

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081718\
 Data File : BF108247.D
 Acq On : 17 Aug 2018 17:04
 Operator : JU/SJ
 Sample : J4531-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-036

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-BF080818.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	5.260	493	497	504	rVB	177019	211809	4.97%	0.594%
2	5.643	557	562	565	rBV	3599219	3608557	84.74%	10.113%
3	6.637	726	731	734	rBV	3821398	3848789	90.39%	10.787%
4	6.784	752	756	760	rBV	3764037	3799613	89.23%	10.649%
5	7.013	792	795	799	rBV	1114074	965617	22.68%	2.706%
6	7.172	818	822	826	rBV	3465963	2965734	69.65%	8.312%
7	7.578	886	891	894	rBV	2748495	2475630	58.14%	6.938%
8	8.301	1010	1014	1017	rBV	1314855	1180725	27.73%	3.309%
9	8.907	1115	1117	1121	rBV	79710	67556	1.59%	0.189%
10	9.372	1189	1196	1199	rBV	4999137	4258199	100.00%	11.934%
11	9.760	1258	1262	1267	rBV	443992	340407	7.99%	0.954%
12	10.060	1309	1313	1323	rBV	1489806	1287285	30.23%	3.608%
13	10.854	1443	1448	1461	rBV	2617731	2477995	58.19%	6.945%
14	11.554	1563	1567	1571	rBV	1361862	1217530	28.59%	3.412%
15	12.807	1777	1780	1783	rVB	107769	84942	1.99%	0.238%
16	13.142	1833	1837	1840	rBV	3960321	3664247	86.05%	10.269%
17	14.048	1984	1991	2000	rBV2	162554	383837	9.01%	1.076%
18	14.207	2014	2018	2022	rBV	1270599	1204613	28.29%	3.376%
19	14.648	2090	2093	2097	rVB2	53528	57968	1.36%	0.162%
20	14.977	2146	2149	2153	rVB	55864	61351	1.44%	0.172%
21	15.060	2160	2163	2171	rVB	99218	111509	2.62%	0.313%
22	15.342	2207	2211	2215	rVB	124142	145663	3.42%	0.408%
23	15.771	2278	2284	2291	rVB	780333	1109083	26.05%	3.108%
