

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
 Data File : BF110640.D
 Acq On : 9 Nov 2018 21:09
 Operator : JU/SJ
 Sample : J5269-21
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-14

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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	2.281	28	33	49	rVB	102278	145532	2.87%	0.490%
2	4.093	332	341	345	rBV	3391231	5071700	100.00%	17.090%
3	5.198	525	529	546	rBV	72025	110366	2.18%	0.372%
4	5.569	587	592	595	rBV	2311327	2439308	48.10%	8.220%
5	6.575	757	763	778	rBV	2327834	2752297	54.27%	9.274%
6	6.716	782	787	790	rBV	2731769	2659334	52.43%	8.961%
7	6.945	822	826	832	rBV	544797	509439	10.04%	1.717%
8	7.098	848	852	856	rBV	2130516	2021824	39.86%	6.813%
9	7.510	917	922	925	rBV	1621185	1676413	33.05%	5.649%
10	8.222	1039	1043	1055	rBV	624694	674034	13.29%	2.271%
11	9.298	1220	1226	1230	rBV	3038132	3209128	63.28%	10.814%
12	9.692	1289	1293	1298	rBV	141005	128670	2.54%	0.434%
13	9.986	1338	1343	1354	rVB	824368	795438	15.68%	2.680%
14	10.780	1473	1478	1490	rBV	1993620	1988411	39.21%	6.700%
15	11.480	1593	1597	1605	rBV	872396	837153	16.51%	2.821%
16	13.069	1861	1867	1870	rBV	3160016	3171053	62.52%	10.685%
17	13.933	2011	2014	2027	rVB	90437	126338	2.49%	0.426%
18	14.127	2044	2047	2058	rBV	677354	646904	12.76%	2.180%
19	14.874	2169	2174	2181	rVB2	48569	62748	1.24%	0.211%
20	15.227	2230	2234	2237	rBV	49633	59375	1.17%	0.200%
21	15.621	2296	2301	2303	rBV	52836	75183	1.48%	0.253%
22	15.651	2303	2306	2318	rVB	278546	392427	7.74%	1.322%
23	16.074	2373	2378	2384	rVB2	47835	70430	1.39%	0.237%
24	16.604	2462	2468	2477	rVB	27332	53546	1.06%	0.180%

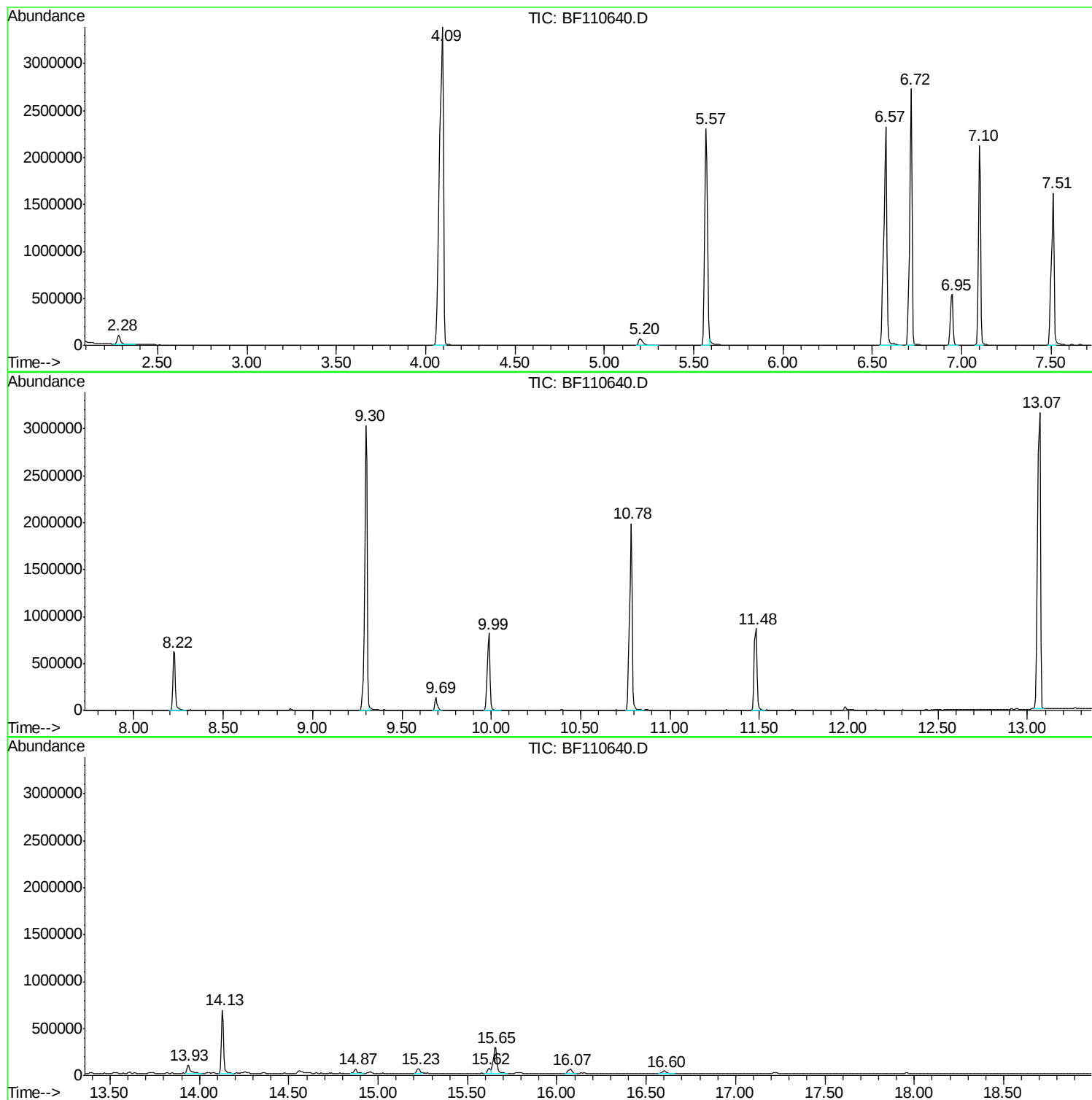
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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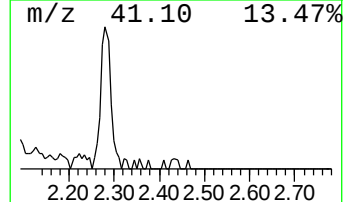
