

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101018\
 Data File : BF109741.D
 Acq On : 10 Oct 2018 14:41
 Operator : JU/SJ
 Sample : J5326-17
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FL-PIT-5

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-BF100818.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	4.904	475	479	489	rBV	47032	75706	2.58%	0.334%
2	5.316	545	549	578	rBV	1690814	2013065	68.73%	8.871%
3	6.345	720	724	741	rBV	1721642	2272410	77.58%	10.014%
4	6.469	741	745	770	rVB	2156429	2362328	80.65%	10.410%
5	6.698	780	784	794	rBV	268465	394498	13.47%	1.738%
6	6.851	806	810	837	rVB	1653784	1681872	57.42%	7.412%
7	7.257	875	879	914	rBV	1086066	1517219	51.80%	6.686%
8	7.975	997	1001	1027	rBV	430234	576164	19.67%	2.539%
9	9.051	1179	1184	1223	rBV	2381263	2676881	91.39%	11.796%
10	9.445	1247	1251	1262	rBV	169802	193720	6.61%	0.854%
11	9.722	1294	1298	1310	rBV	674034	677858	23.14%	2.987%
12	10.510	1428	1432	1451	rBV	1585089	1876119	64.05%	8.268%
13	11.198	1546	1549	1573	rBV	566663	799106	27.28%	3.522%
14	11.739	1638	1641	1651	rBV2	59549	87760	3.00%	0.387%
15	12.410	1751	1755	1769	rBV	65734	94965	3.24%	0.418%
16	12.633	1787	1793	1797	rBV	64114	83959	2.87%	0.370%
17	12.786	1814	1819	1835	rBV	2542301	2929047	100.00%	12.908%
18	13.686	1968	1972	1987	rBV	116488	203240	6.94%	0.896%
19	13.827	1990	1996	2009	rBV	701622	875705	29.90%	3.859%
20	13.998	2022	2025	2031	rBV	51407	50078	1.71%	0.221%
21	14.304	2074	2077	2080	rBV	63236	59829	2.04%	0.264%
22	14.598	2123	2127	2133	rVB	68990	67806	2.31%	0.299%
23	14.839	2163	2168	2170	rBV	30106	44835	1.53%	0.198%
24	14.904	2175	2179	2183	rVB	86168	88294	3.01%	0.389%
25	15.168	2220	2224	2229	rBV	20364	30713	1.05%	0.135%
26	15.227	2229	2234	2252	rVB	420891	721625	24.64%	3.180%
27	15.645	2300	2305	2311	rBV	76612	108303	3.70%	0.477%
28	16.104	2377	2383	2391	rBV	47790	82633	2.82%	0.364%
29	16.639	2469	2474	2480	rVB2	24275	46445	1.59%	0.205%

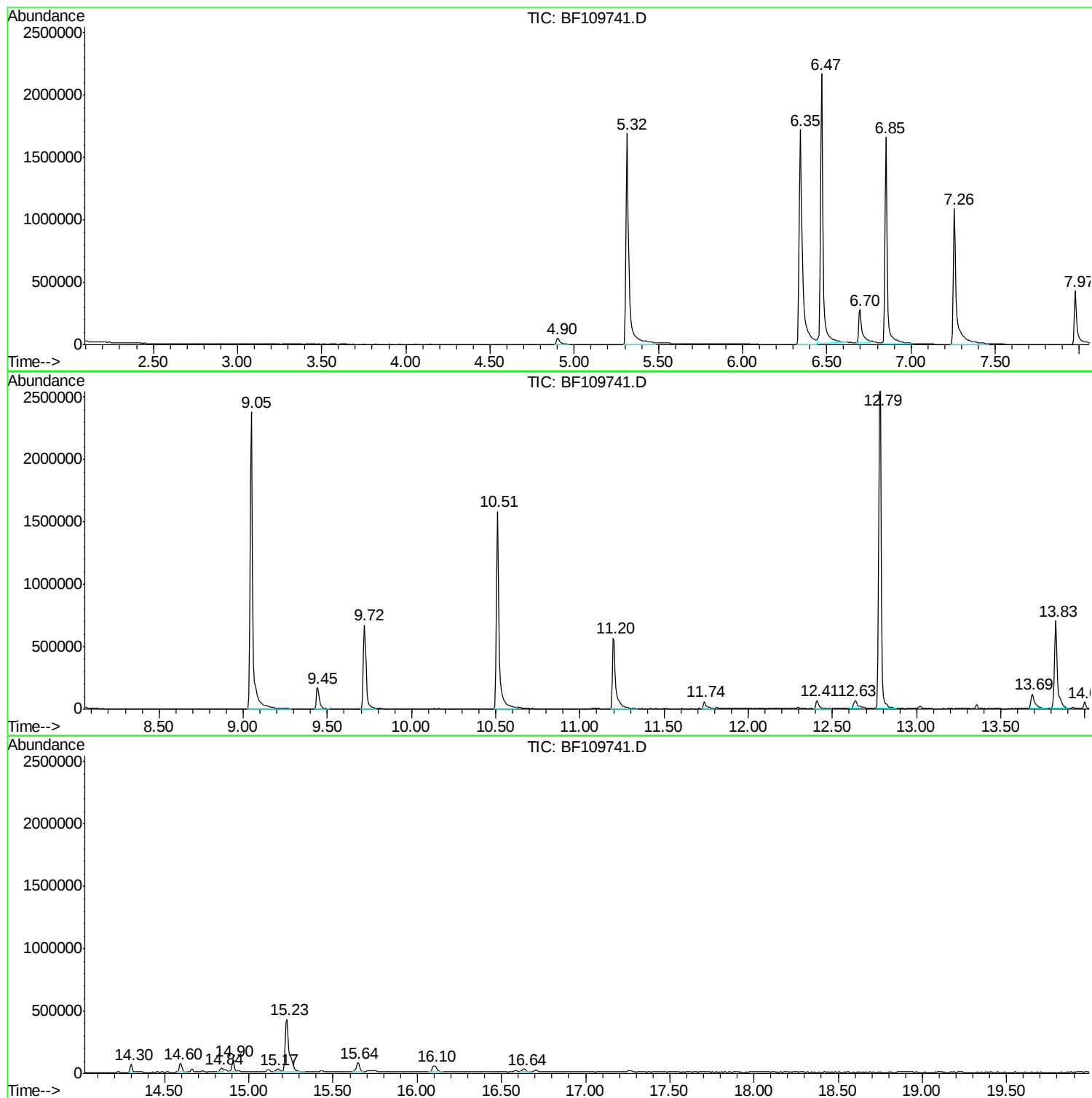