24	16.236	2359	2363	2368	rVB	98120	152664	3.59%	0.428%

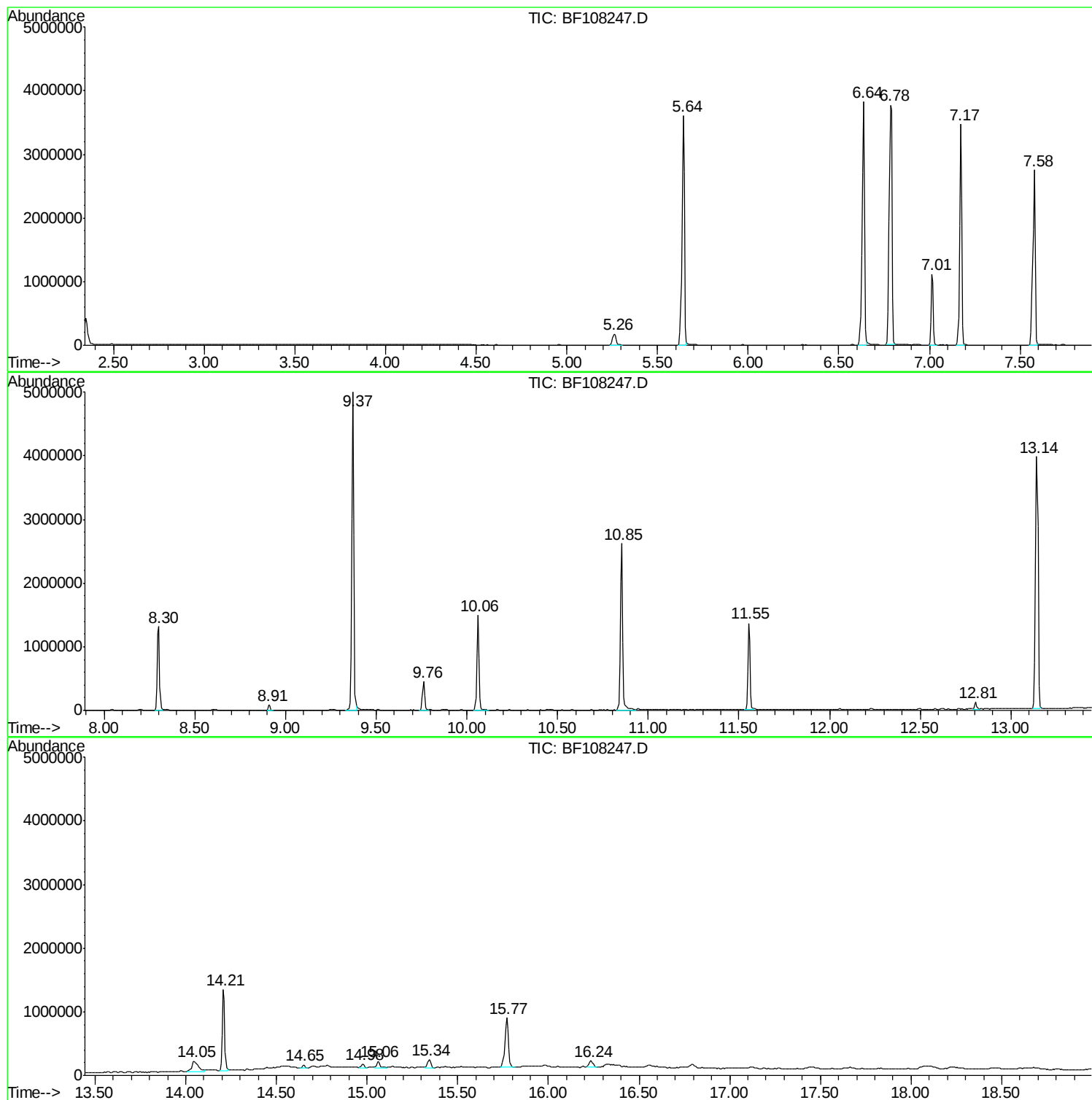
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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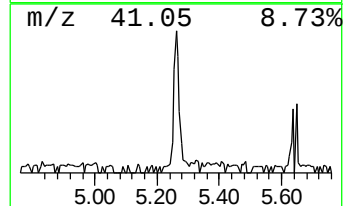
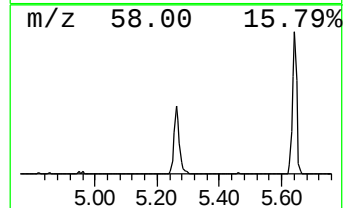
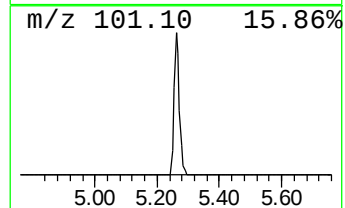
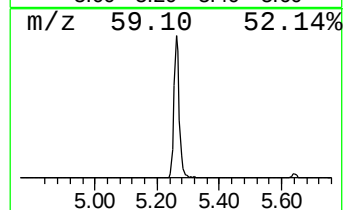
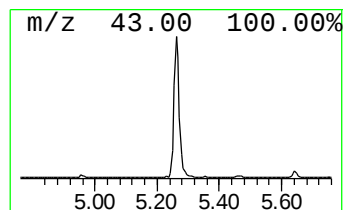
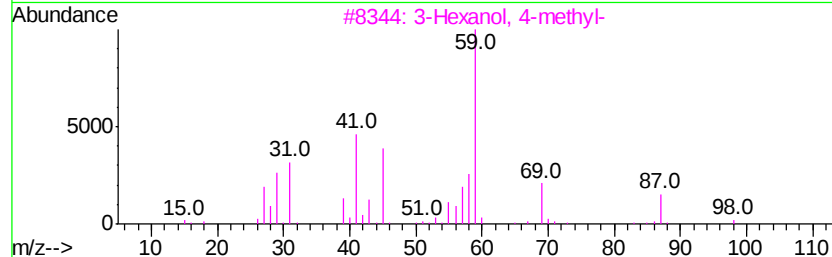
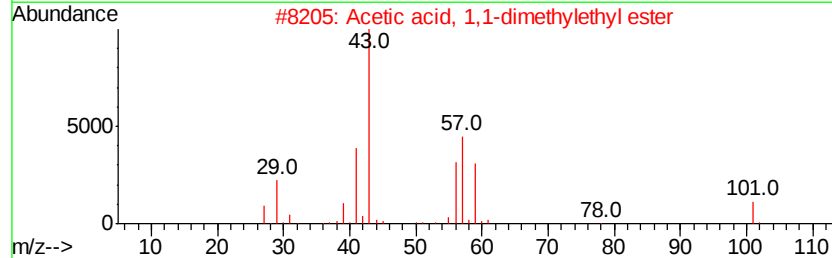
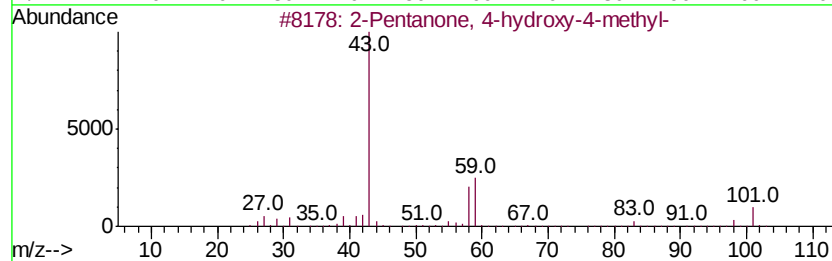
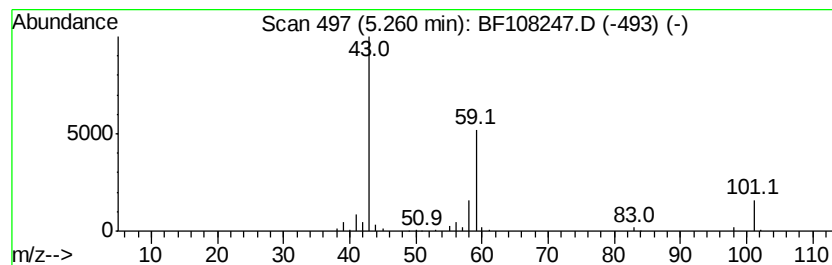
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	4.39 ng	211809	1,4-Dichlorobenzene-d4	7.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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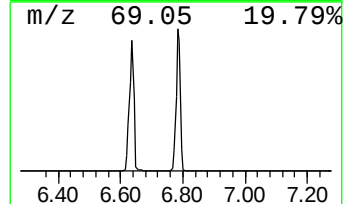
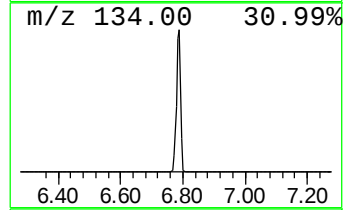