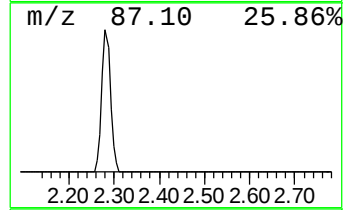
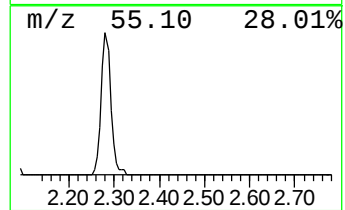
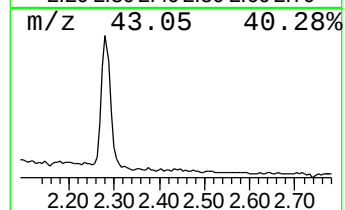
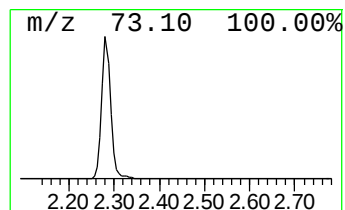
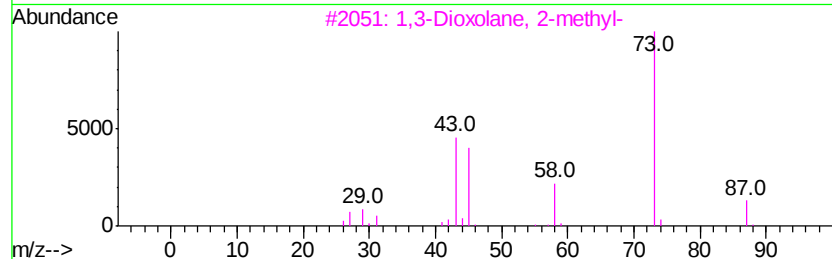
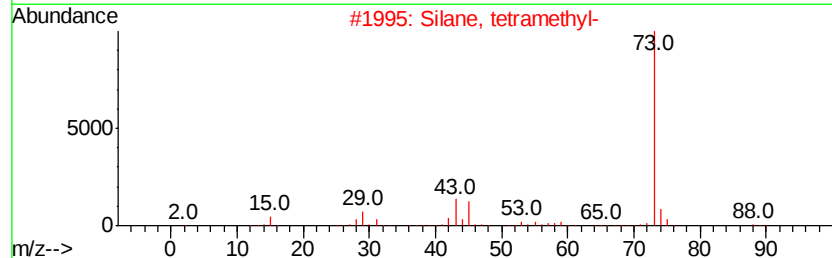
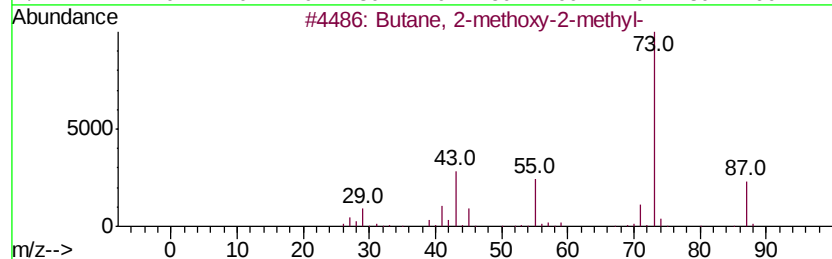
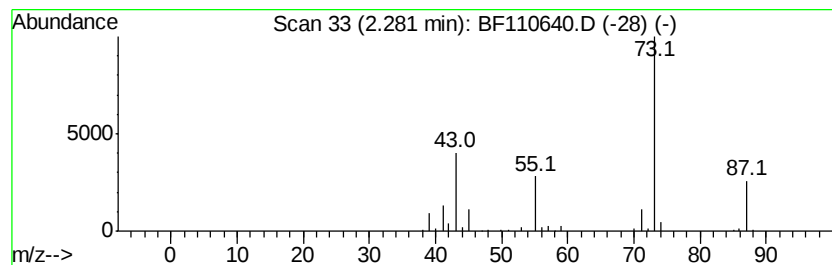
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.28	5.71 ng	145532	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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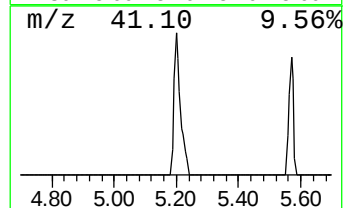
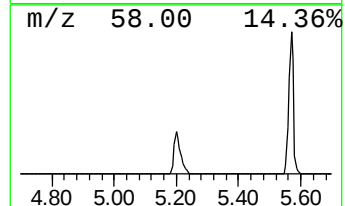
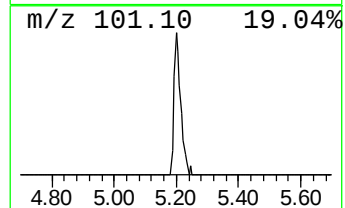
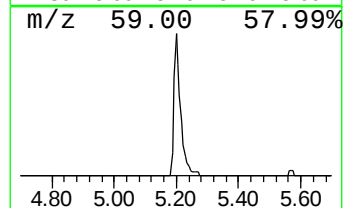
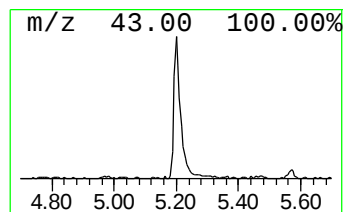
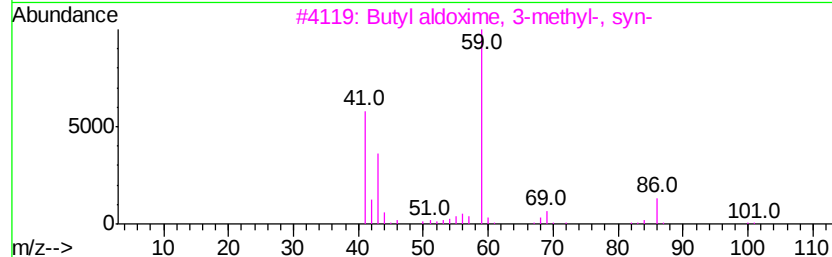
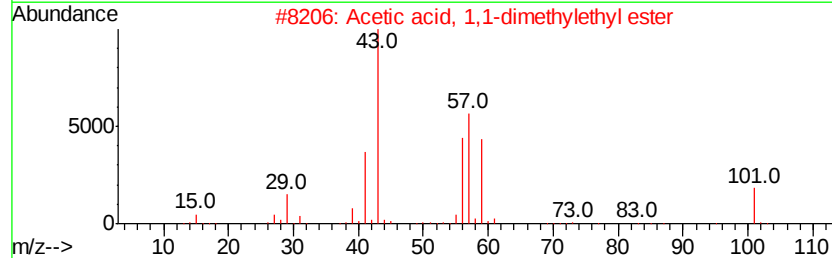
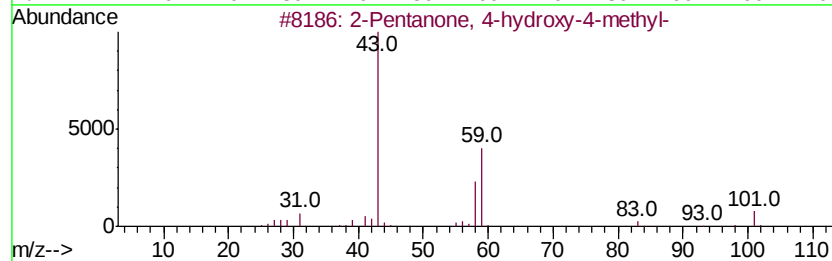
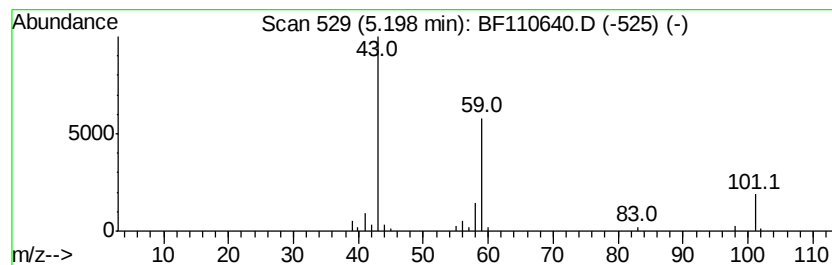
