

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121718\
 Data File : BF111563.D
 Acq On : 18 Dec 2018 2:26
 Operator : JU/SJ
 Sample : J6403-49
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-7-A

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-BF121418.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	3.251	196	198	205	rBV6	27032	48844	1.25%	0.152%
2	4.992	490	494	502	rBV	137270	165516	4.25%	0.515%
3	5.422	563	567	583	rVB	2976340	2729278	70.10%	8.488%
4	6.439	735	740	755	rBV	2991704	3102697	79.69%	9.649%
5	6.563	757	761	764	rBV	3536112	3016474	77.47%	9.381%
6	6.787	795	799	808	rBV	1016106	815844	20.95%	2.537%
7	6.945	822	826	829	rBV	2806981	2260922	58.07%	7.031%
8	7.345	889	894	906	rBV	1668750	1717138	44.10%	5.340%
9	8.069	1013	1017	1032	rBV	1182575	1033555	26.55%	3.214%
10	9.145	1196	1200	1203	rBV	4528909	3893486	100.00%	12.109%
11	9.539	1263	1267	1275	rBV	431111	403522	10.36%	1.255%
12	9.822	1311	1315	1319	rBV2	1668674	1498263	38.48%	4.660%
13	10.610	1445	1449	1462	rBV	2080339	2035342	52.28%	6.330%