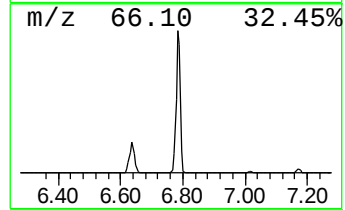
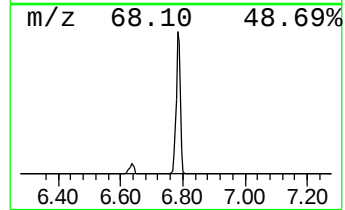
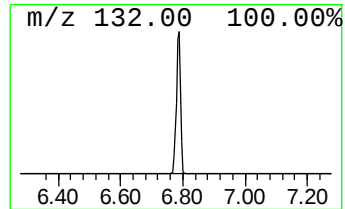
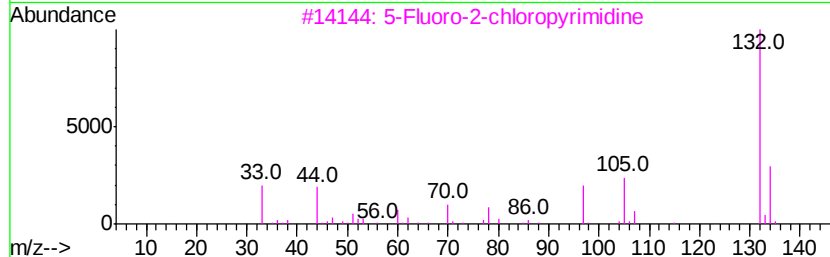
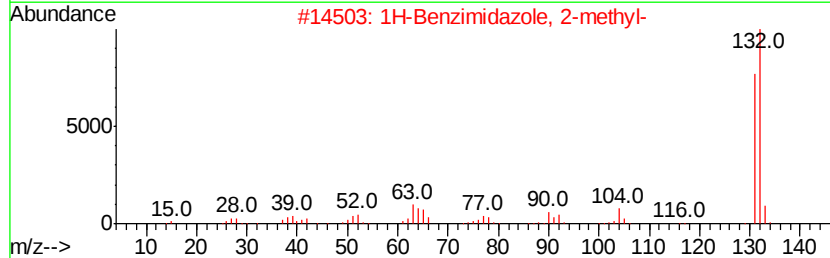
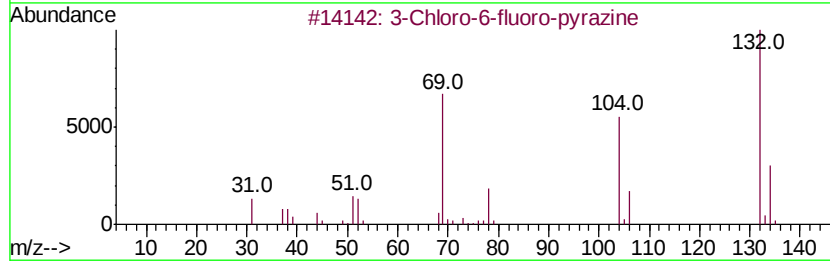
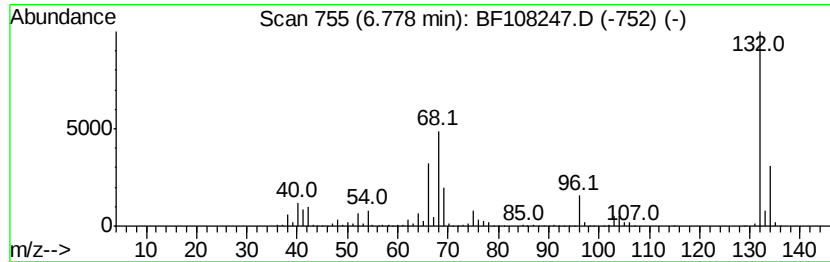
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Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	78.70 ng	3799610	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22	
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
4	5-Aminoindole	132	C8H8N2	005192-03-0	12	
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10	



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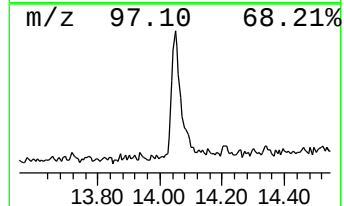
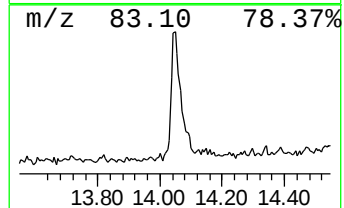
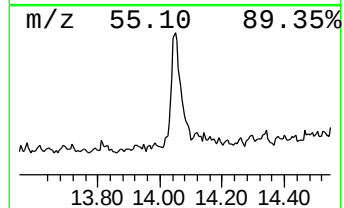
