

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
 Data File : BF111306.D
 Acq On : 12 Dec 2018 5:10
 Operator : JU/SJ
 Sample : J6214-31
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2(15-17)

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-BF120818.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	4.992	483	494	502	rBV	237237	305823	6.16%	0.713%
2	5.410	561	565	582	rVB	4918609	4499589	90.57%	10.496%
3	6.428	733	738	746	rBV	4990649	4968036	100.00%	11.589%
4	6.569	757	762	765	rBV	4851932	4654054	93.68%	10.856%
5	6.628	769	772	777	rVB2	47261	51969	1.05%	0.121%
6	6.798	797	801	804	rBV	1560588	1316563	26.50%	3.071%
7	6.951	823	827	831	rBV	4012261	3471358	69.87%	8.098%
8	7.351	889	895	899	rBV	3111201	2982723	60.04%	6.958%
9	8.081	1015	1019	1022	rBV	1881277	1724671	34.72%	4.023%
10	9.157	1198	1202	1205	rBV	5410082	4430862	89.19%	10.336%
11	9.245	1214	1217	1222	rVB3	39054	53079	1.07%	0.124%
12	9.545	1265	1268	1276	rBV	479217	376779	7.58%	0.879%
13	9.751	1301	1303	1305	rVB2	75825	53730	1.08%	0.125%
14	9.833	1311	1317	1320	rBV	2003597	1690924	34.04%	3.944%
15	9.863	1320	1322	1325	rVB	83732	66843	1.35%	0.156%
16	10.116	1362	1365	1369	rBV	100462	90707	1.83%	0.212%
17	10.374	1407	1409	1412	rBV	75248	68397	1.38%	0.160%
18	10.616	1446	1450	1454	rBV	2586334	2201574	44.31%	5.136%
19	11.069	1524	1527	1529	rBV4	86560	83588	1.68%	0.195%
20	11.316	1565	1569	1571	rBV	1633310	1336927	26.91%	3.119%
21	11.339	1571	1573	1576	rVV	479225	379401	7.64%	0.885%
22	11.386	1579	1581	1584	rVB	123665	118736	2.39%	0.277%
23	11.851	1657	1660	1665	rBV2	918292	859051	17.29%	2.004%
24	12.527	1772	1775	1778	rBV	680701	608331	12.24%	1.419%
25	12.639	1791	1794	1799	rBV	505050	579137	11.66%	1.351%
26	12.757	1811	1814	1816	rVB	441307	373797	7.52%	0.872%
