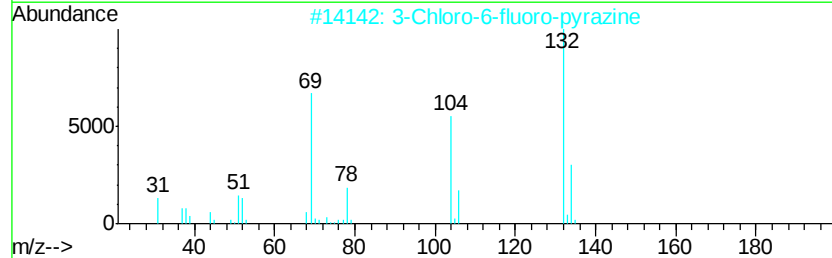
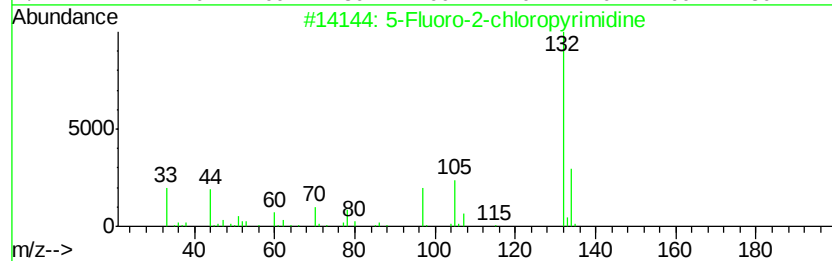
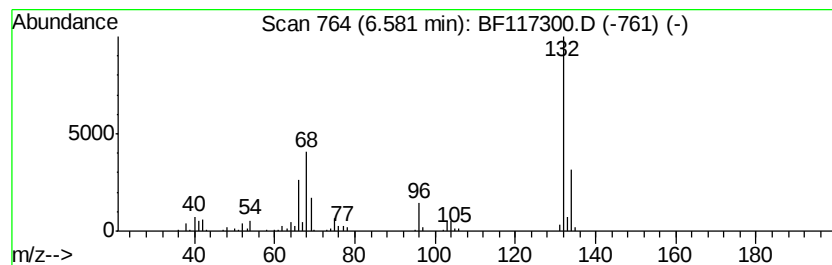
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	34.35 ng	202429	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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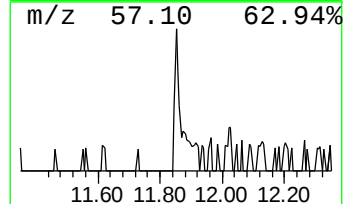
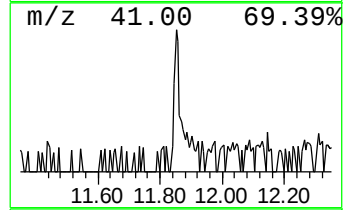
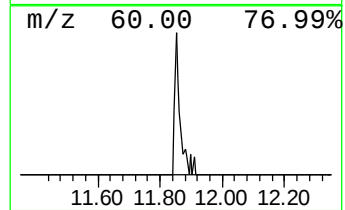
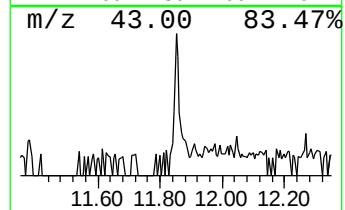
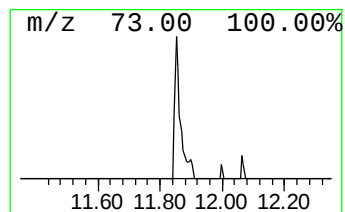
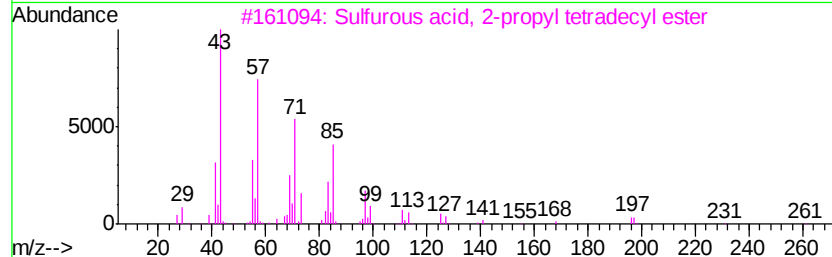
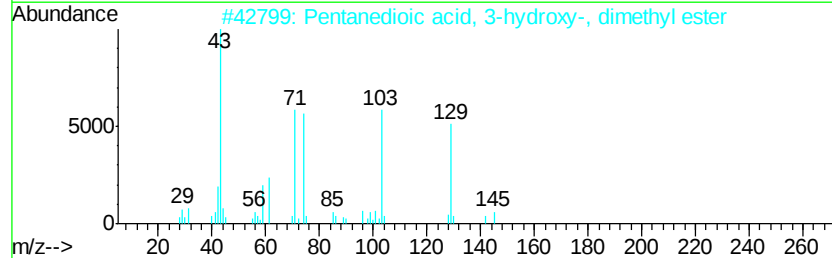
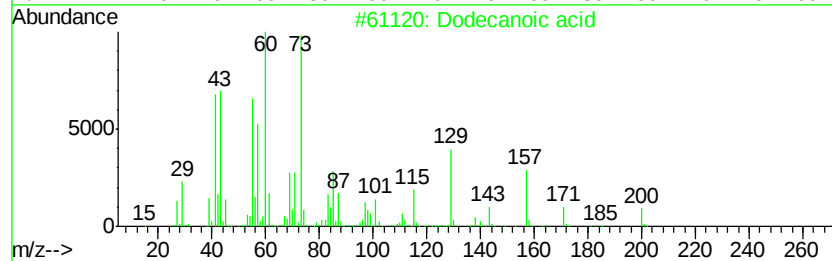
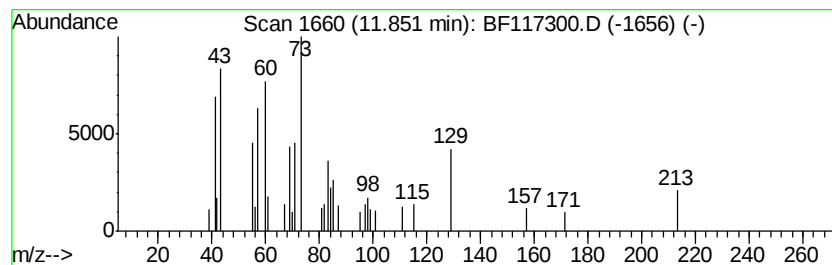
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	3.11 ng	30522	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	53	
2	Pentanedioic acid, 3-hydroxy-, d...	176	C7H12O5	007250-55-7	14	
3	Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	14	
4	Undecane, 5-methyl-	170	C12H26	001632-70-8	14	
5	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	14	