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Peak Number 3 unknown5.20 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	4.33 ng	110366	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5		3-Hexanol	102	C6H14O	000623-37-0	25



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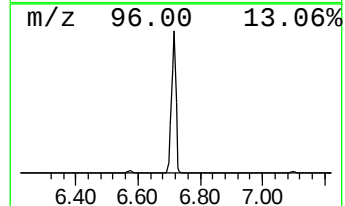
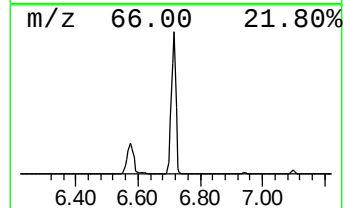
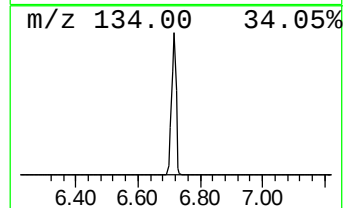
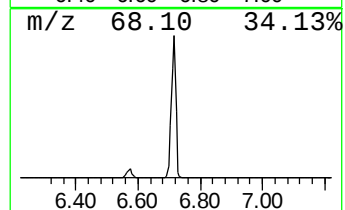
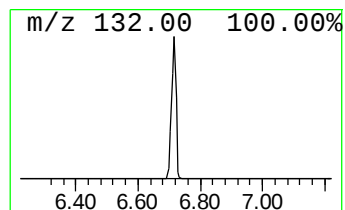
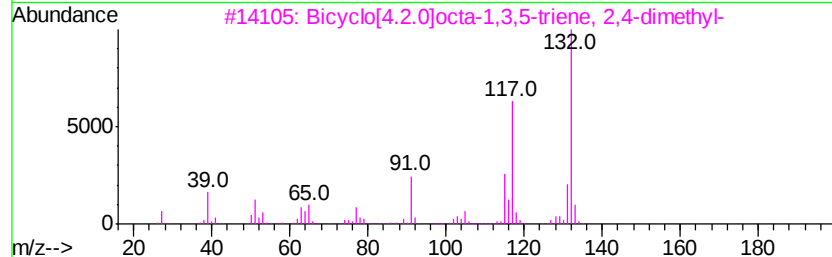
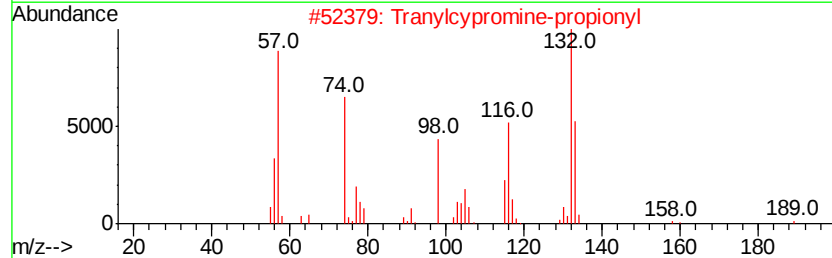
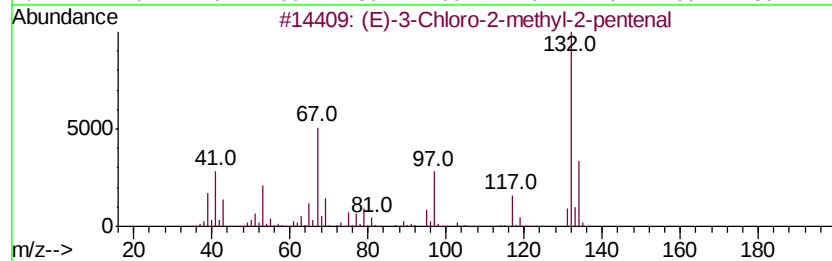
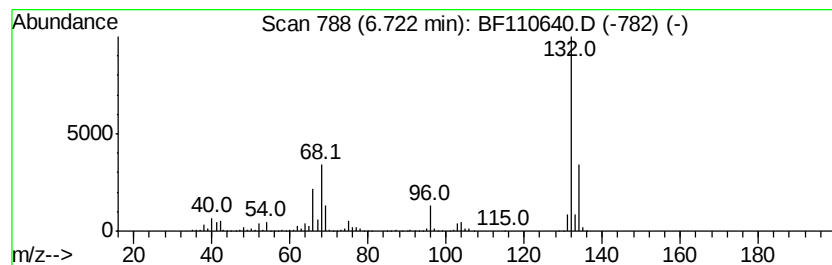
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Peak Number 4 unknown6.72 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	104.40 ng	2659330	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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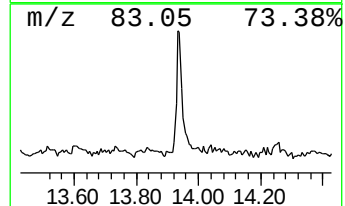