27	12.904	1835	1839	1843	rBV	3392334	2877310	57.92%	6.712%
28	13.821	1992	1995	2001	rVB	467830	501496	10.09%	1.170%
29	13.957	2014	2018	2020	rBV2	1429712	1430074	28.79%	3.336%
30	15.398	2260	2263	2266	rVB	654509	713301	14.36%	1.664%

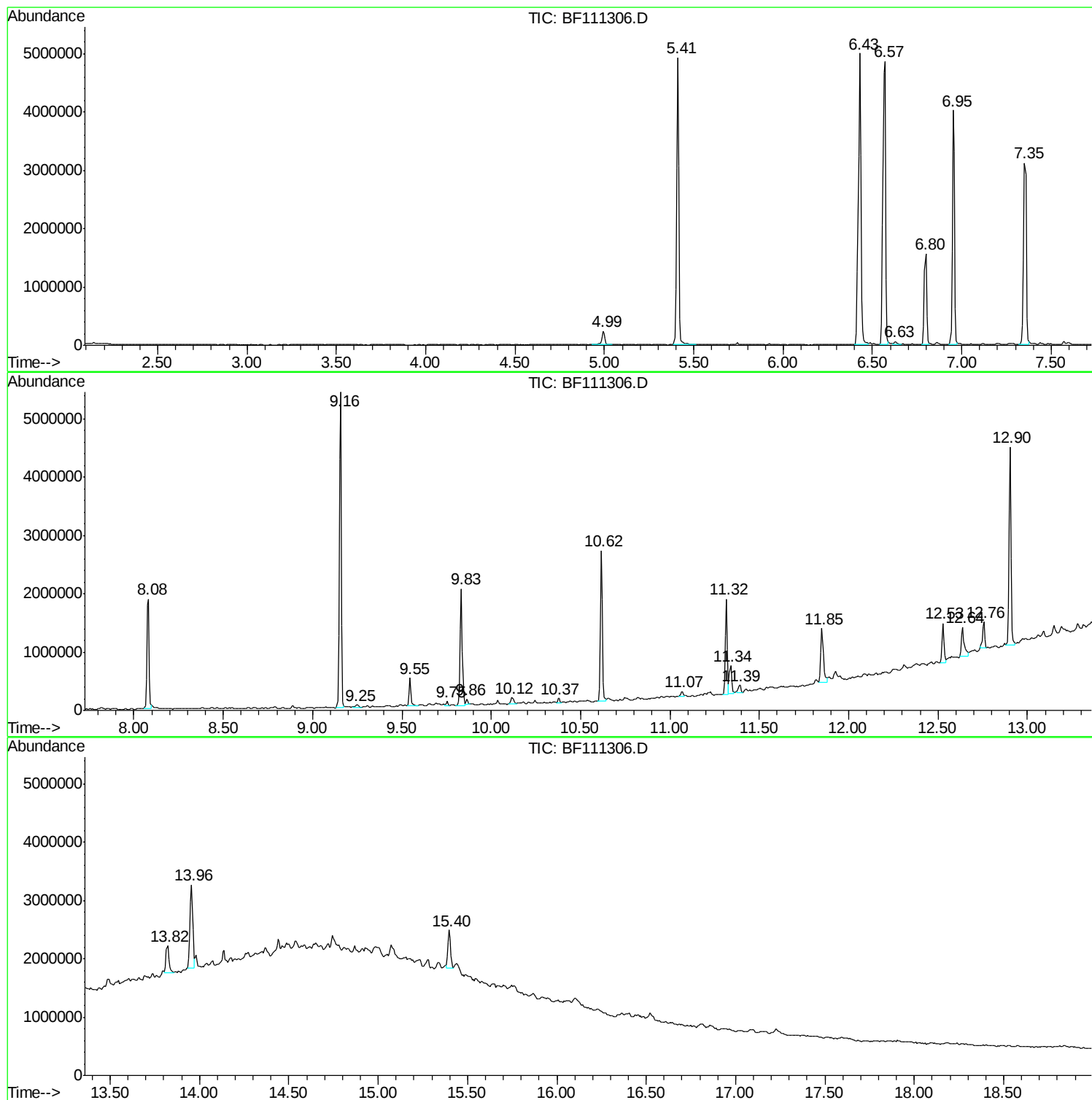
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(15-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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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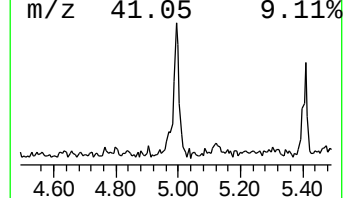
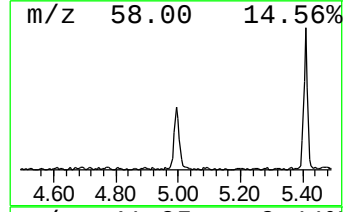
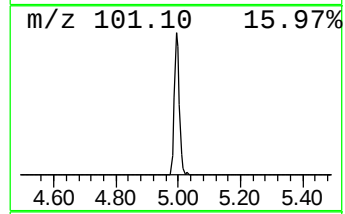
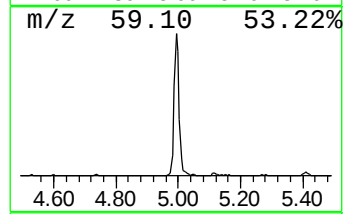
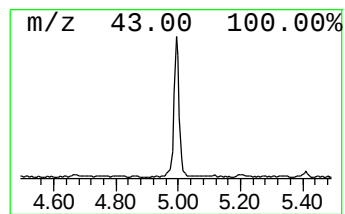
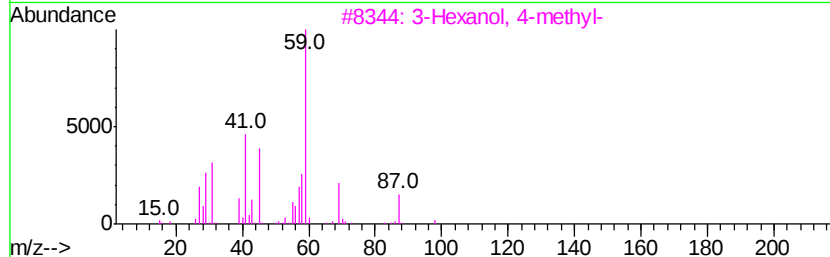
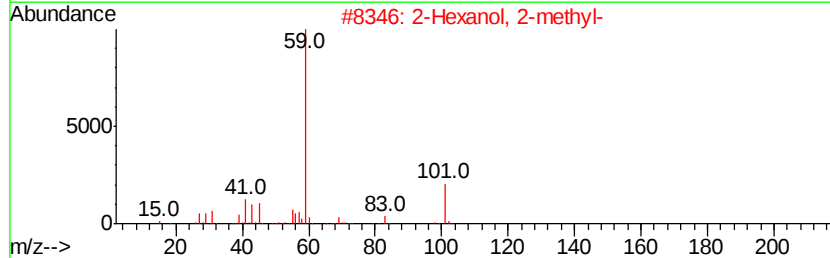
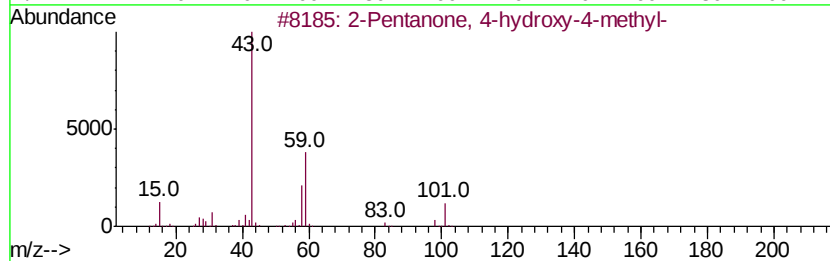
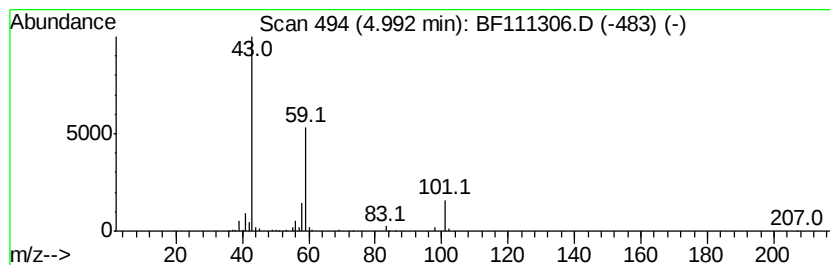