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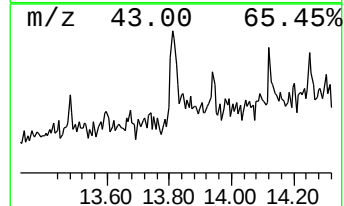
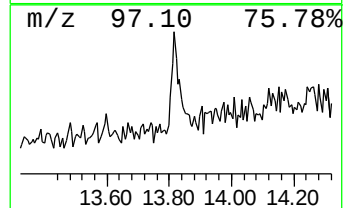
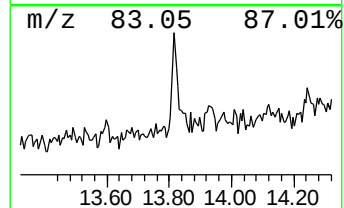
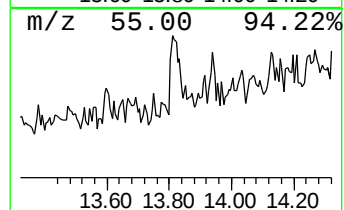
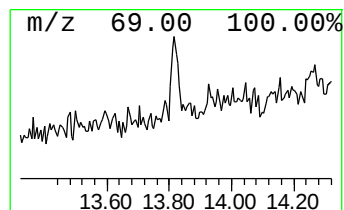
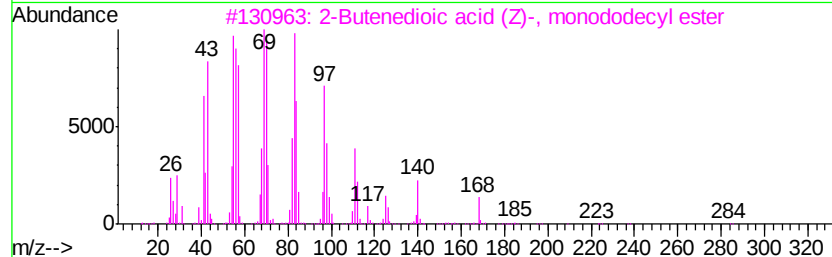
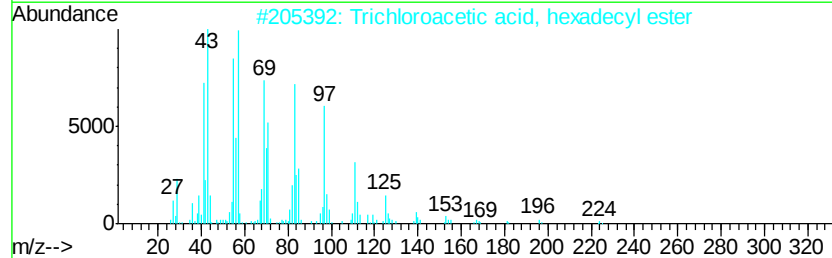
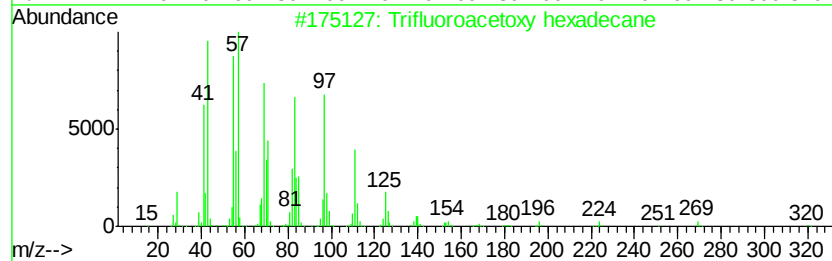
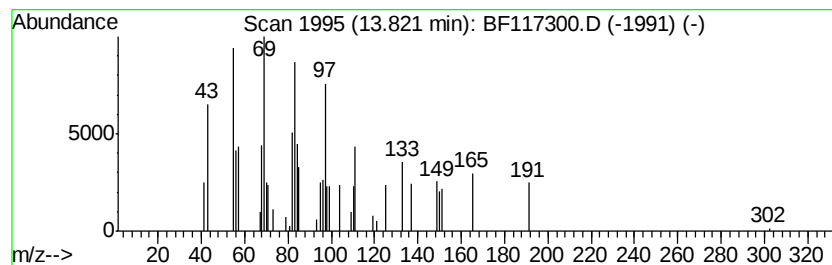
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	4.18 ng	40842	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	59
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	59
3		2-Butenedioic acid (Z)-, monodod...	284	C16H28O4	002424-61-5	58
4		Isobutyl tridecyl carbonate	300	C18H36O3	959275-44-6	38
5		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	38



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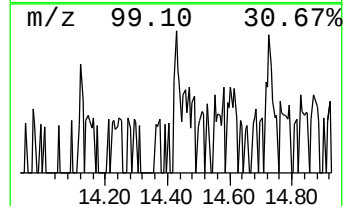
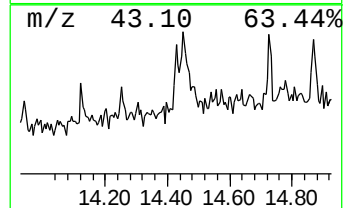
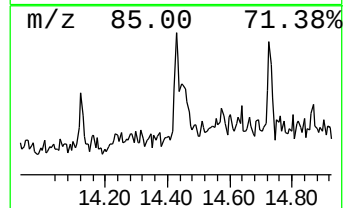
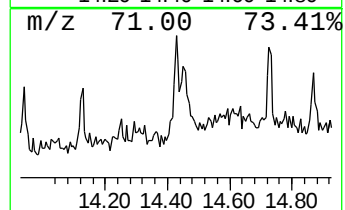