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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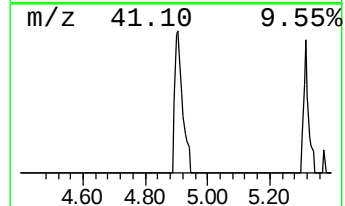
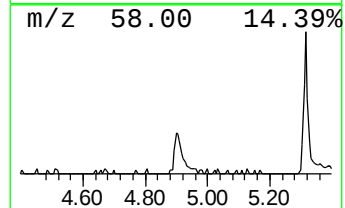
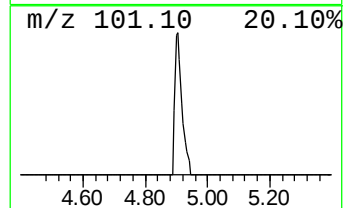
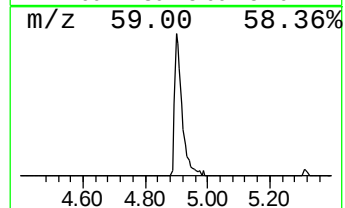
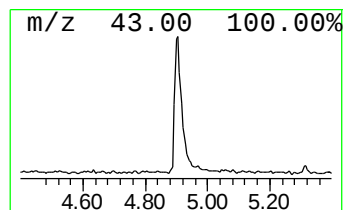
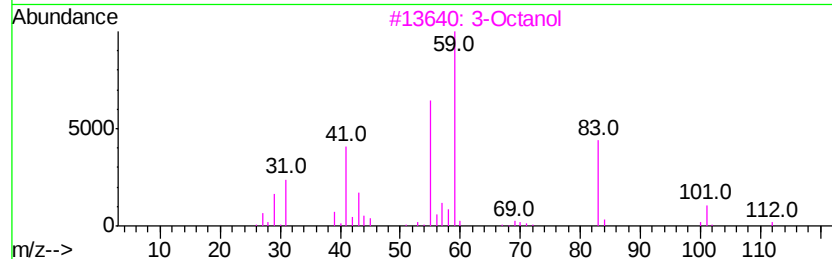
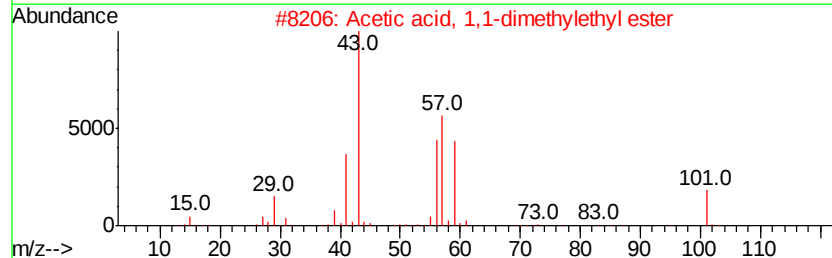
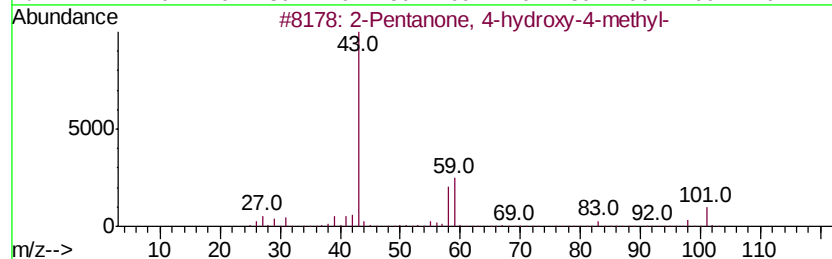
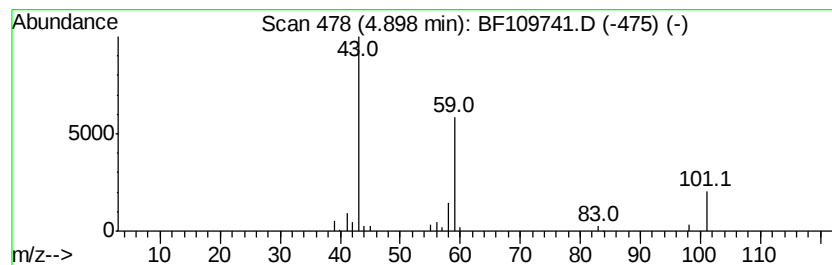
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.84 ng	75706	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl ester	116	C6H12O2	000540-88-5	39
3			3-Octanol	130	C8H18O	000589-98-0	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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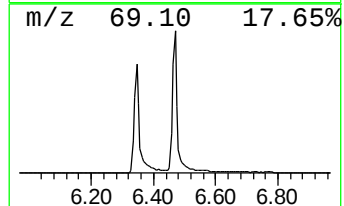
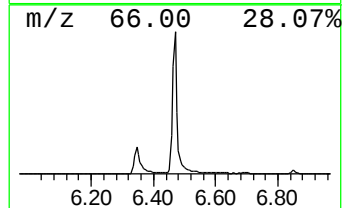
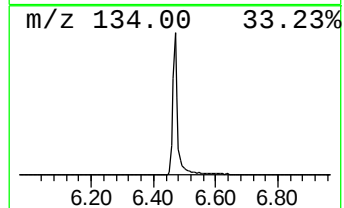
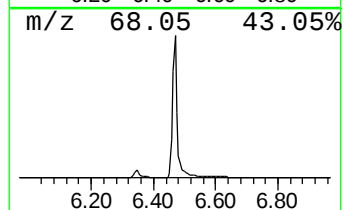