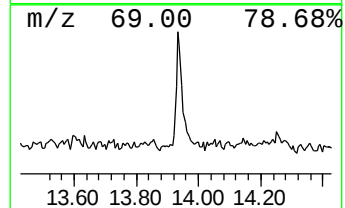
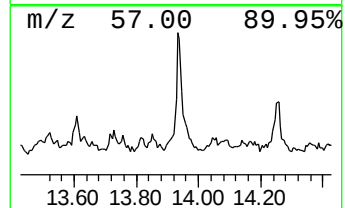
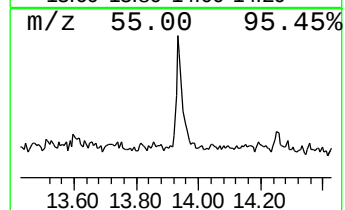
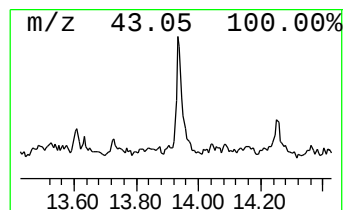
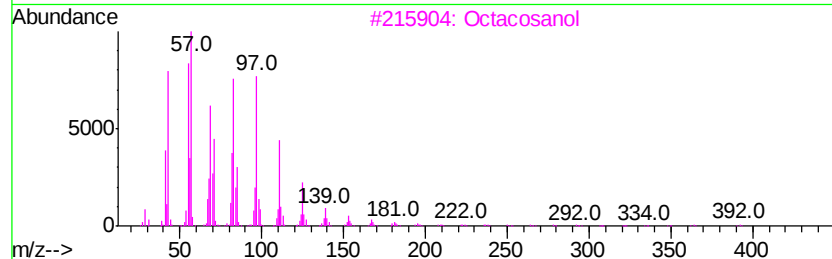
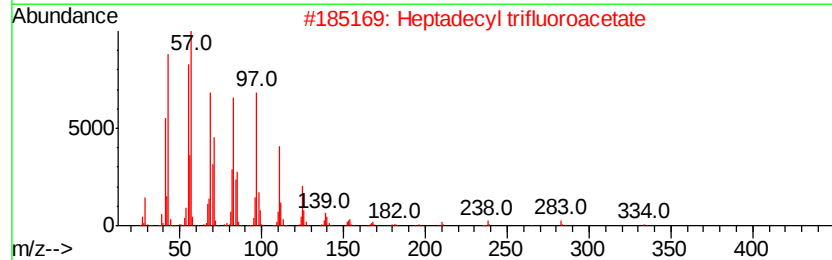
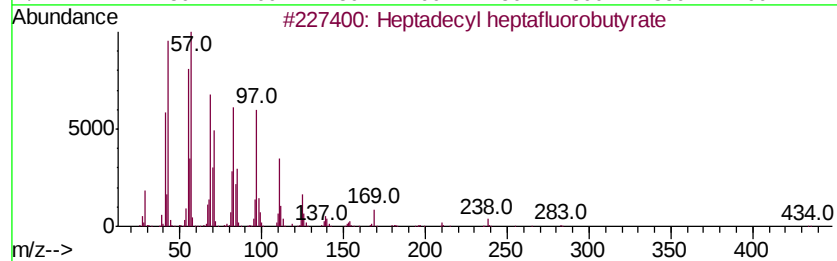
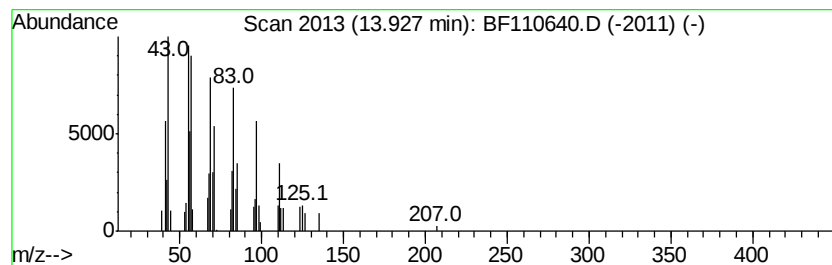
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Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	3.91 ng	126338	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		Octacosanol	410	C28H58O	000557-61-9	91
4		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



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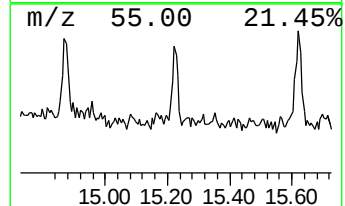
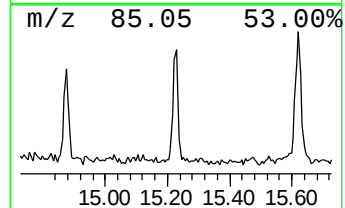
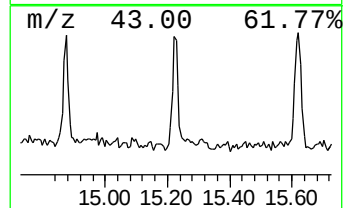