14	11.304	1564	1567	1570	rBV	1291061	1233228	31.67%	3.835%
15	11.327	1570	1571	1575	rVV	292965	229348	5.89%	0.713%
16	11.380	1578	1580	1584	rVB	67155	62773	1.61%	0.195%
17	11.539	1601	1607	1610	rBV2	41973	55088	1.41%	0.171%
18	11.839	1655	1658	1662	rBV	251380	242630	6.23%	0.755%
19	11.921	1668	1672	1674	rBV2	64378	65766	1.69%	0.205%
20	12.357	1743	1746	1750	rBV3	50068	62843	1.61%	0.195%
21	12.398	1750	1753	1758	rVB6	42669	66973	1.72%	0.208%
22	12.516	1770	1773	1777	rBV	400272	375685	9.65%	1.168%
23	12.621	1787	1791	1796	rBV6	53074	96397	2.48%	0.300%
24	12.745	1807	1812	1815	rBV	412682	394981	10.14%	1.228%
25	12.892	1833	1837	1840	rBV	2946053	2552462	65.56%	7.938%
26	13.074	1866	1868	1871	rVB	63156	49294	1.27%	0.153%
27	13.180	1883	1886	1889	rBV2	42641	46053	1.18%	0.143%
28	13.580	1952	1954	1960	rVB2	43573	49293	1.27%	0.153%
29	13.792	1987	1990	2000	rVB3	116277	149268	3.83%	0.464%
30	13.945	2011	2016	2019	rBV2	1143429	1276336	32.78%	3.969%
31	13.968	2019	2020	2023	rVB	235349	135162	3.47%	0.420%