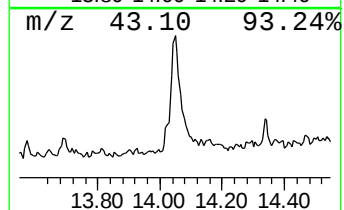
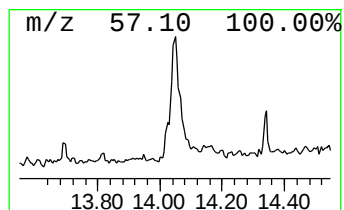
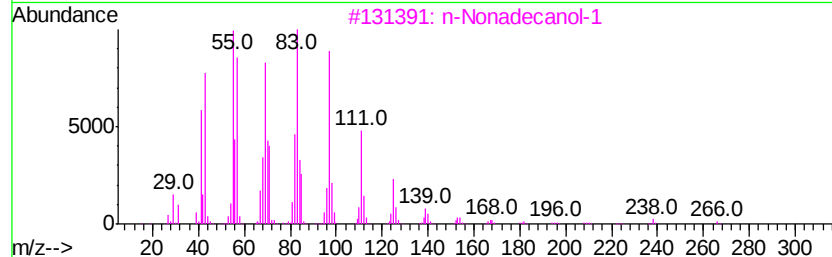
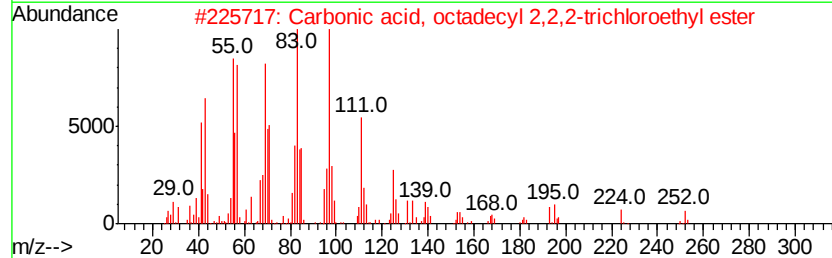
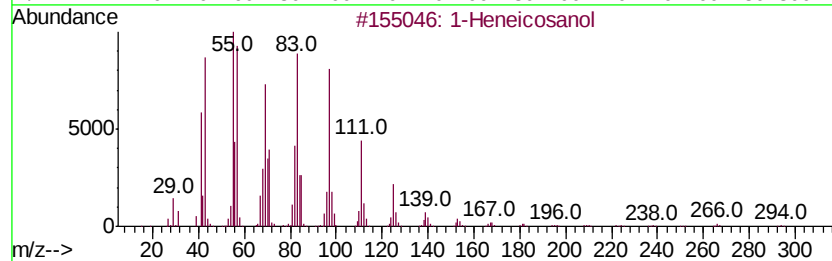
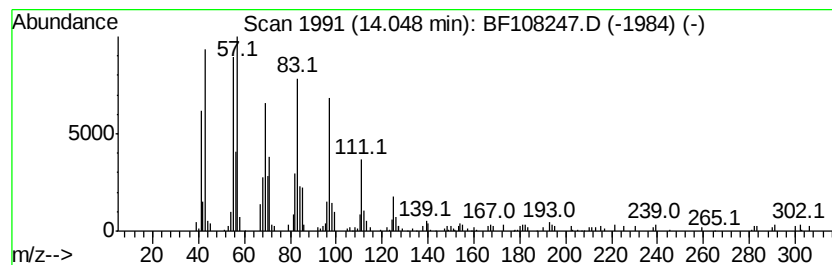
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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.05	6.37 ng	383837	Chrysene-d12		14.21		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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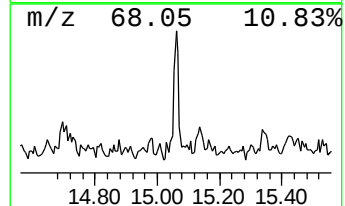
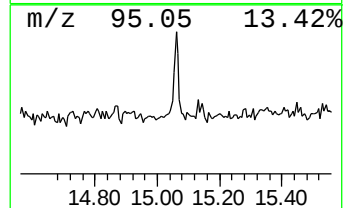
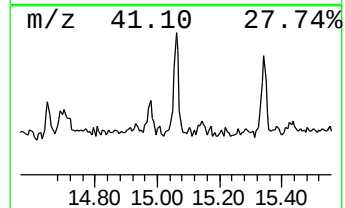
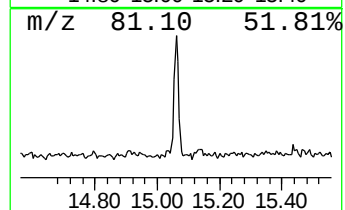
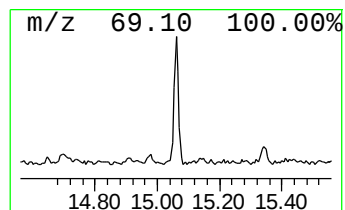
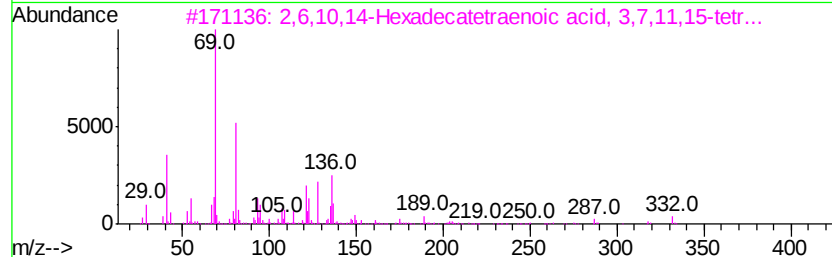
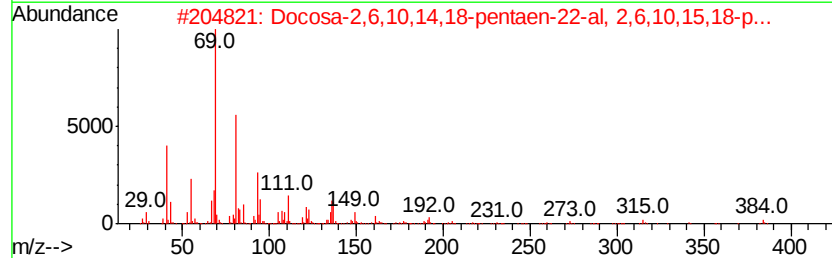
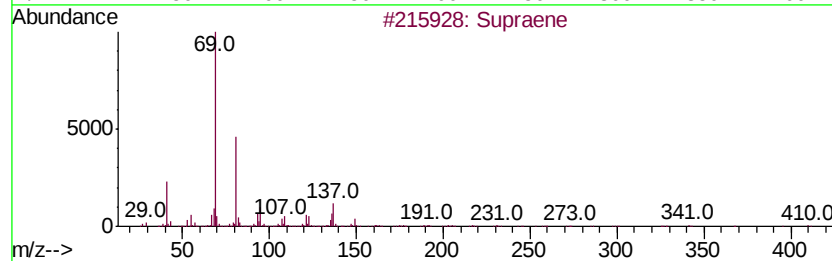