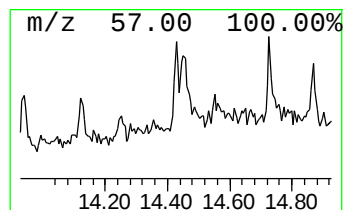
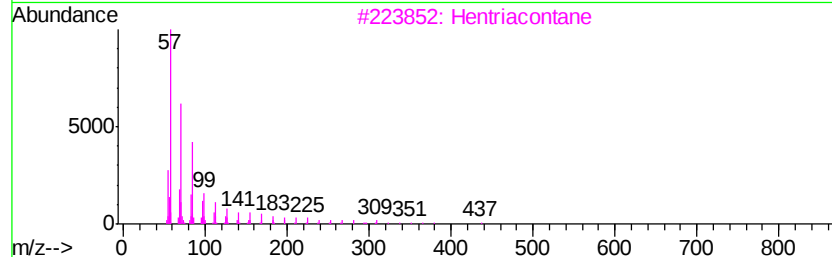
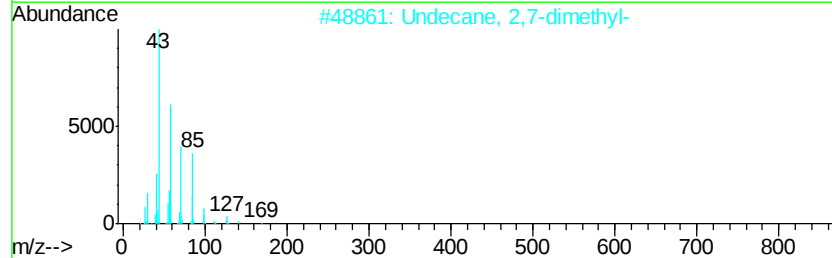
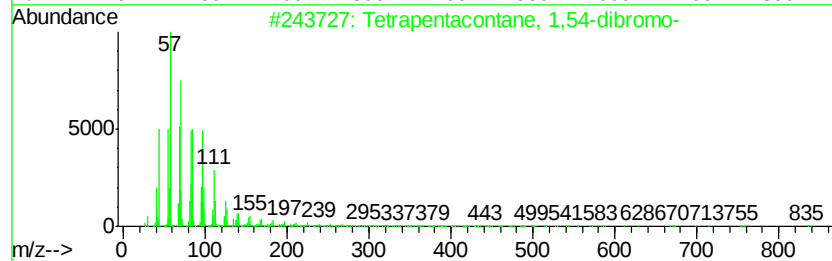
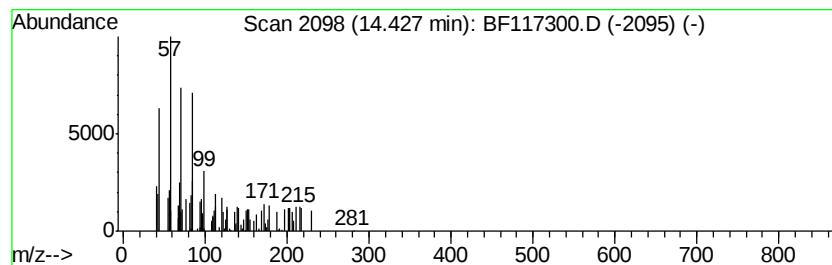
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetrapentacontane, 1,54-dib... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	3.01 ng	29462	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	52
2		Undecane, 2,7-dimethyl-	184	C13H28	017301-24-5	50
3		Hentriacontane	437	C31H64	000630-04-6	47
4		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	47
5		1-Decanol, 2,2-dimethyl-	186	C12H26O	002370-15-2	47



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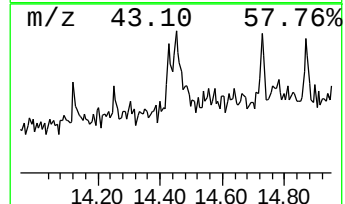
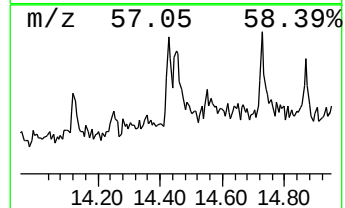
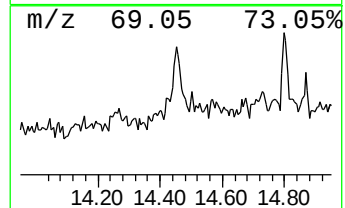
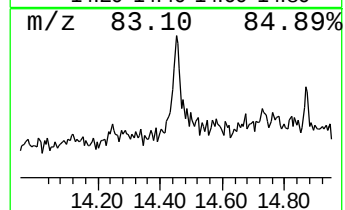
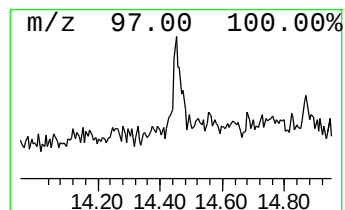
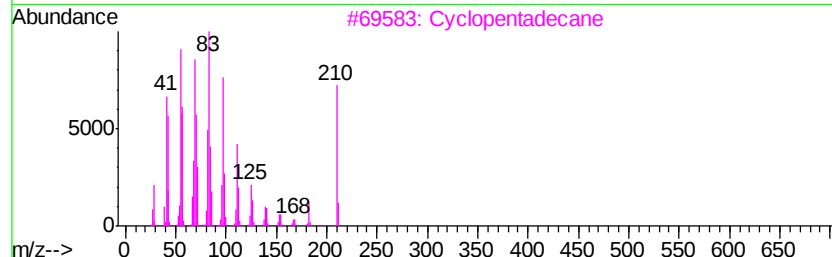
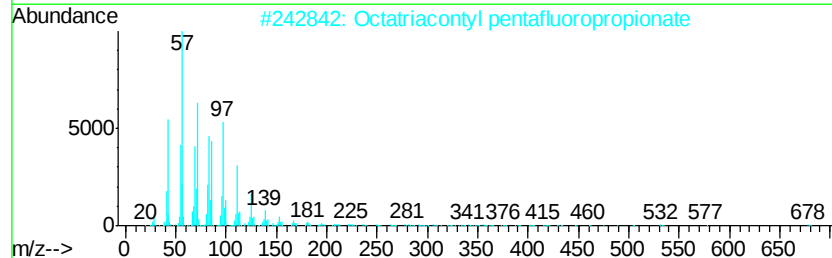
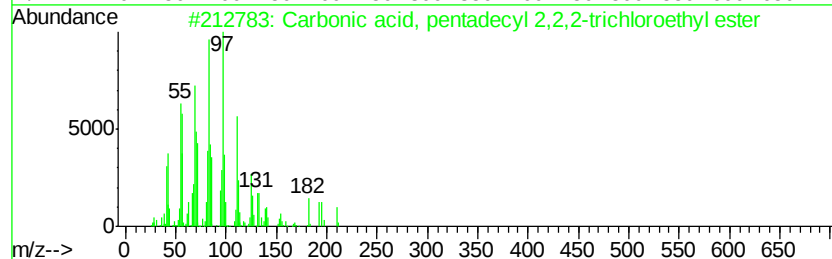