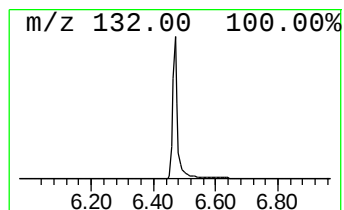
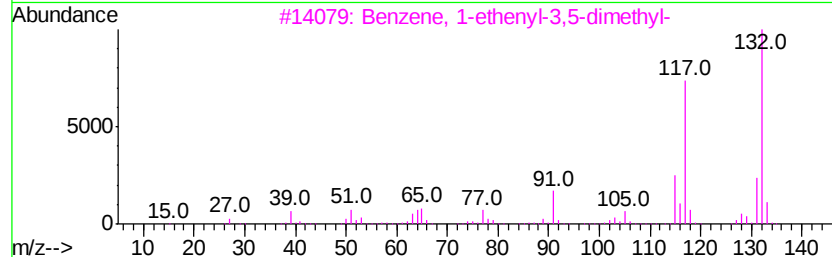
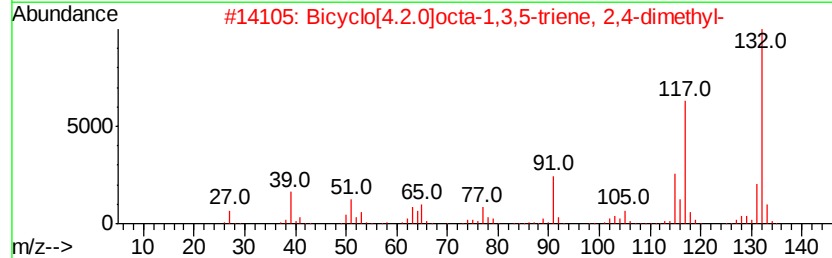
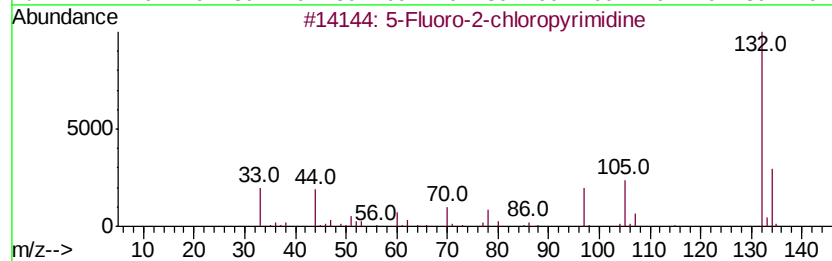
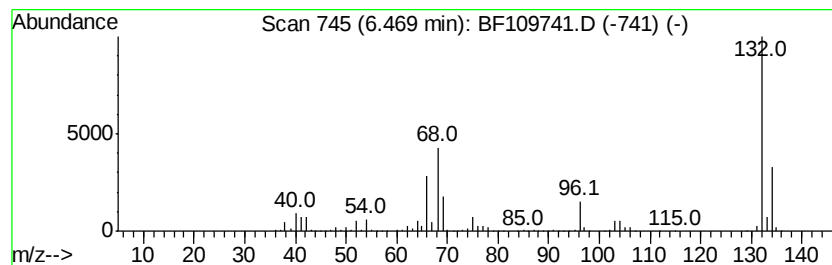
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	119.76 ng	2362330	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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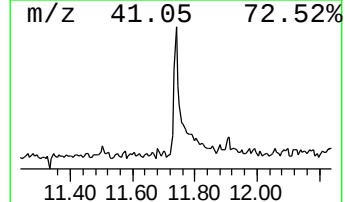
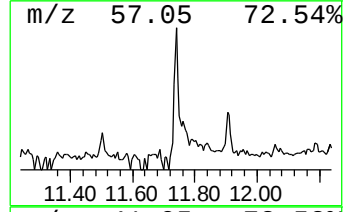
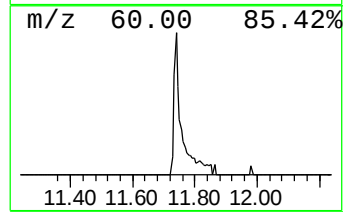
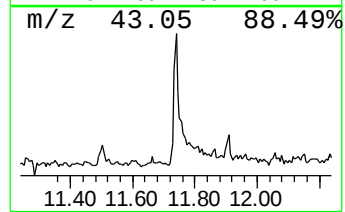
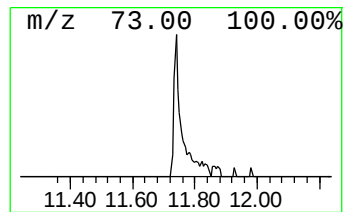
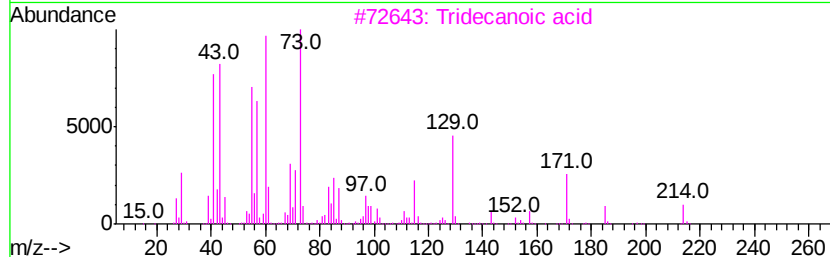
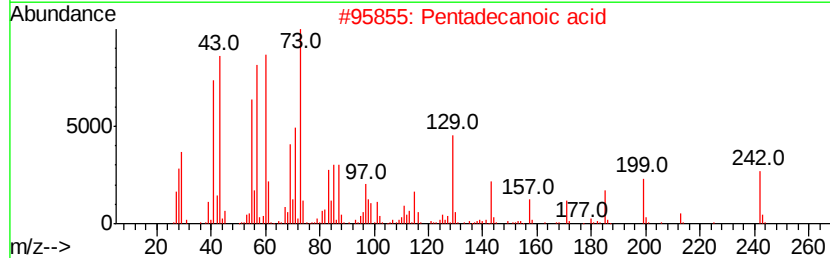
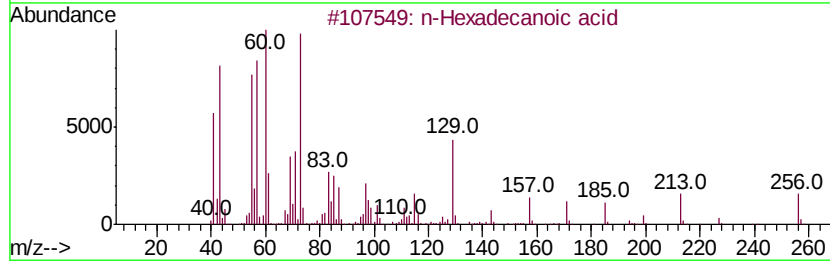
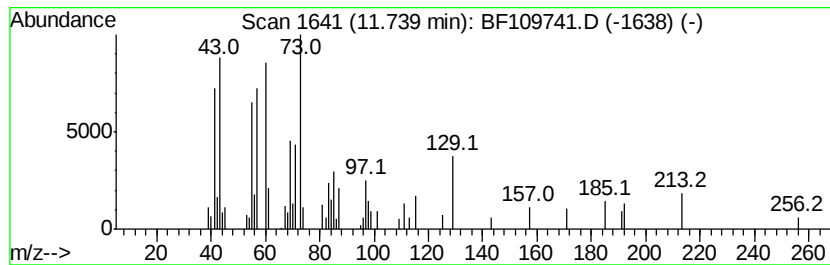
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	2.20 ng	87760	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	64
4		n-Decanoic acid	172	C10H20O2	000334-48-5	59
5		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	20