32	14.115	2042	2045	2047	rBV	46178	49090	1.26%	0.153%
33	14.421	2094	2097	2100	rBV3	94882	84456	2.17%	0.263%
34	14.721	2145	2148	2152	rVB	94679	90105	2.31%	0.280%

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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 >
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35	14.792	2157	2160	2164	rBV	218402	202074	5.19%	0.628%
36	14.968	2186	2190	2199	rBV	203947	400074	10.28%	1.244%
37	15.045	2200	2203	2206	rBV	114519	118990	3.06%	0.370%
38	15.262	2236	2240	2245	rVB	121325	172382	4.43%	0.536%
39	15.321	2246	2250	2256	rBV	158196	209112	5.37%	0.650%
40	15.386	2256	2261	2264	rBV	660428	843375	21.66%	2.623%
41	15.839	2335	2338	2343	rVB2	87813	120394	3.09%	0.374%

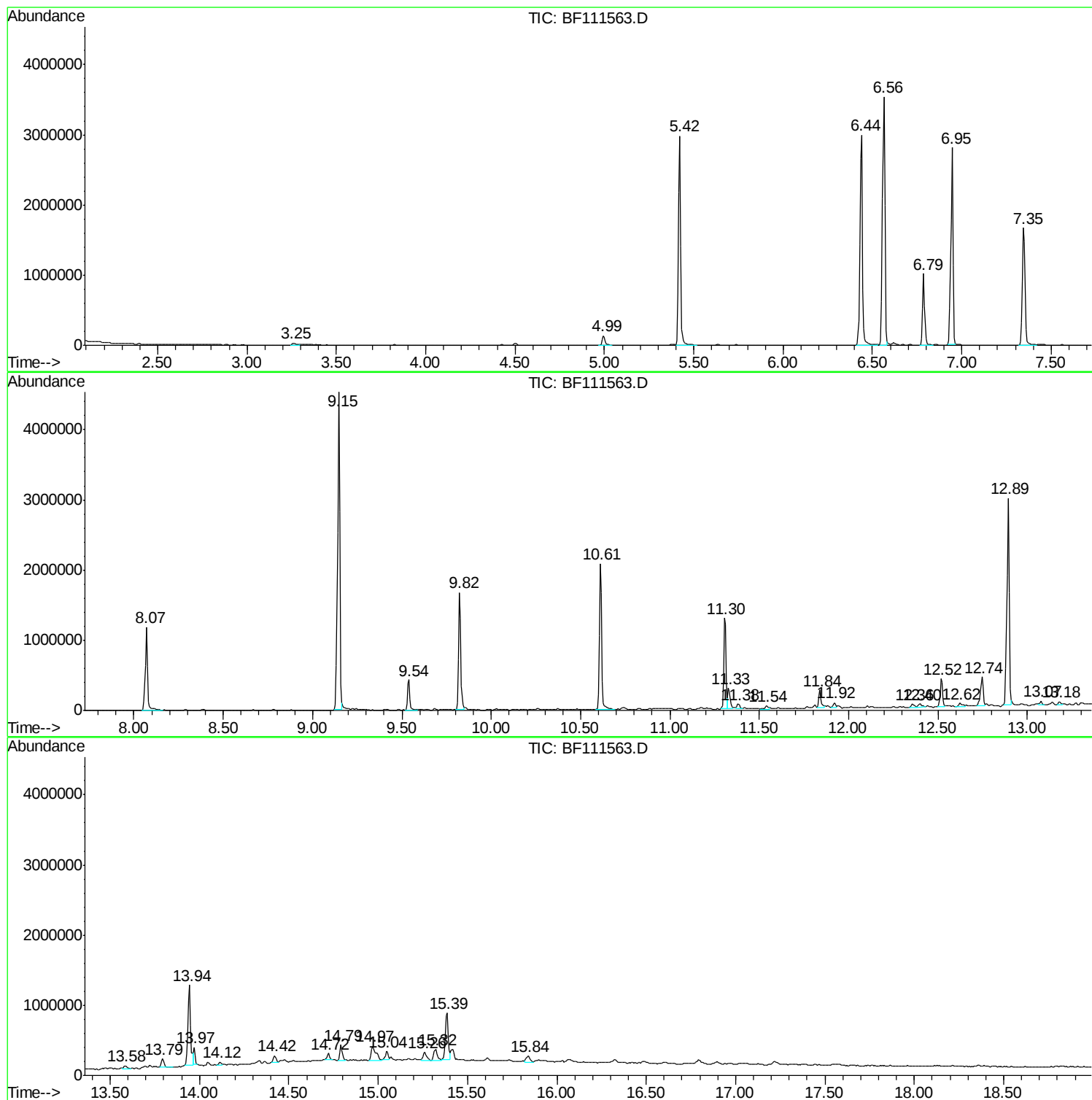
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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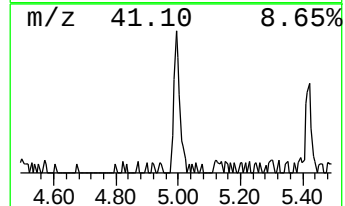
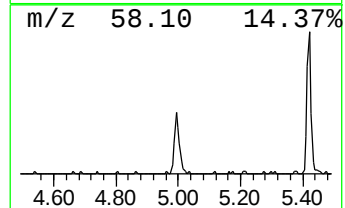
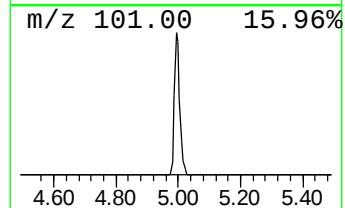