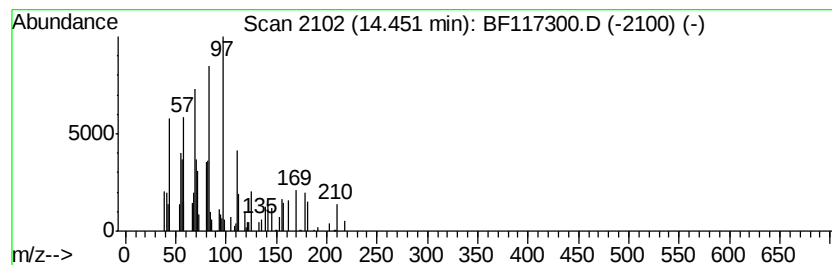
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Peak Number 6 Carbonic acid, pentadecyl 2... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	6.40 ng	62583	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, pentadecyl 2,2,2-...	402	C18H33Cl3O3	1000314-56-1	72
2		Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	53
3		Cyclopentadecane	210	C15H30	000295-48-7	52
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	47
5		Cyclopentane, decyl-	210	C15H30	001795-21-7	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100219\
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Sample : K5128-01
Misc :
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ClientSampleId :
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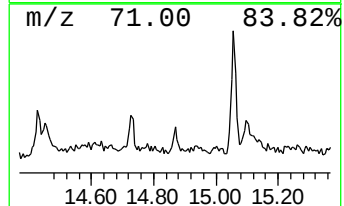
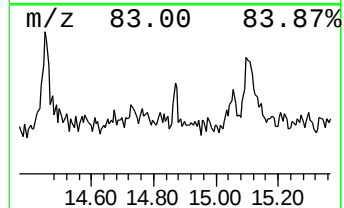
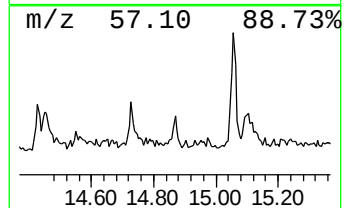
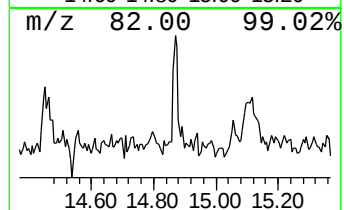
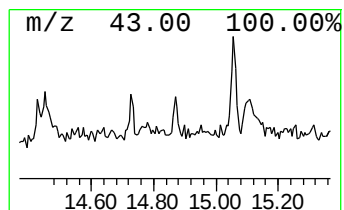
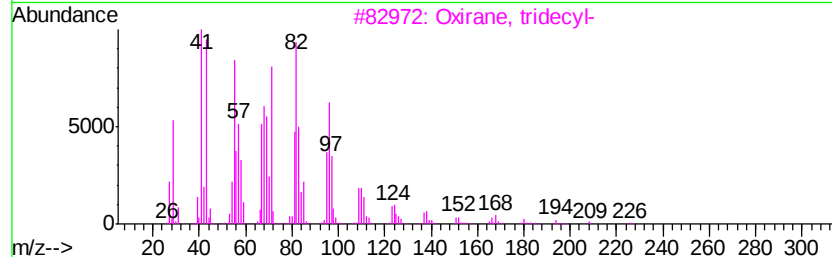