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	4.65 ng	305823	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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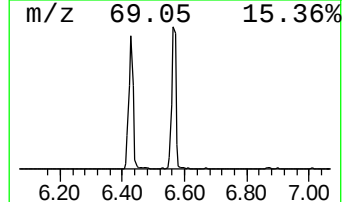
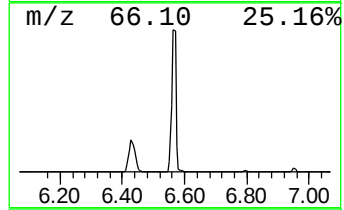
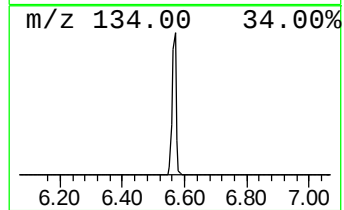
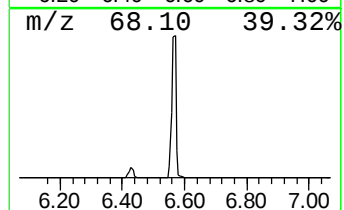
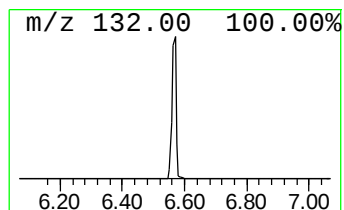
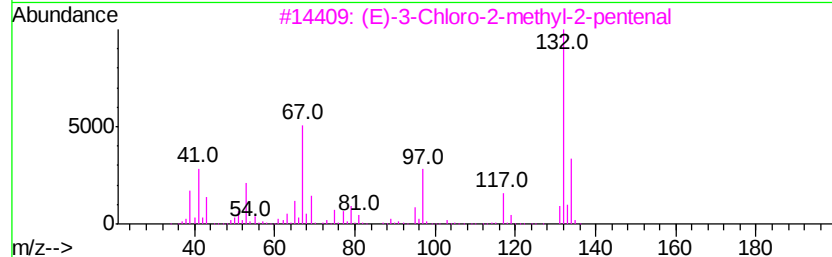
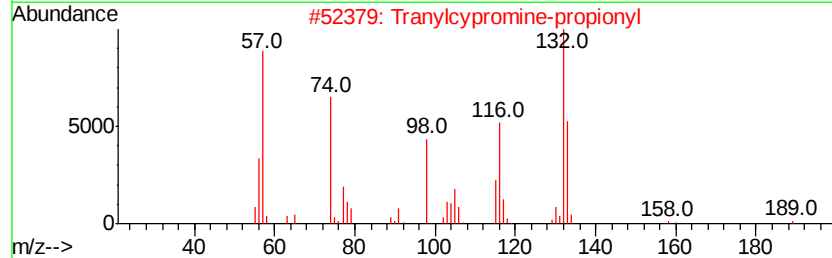
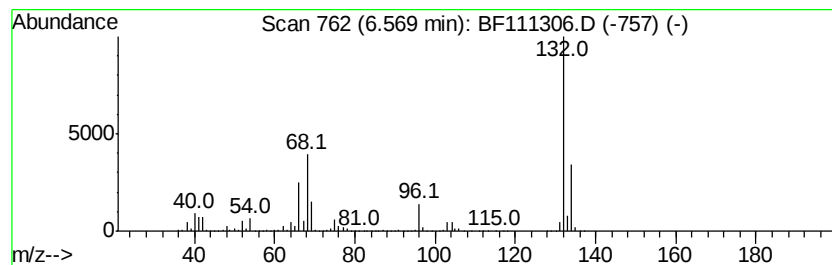
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	70.70 ng	4654050	1,4-Dichlorobenzene-d4	6.80

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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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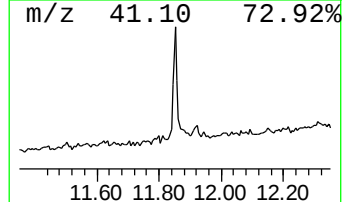
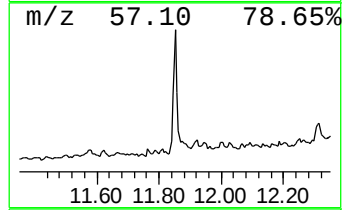
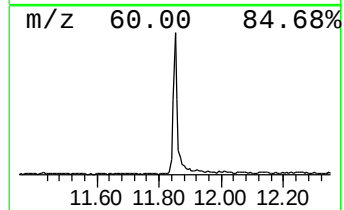
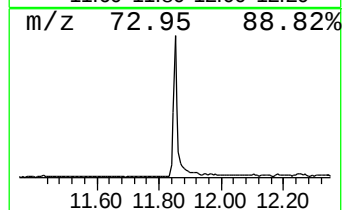