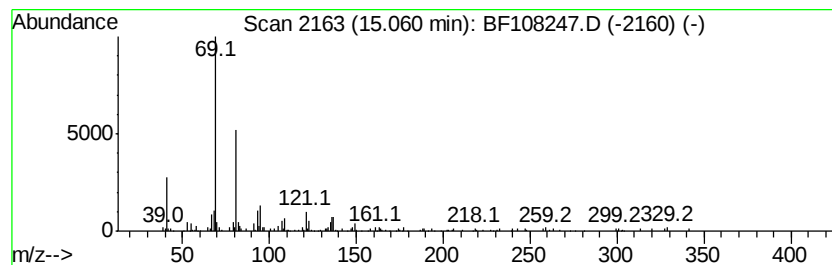
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Peak Number 5 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	2.01 ng	111509	Perylene-d12	15.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	83
2	Docosa-2,6,10,14,18-pentaen-22-a...		384	C27H44O	1000163-04-7	72
3	2,6,10,14-Hexadecatetraenoic aci...		332	C22H36O2	024035-35-6	64
4	2,6-Octadiene, 2,6-dimethyl-		138	C10H18	002792-39-4	59
5	trans-Farnesol		222	C15H26O	000106-28-5	59



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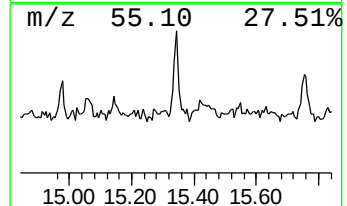
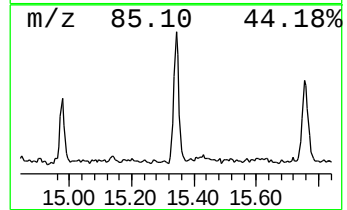
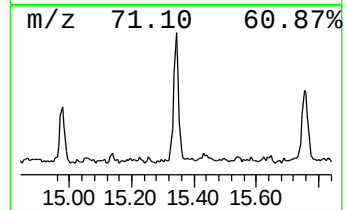
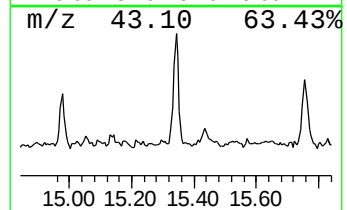
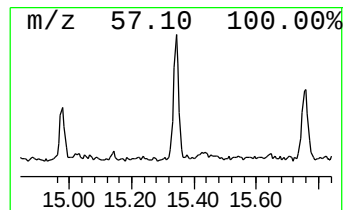
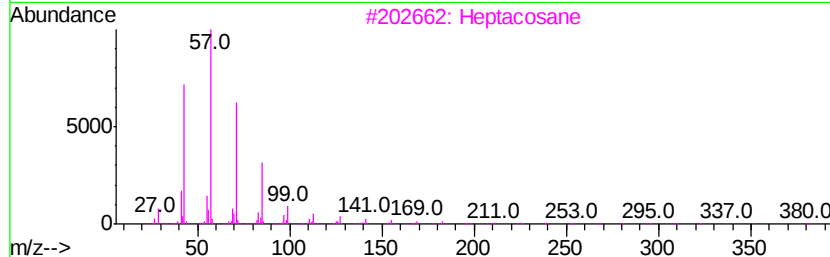
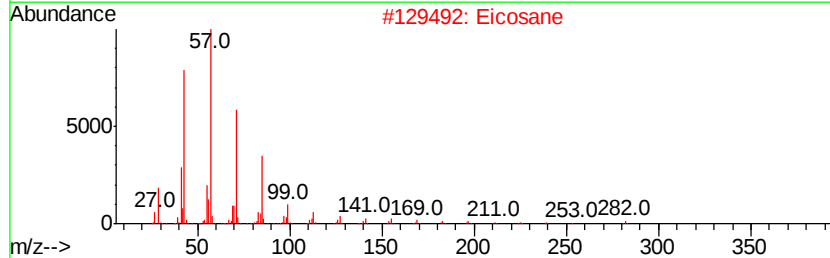