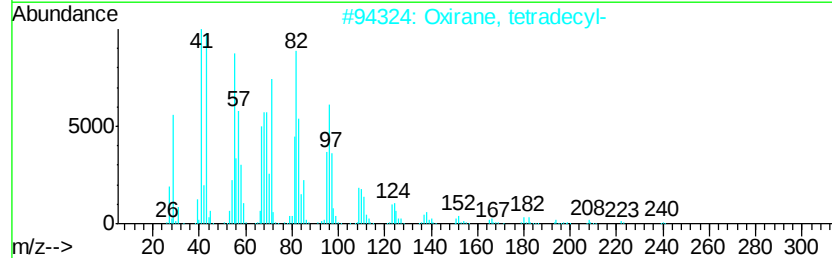
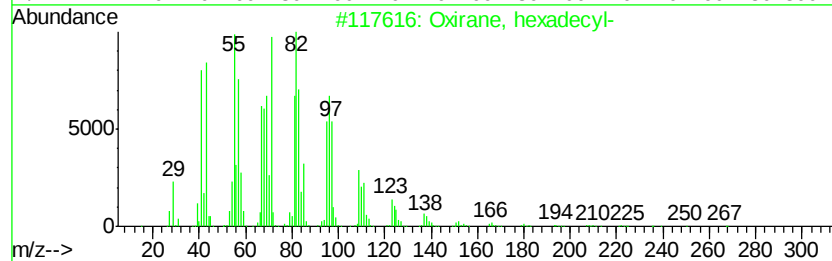
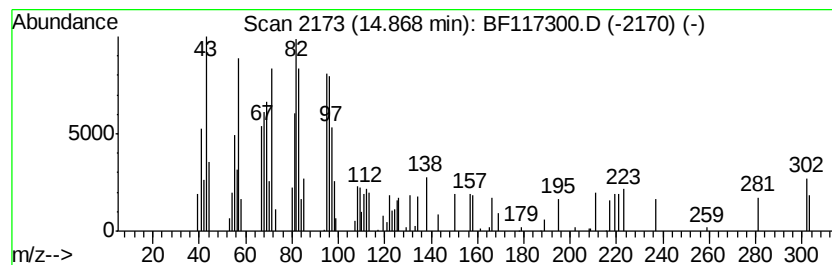
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	4.00 ng	35116	Perylene-d12	15.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74	
2	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	62	
3	Oxirane, tridecyl-	226	C15H30O	018633-25-5	58	
4	Pentadecanal-	226	C15H30O	002765-11-9	53	
5	Octadecanal	268	C18H36O	000638-66-4	52	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100219\
Data File : BF117300.D
Acq On : 2 Oct 2019 15:32
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ClientSampleId :
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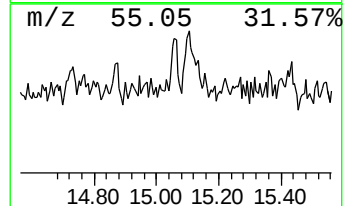
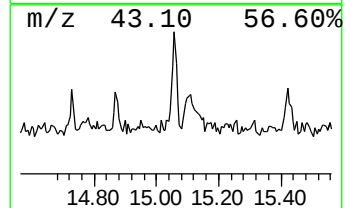
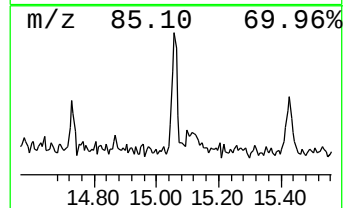
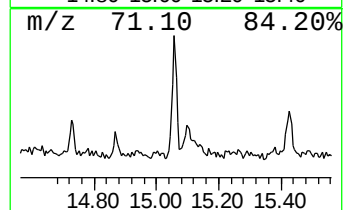
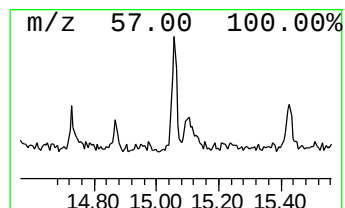
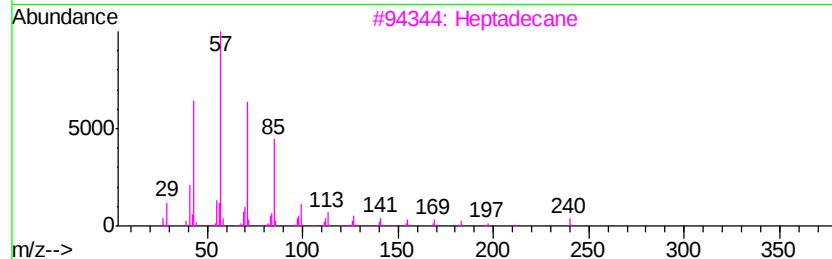
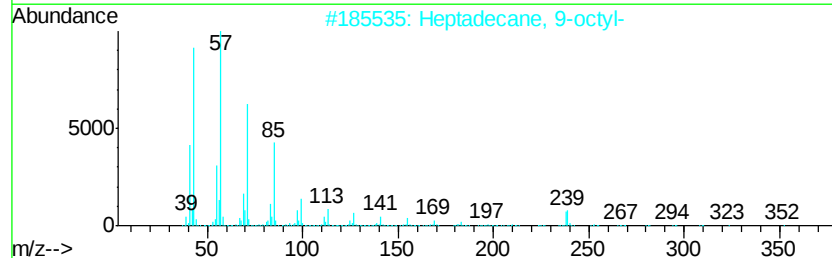
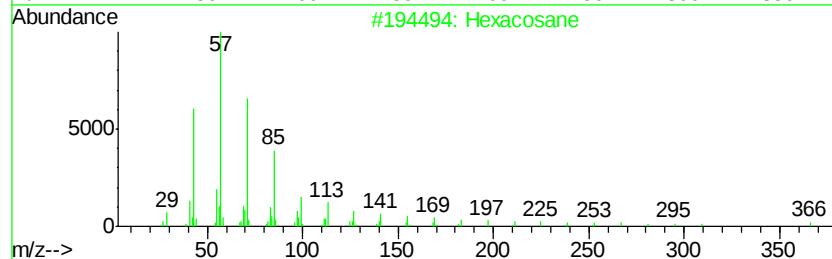