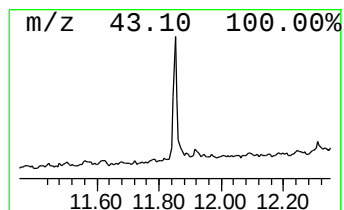
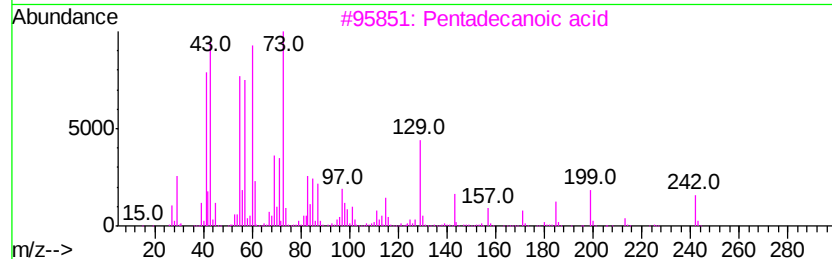
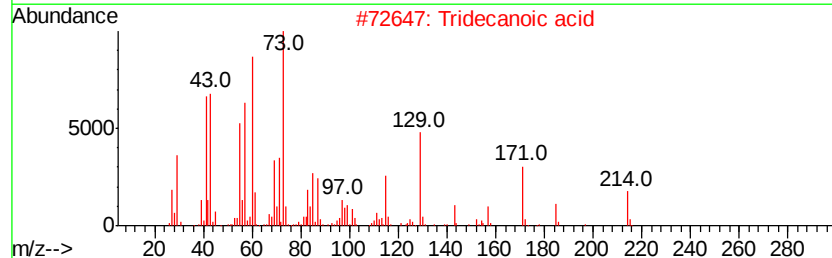
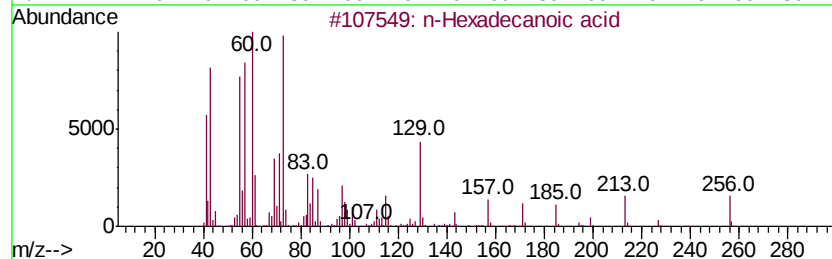
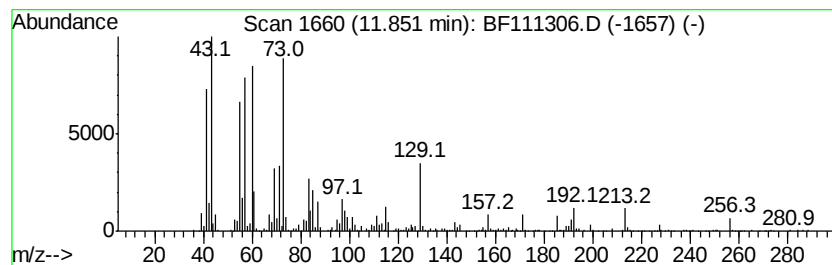
Instrument :
 BNA_F
 ClientSampleId :
 SB-2(15-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.85	12.85 ng	859051	Phenanthrene-d10		11.32	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Octadecanoic acid	284	C18H36O2	000057-11-4	90
5		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86



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Misc :
ALS Vial : 25 Sample Multiplier: 1

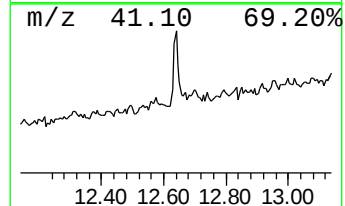
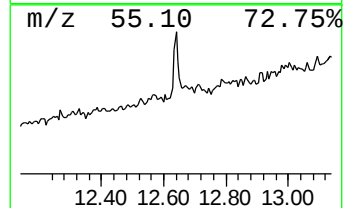
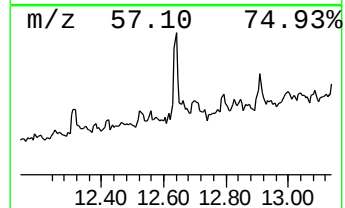
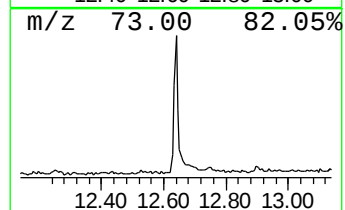
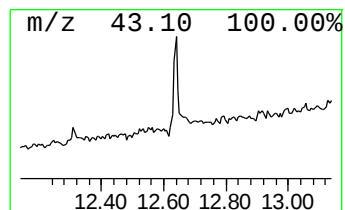
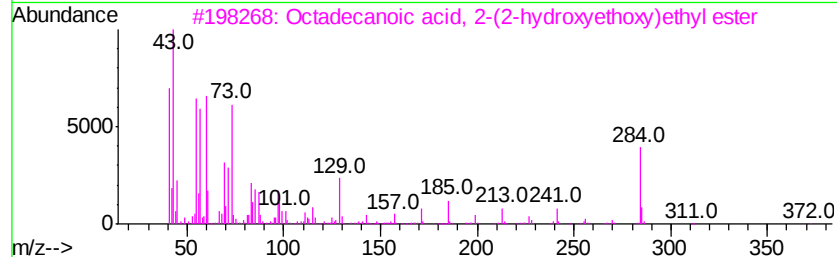
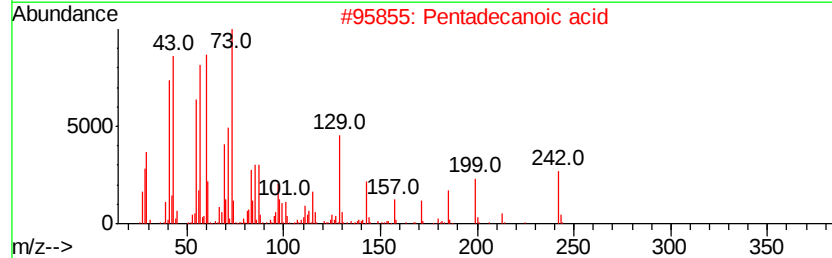