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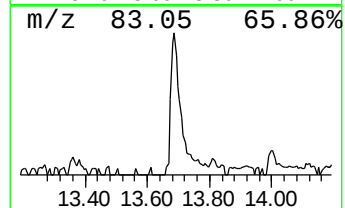
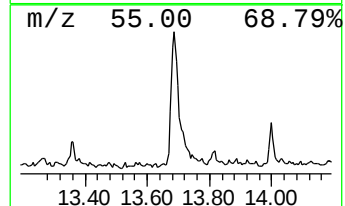
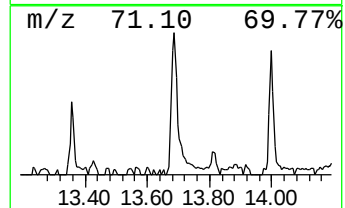
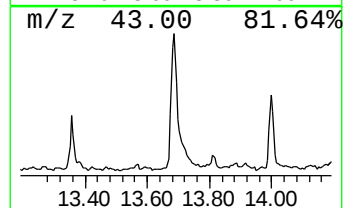
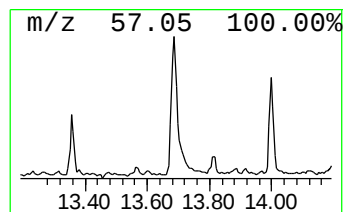
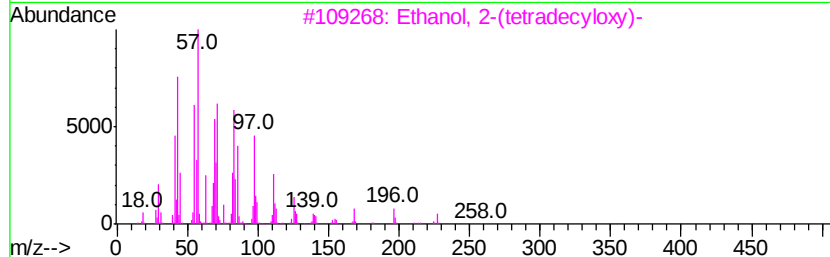
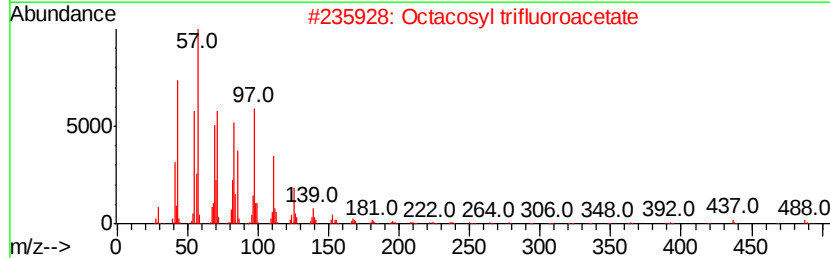
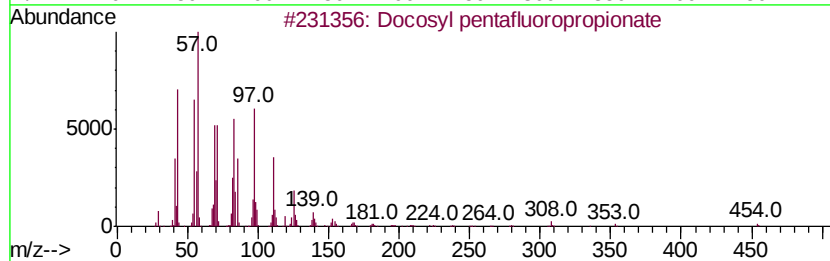
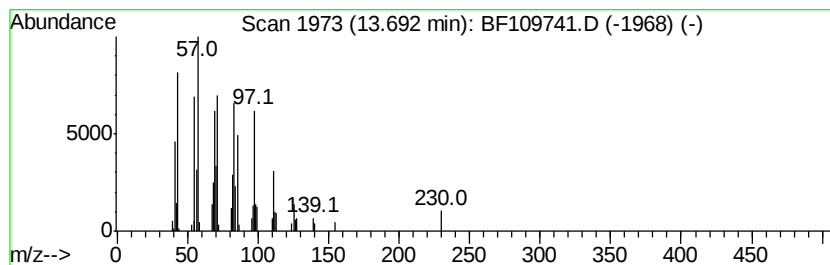
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Peak Number 5 Docosyl pentafluoropropionate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	4.64 ng	203240	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	83
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	83
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81
4		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	81
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	76



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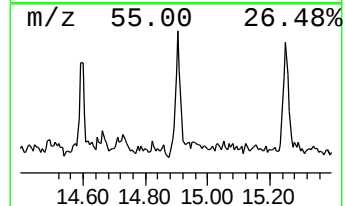