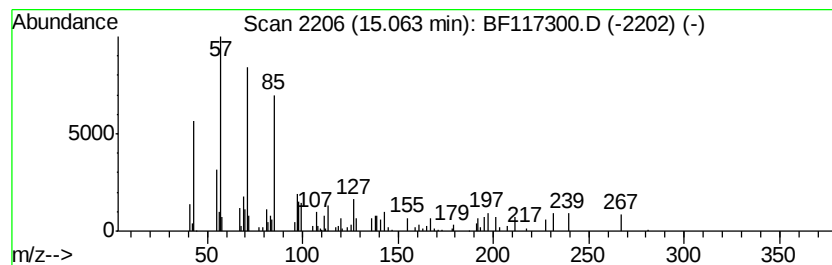
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	5.93 ng	52144	Perylene-d12	15.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	90
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	86
3	Heptadecane		240	C17H36	000629-78-7	80
4	2,6-Dimethyldecane		170	C12H26	013150-81-7	68
5	Heneicosane		296	C21H44	000629-94-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100219\
Data File : BF117300.D
Acq On : 2 Oct 2019 15:32
Operator : JU
Sample : K5128-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-1A

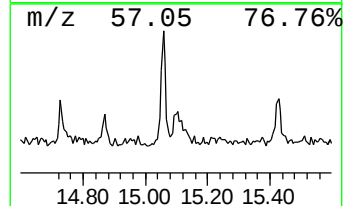
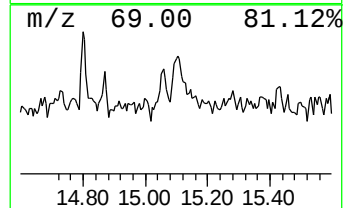
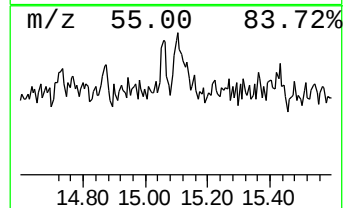
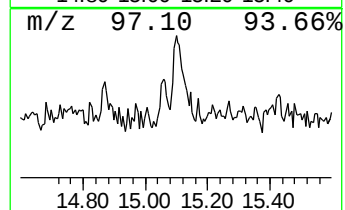
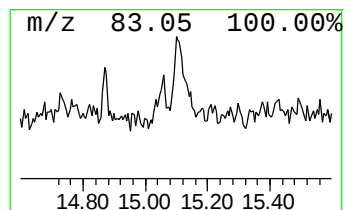
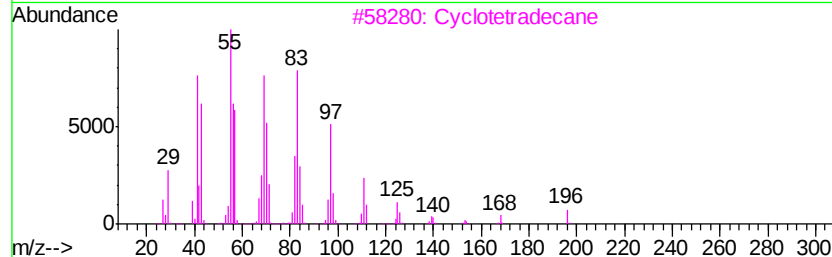
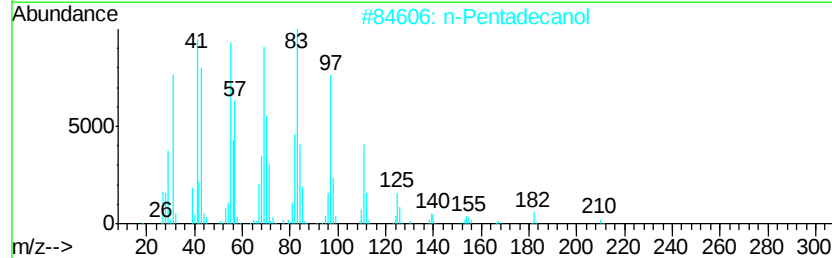
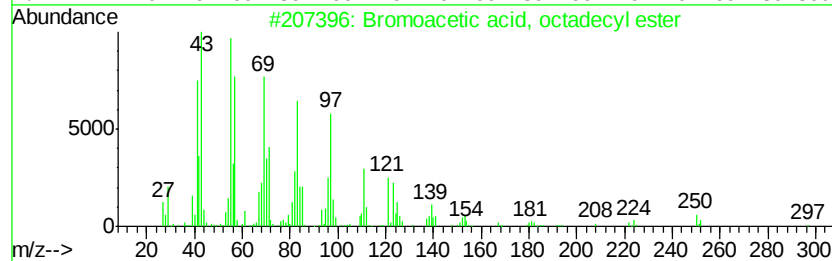
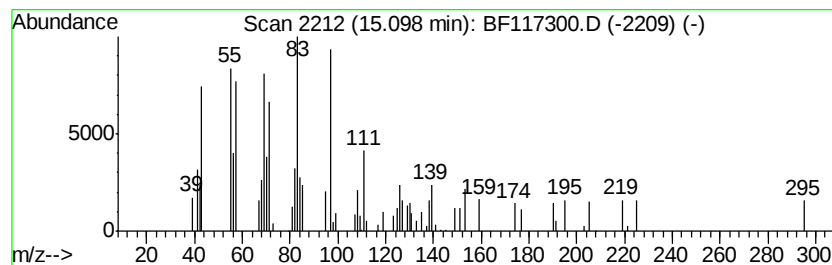