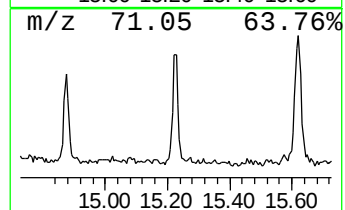
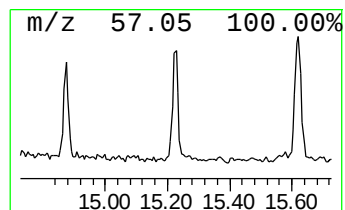
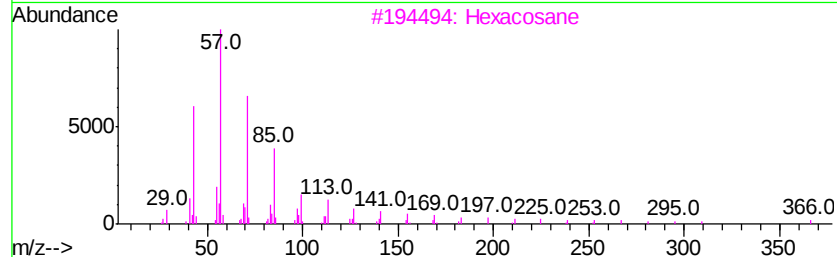
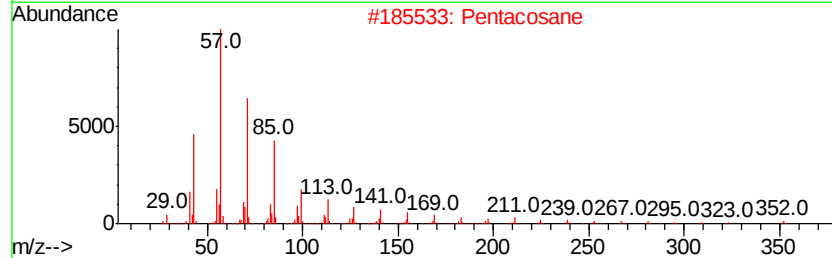
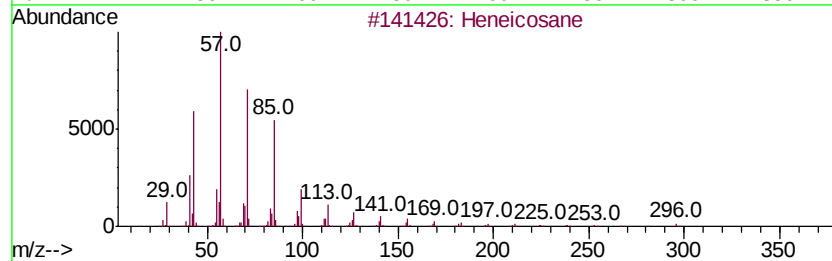
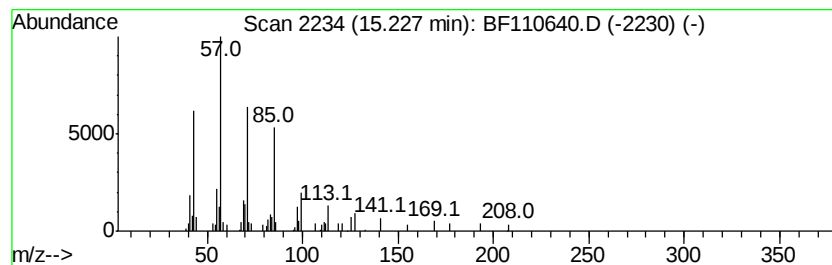
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	3.03 ng	59375	Perylene-d12	15.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Pentacosane		352	C25H52	000629-99-2	87
3	Hexacosane		366	C26H54	000630-01-3	87
4	Hentriacontane		437	C31H64	000630-04-6	87
5	Heptadecane		240	C17H36	000629-78-7	87



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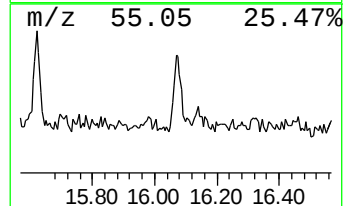
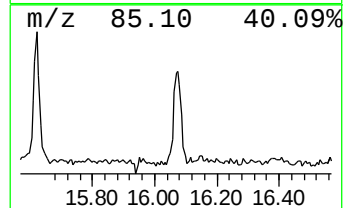
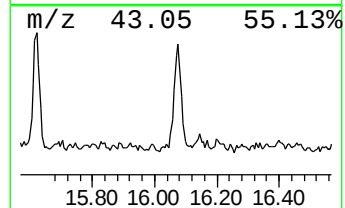
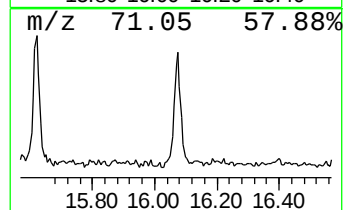
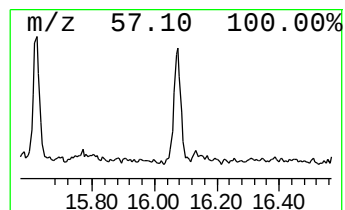
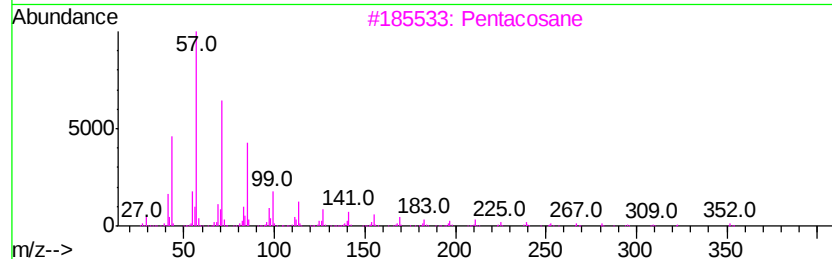
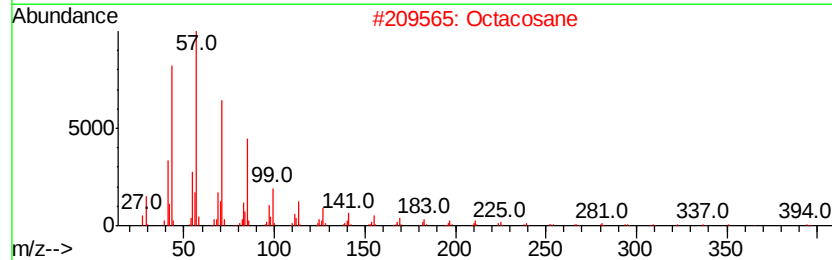