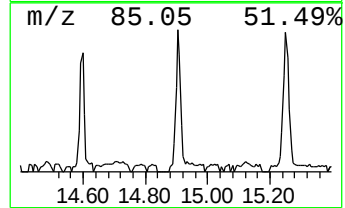
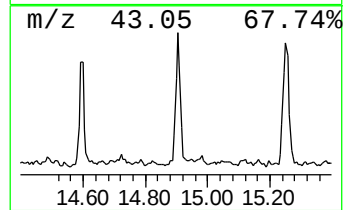
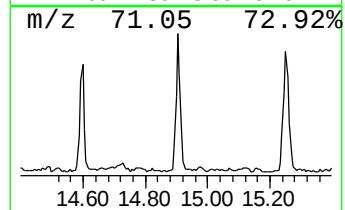
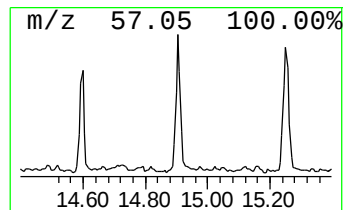
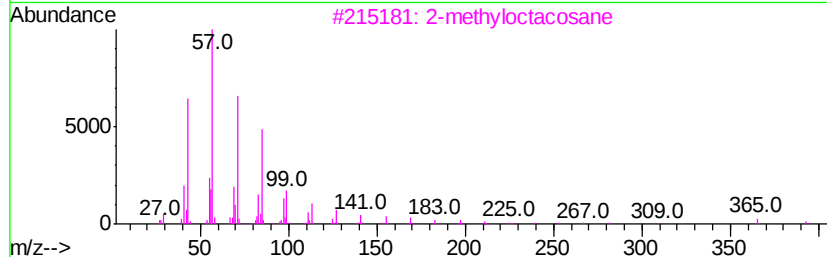
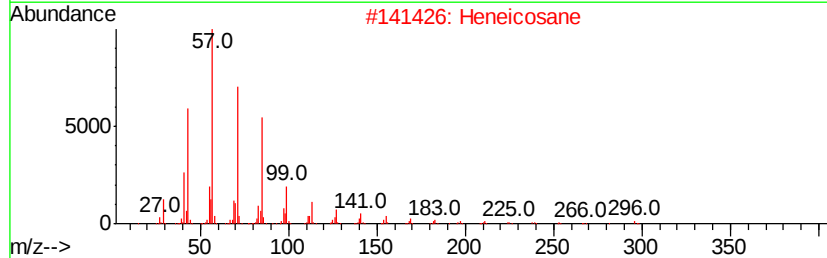
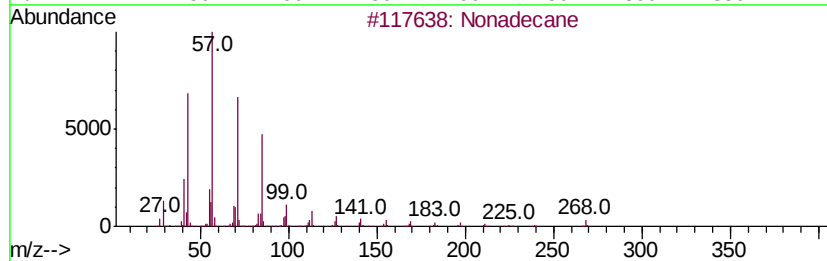
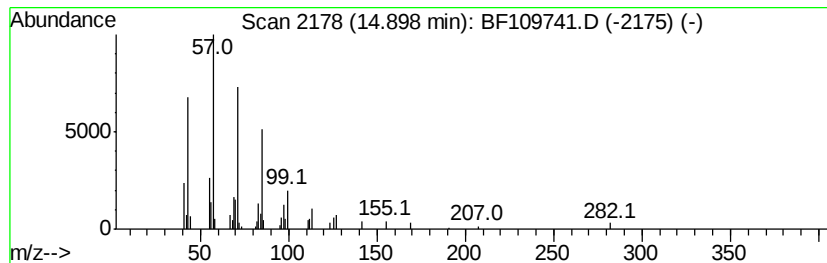
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Peak Number 6 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.45 ng	88294	Perylene-d12	15.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonadecane	268 C19H40	000629-92-5	93
2	Heneicosane	296 C21H44	000629-94-7	91
3	2-methyloctacosane	408 C29H60	1000376-72-8	91
4	Hexacosane	366 C26H54	000630-01-3	90
5	Octacosane	394 C28H58	000630-02-4	90



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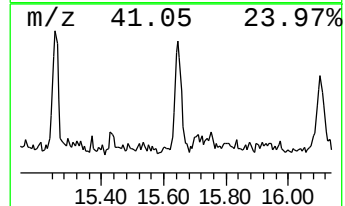
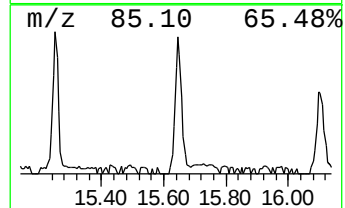
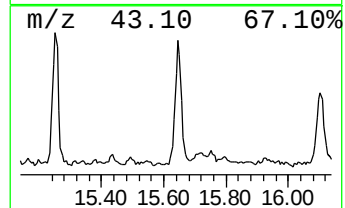
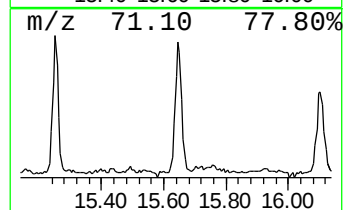
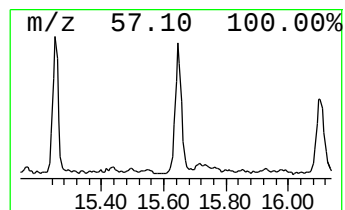