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bromoacetic acid, octadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	8.94 ng	78578	Perylene-d12	15.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	68
2		n-Pentadecanol	228	C15H32O	000629-76-5	53
3		Cyclotetradecane	196	C14H28	000295-17-0	49
4		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	46
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100219\
Data File : BF117300.D
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Operator : JU
Sample : K5128-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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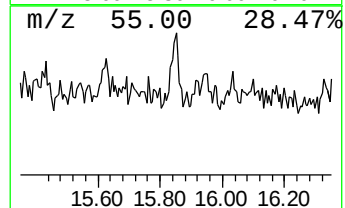
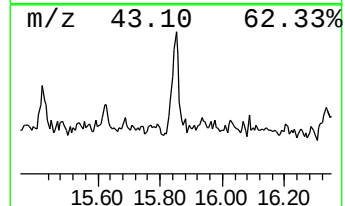
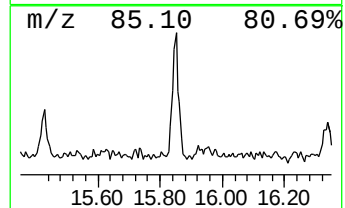
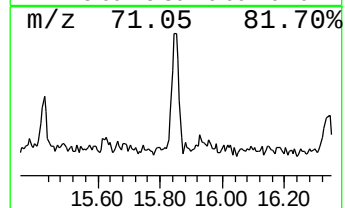
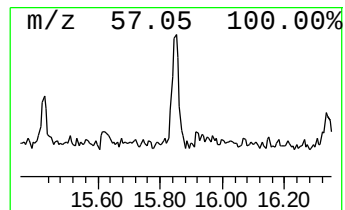
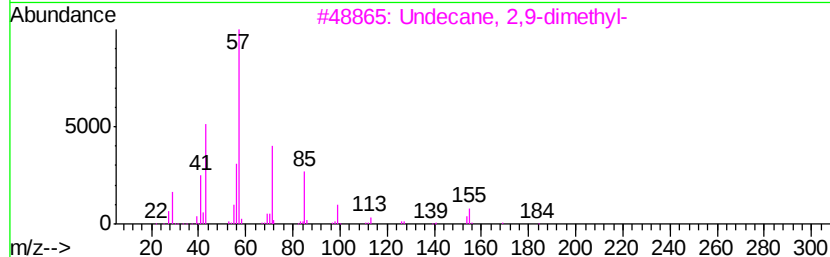
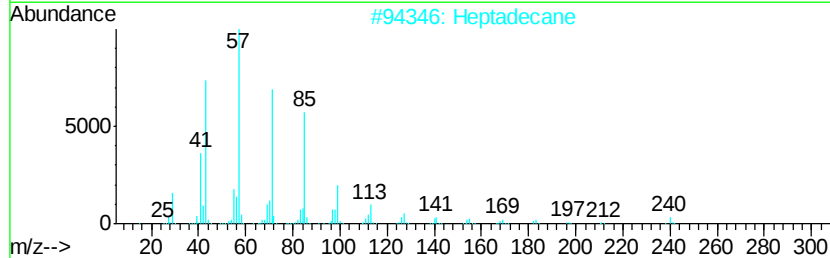
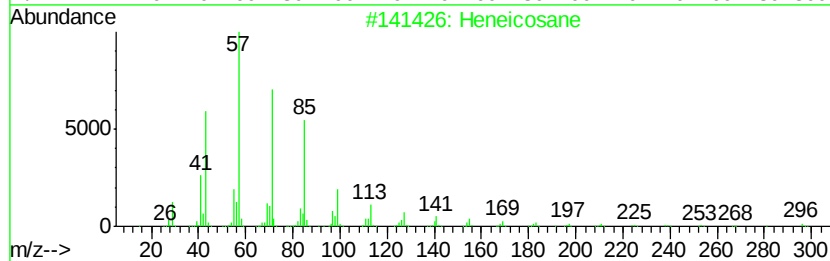
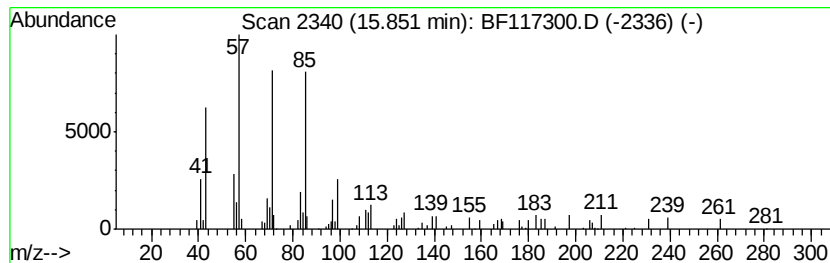
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	7.28 ng	64014	Perylene-d12	15.43

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Heptadecane	240	C17H36	000629-78-7	83
3			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	80
4			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	64
5			Hexacosane	366	C26H54	000630-01-3	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100219\
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Acq On : 2 Oct 2019 15:32
Operator : JU
Sample : K5128-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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
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Dodecanoic acid	11.85	3.1	ng	30522	4	11.33	196188	20.0
Trifluoroacetoxy ...	13.82	4.2	ng	40842	5	13.97	195597	20.0
Tetrapentacontane...	14.43	3.0	ng	29462	5	13.97	195597	20.0
Carbonic acid, pe...	14.45	6.4	ng	62583	5	13.97	195597	20.0
Oxirane, hexadecyl-	14.87	4.0	ng	35116	6	15.43	175761	20.0
Hexacosane	15.06	5.9	ng	52144	6	15.43	175761	20.0
Bromoacetic acid,...	15.10	8.9	ng	78578	6	15.43	175761	20.0
Heneicosane	15.85	7.3	ng	64014	6	15.43	175761	20.0