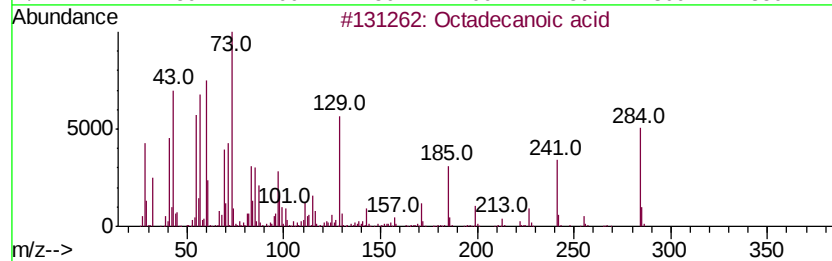
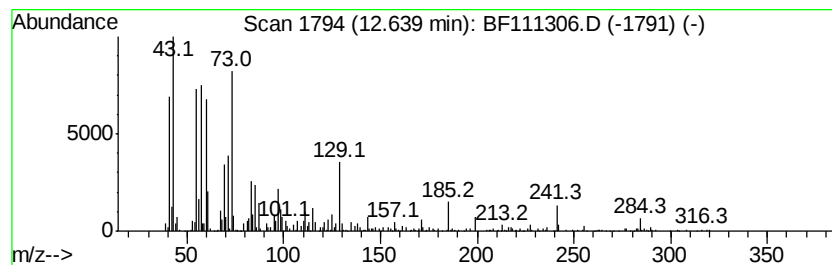
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	8.10 ng	579137	Chrysene-d12	13.96
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecanoic acid	284 C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242 C15H30O2	001002-84-2	74
3	Octadecanoic acid, 2-(2-hydroxyve...	372 C22H44O4	000106-11-6	72
4	Tridecanoic acid	214 C13H26O2	000638-53-9	70
5	n-Decanoic acid	172 C10H20O2	000334-48-5	64



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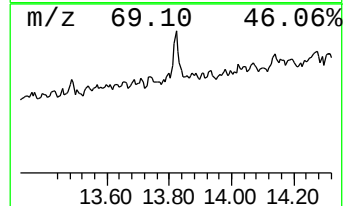
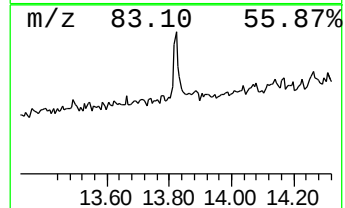
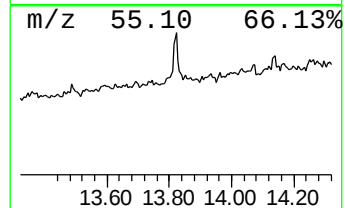
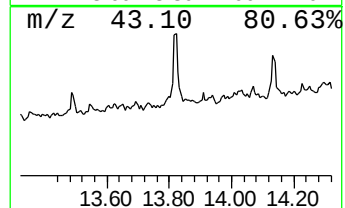
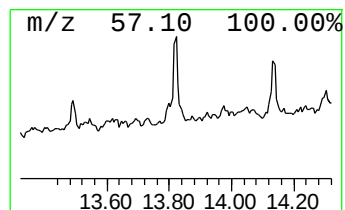
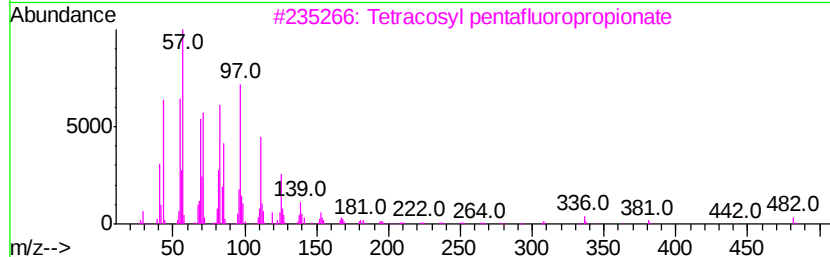
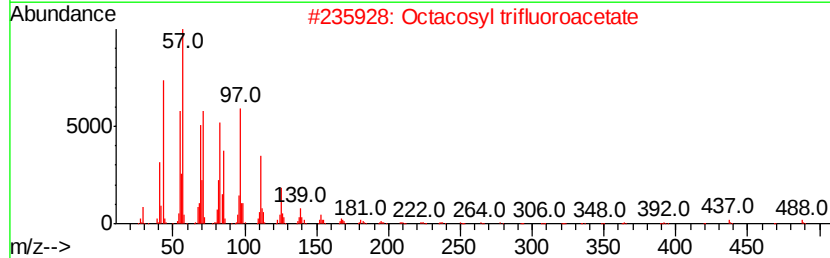
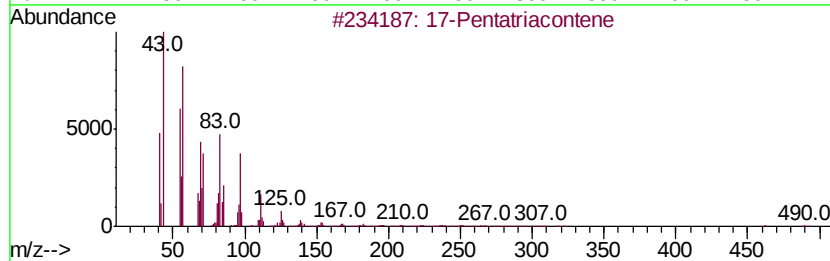
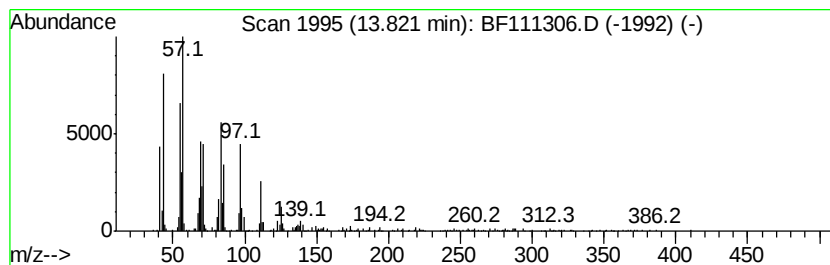
Instrument :
BNA_F
ClientSampleId :
SB-2(15-17)

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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 6 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.82	7.01 ng	501496	Chrysene-d12		13.96		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
3			Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	87
4			Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	87
5			Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	87



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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
2-Pentanone, 4-hy...	4.99	4.7	ng	305823	1	6.80	1316560	20.0
unknown6.57	6.57	70.7	ng	4654050	1	6.80	1316560	20.0
n-Hexadecanoic acid	11.85	12.9	ng	859051	4	11.32	1336930	20.0
Octadecanoic acid	12.64	8.1	ng	579137	5	13.96	1430070	20.0
17-Pentatriacontene	13.82	7.0	ng	501496	5	13.96	1430070	20.0