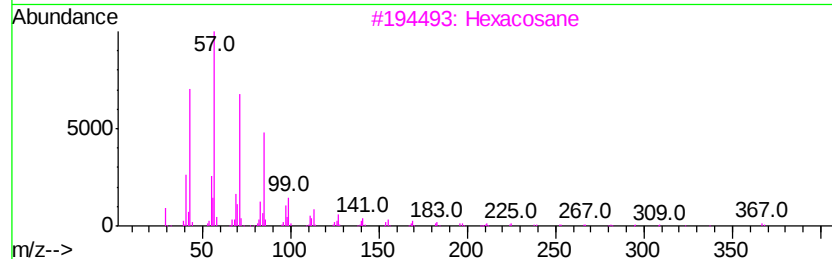
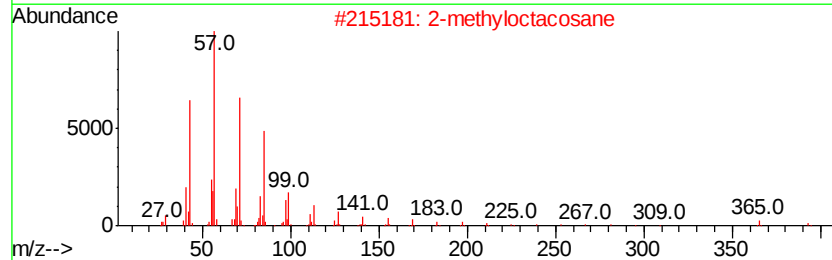
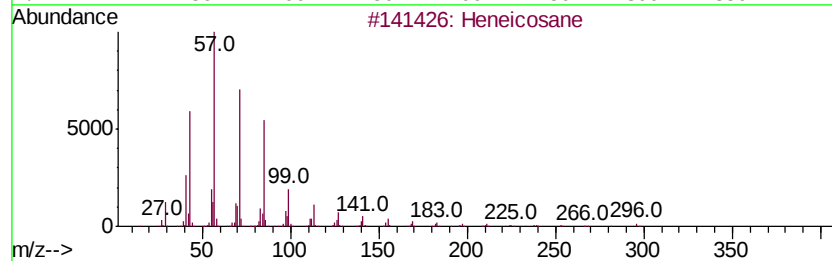
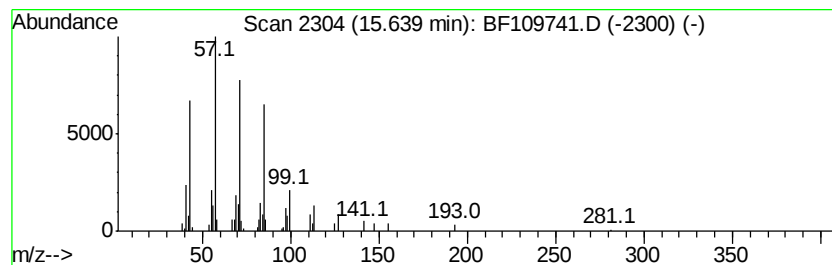
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	3.00 ng	108303	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Hexacosane	366	C26H54	000630-01-3	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Octacosane	394	C28H58	000630-02-4	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109741.D
Acq On : 10 Oct 2018 14:41
Operator : JU/SJ
Sample : J5326-17
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FL-PIT-5

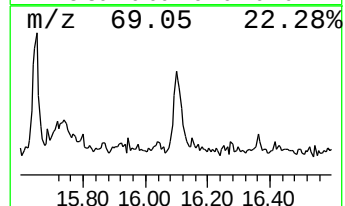
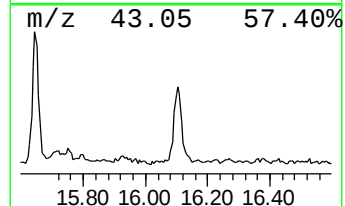
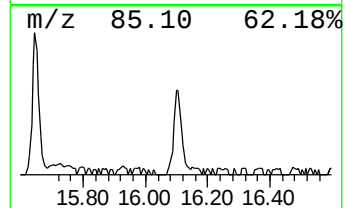
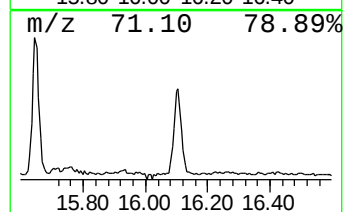
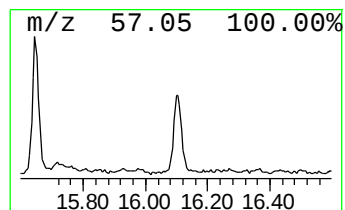
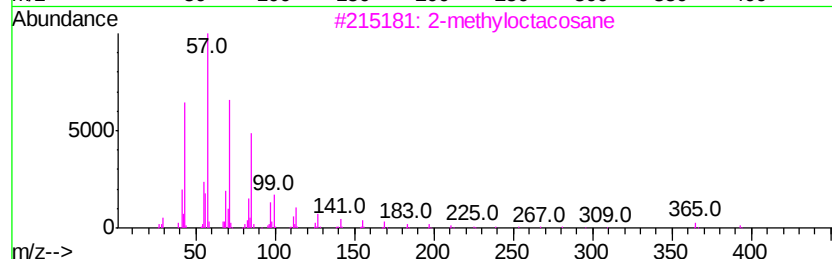
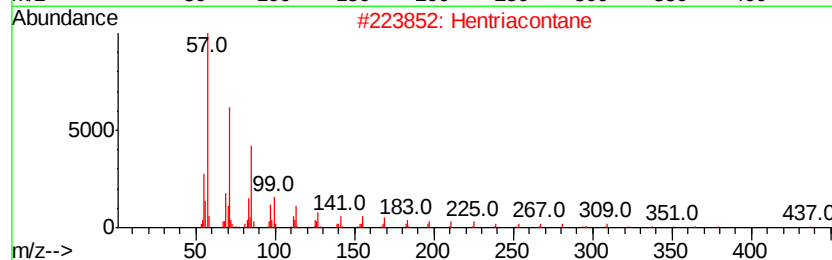
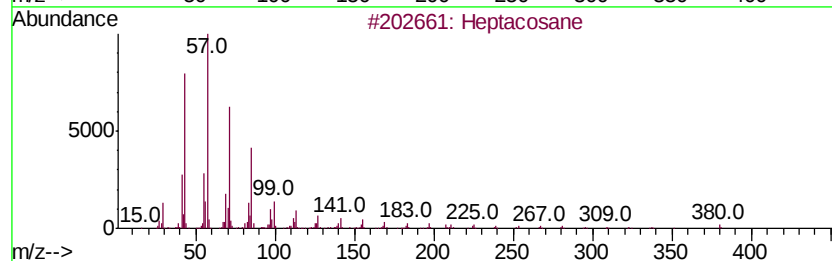
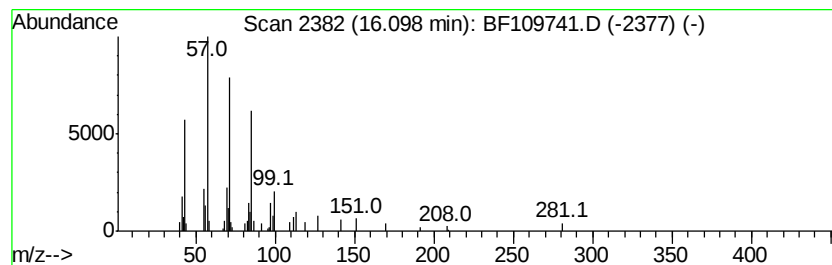
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.29 ng	82633	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Hentriacontane		437	C31H64	000630-04-6	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	2-methyltetracosane		352	C25H52	1000376-72-6	91
5	Heneicosane		296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101018\
Data File : BF109741.D
Acq On : 10 Oct 2018 14:41
Operator : JU/SJ
Sample : J5326-17
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FL-PIT-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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
2-Pentanone, 4-hy...	4.90	3.8	ng	75706	1	6.70	394498	20.0
unknown6.47	6.47	119.8	ng	2362330	1	6.70	394498	20.0
n-Hexadecanoic acid	11.74	2.2	ng	87760	4	11.20	799106	20.0
Docosyl pentaflu...	13.69	4.6	ng	203240	5	13.83	875705	20.0
Nonadecane	14.90	2.5	ng	88294	6	15.23	721625	20.0
Heneicosane	15.64	3.0	ng	108303	6	15.23	721625	20.0
Heptacosane	16.10	2.3	ng	82633	6	15.23	721625	20.0