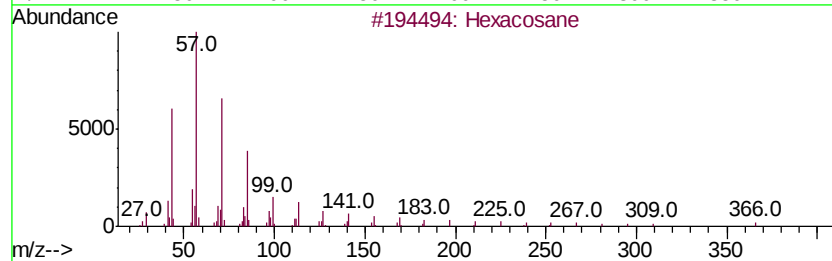
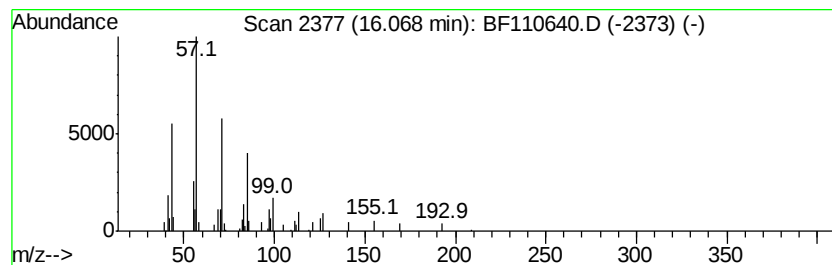
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	3.59 ng	70430	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Pentacosane	352	C25H52	000629-99-2	87
4		Tetratetracontane	619	C44H90	007098-22-8	87
5		2-methyloctacosane	408	C29H60	1000376-72-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110640.D
Acq On : 9 Nov 2018 21:09
Operator : JU/SJ
Sample : J5269-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-14

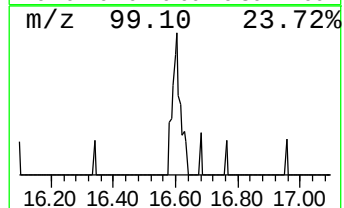
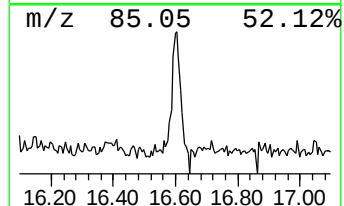
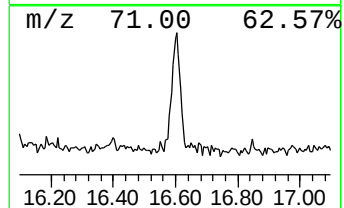
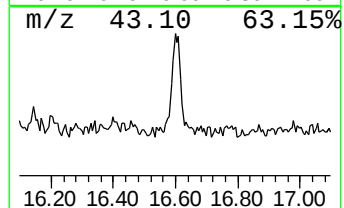
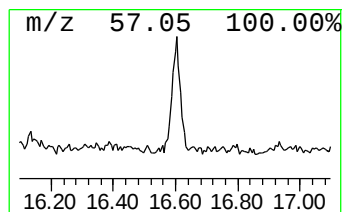
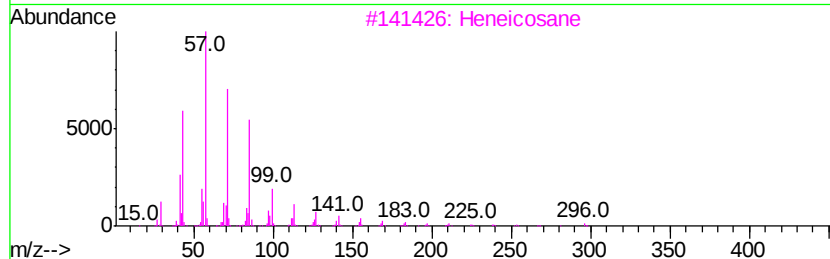
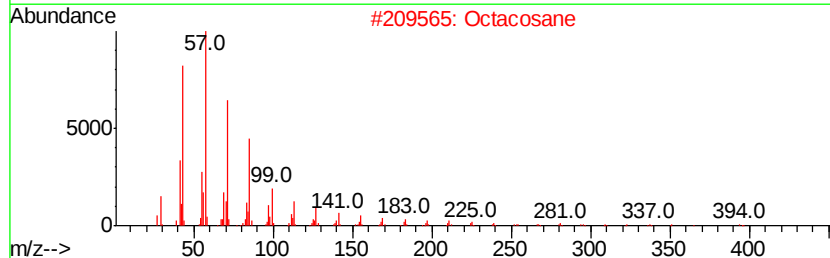
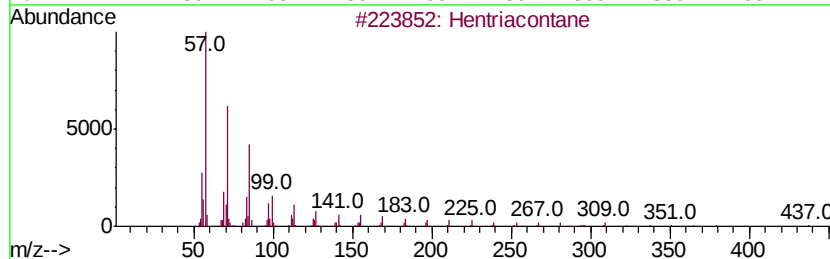
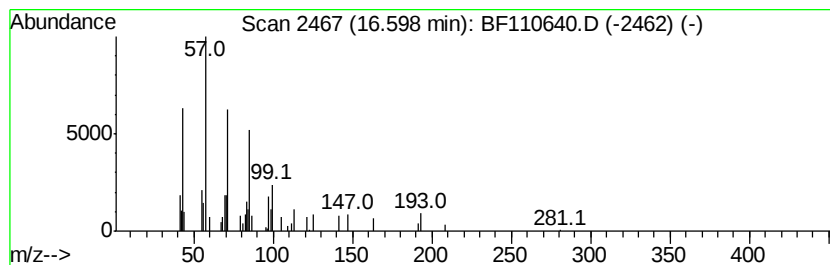
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	2.73 ng	53546	Perylene-d12	15.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	86
2	Octacosane		394	C28H58	000630-02-4	86
3	Heneicosane		296	C21H44	000629-94-7	80
4	Hexacosane		366	C26H54	000630-01-3	80
5	Pentacosane		352	C25H52	000629-99-2	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
Data File : BF110640.D
Acq On : 9 Nov 2018 21:09
Operator : JU/SJ
Sample : J5269-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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
Butane, 2-methoxy...	2.28	5.7	ng	145532	1	6.95	509439	20.0
unknown5.20	5.20	4.3	ng	110366	1	6.95	509439	20.0
unknown6.72	6.72	104.4	ng	2659330	1	6.95	509439	20.0
Heptadecyl heptaf...	13.93	3.9	ng	126338	5	14.13	646904	20.0
Heneicosane	15.23	3.0	ng	59375	6	15.66	392427	20.0
Hexacosane	16.07	3.6	ng	70430	6	15.66	392427	20.0
Hentriacontane	16.60	2.7	ng	53546	6	15.66	392427	20.0