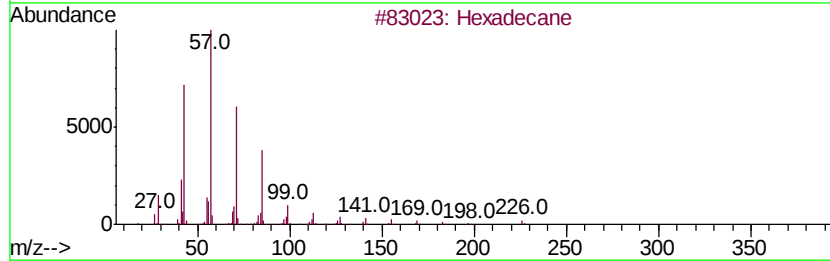
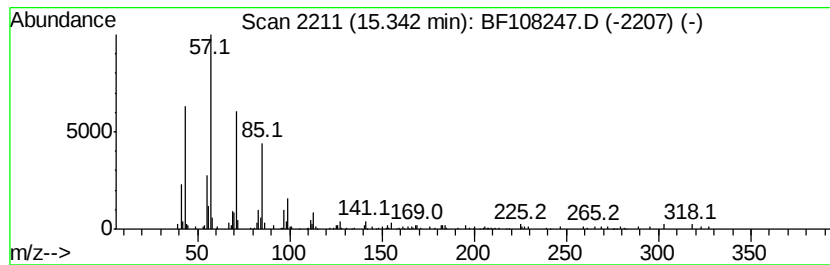
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	2.63 ng	145663	Perylene-d12	15.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	96
2		Eicosane	282	C20H42	000112-95-8	95
3		Heptacosane	380	C27H56	000593-49-7	87
4		Octacosane	394	C28H58	000630-02-4	87
5		Heneicosane	296	C21H44	000629-94-7	86



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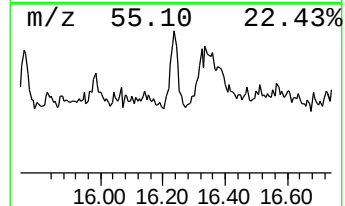
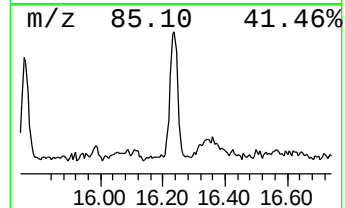
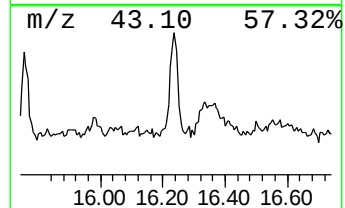
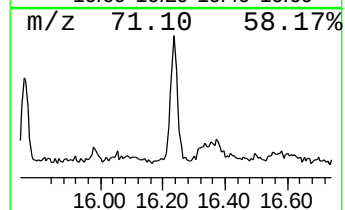
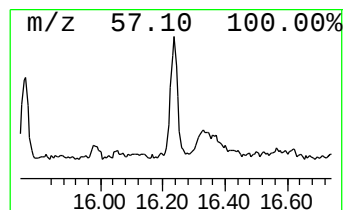
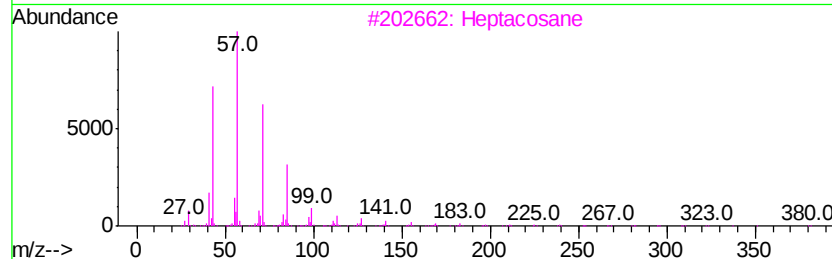
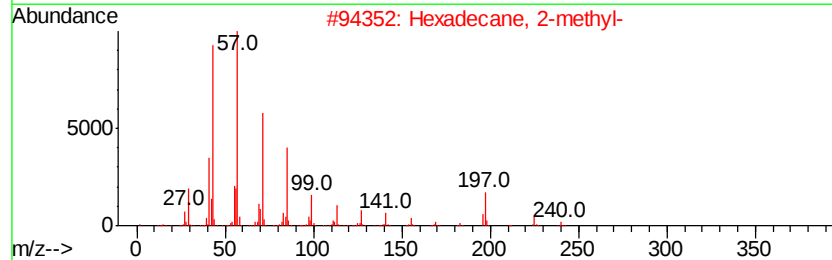
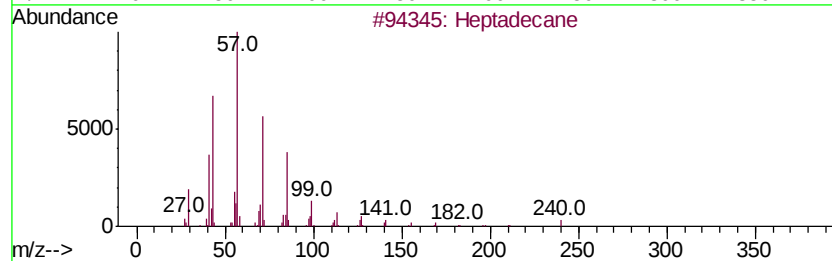
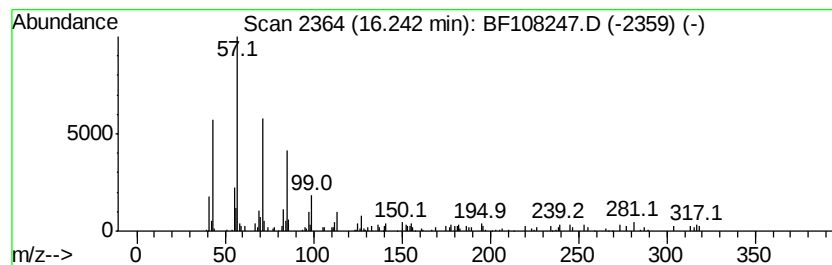
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	2.75 ng	152664	Perylene-d12	15.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Hexadecane, 2-methyl-		240	C17H36	001560-92-5	87
3	Heptacosane		380	C27H56	000593-49-7	83
4	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	80
5	Eicosane		282	C20H42	000112-95-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081718\
Data File : BF108247.D
Acq On : 17 Aug 2018 17:04
Operator : JU/SJ
Sample : J4531-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	5.26	4.4	ng	211809	1	7.01	965617	20.0
unknown6.78	6.78	78.7	ng	3799610	1	7.01	965617	20.0
1-Heneicosanol	14.05	6.4	ng	383837	5	14.21	1204610	20.0
Supraene	15.06	2.0	ng	111509	6	15.77	1109080	20.0
Hexadecane	15.34	2.6	ng	145663	6	15.77	1109080	20.0
Heptadecane	16.24	2.8	ng	152664	6	15.77	1109080	20.0