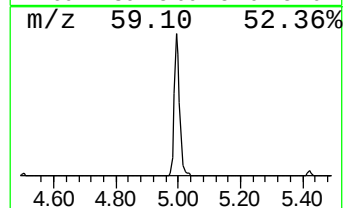
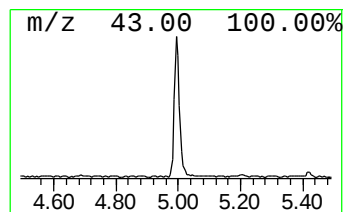
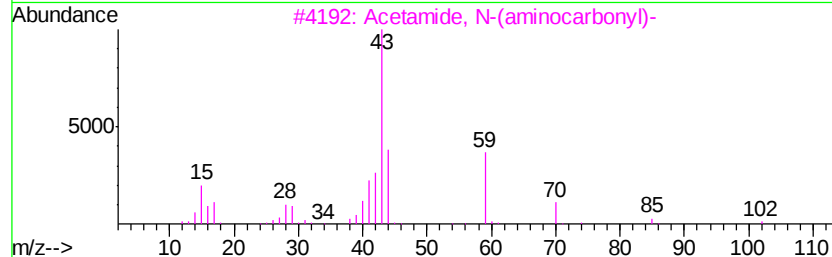
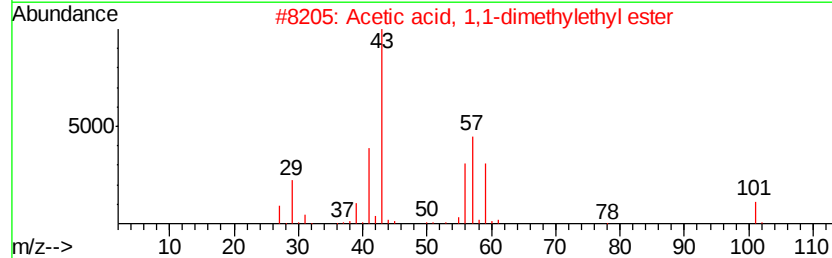
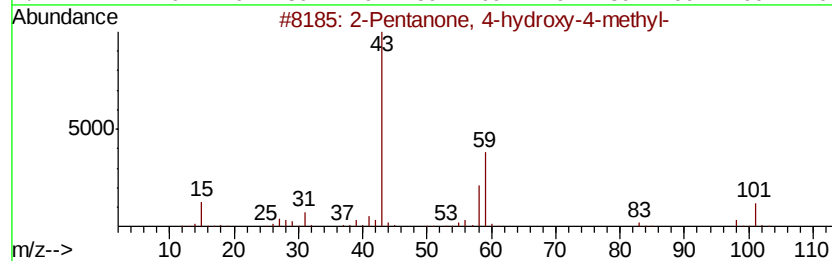
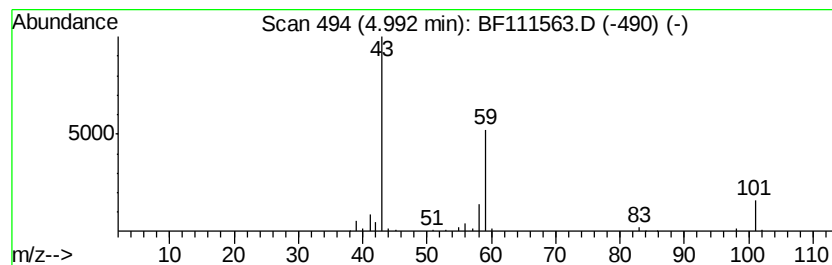
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	4.06 ng	165516	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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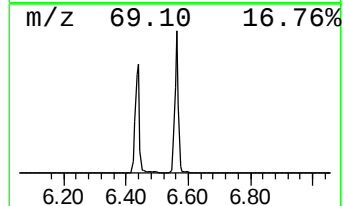
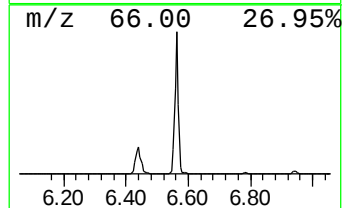
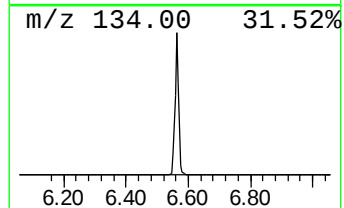
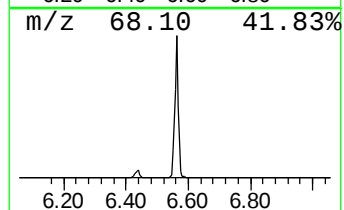
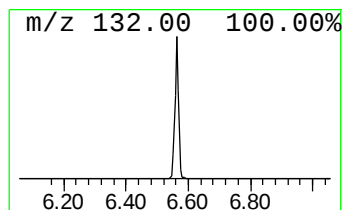
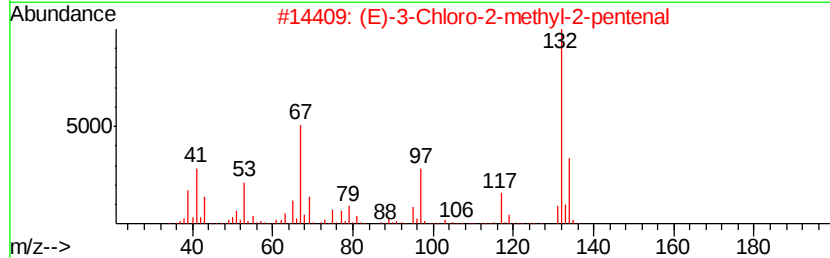
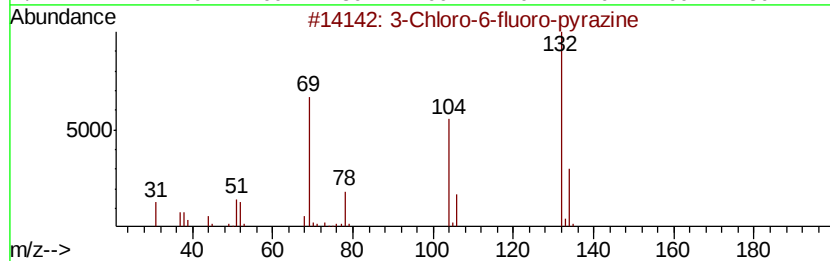
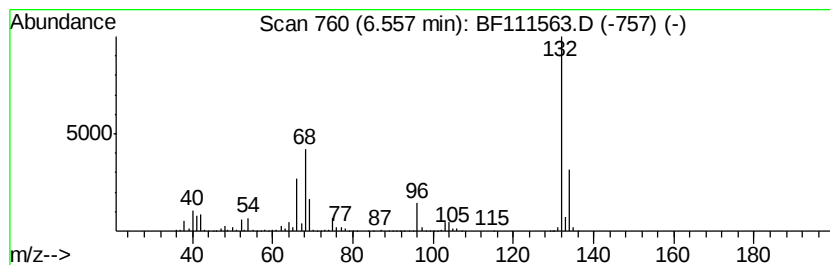
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	73.95 ng	3016470	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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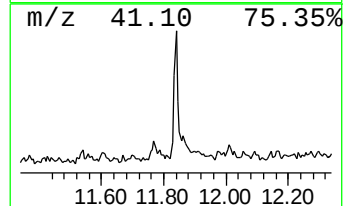
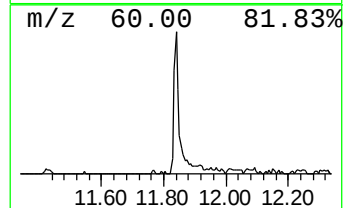
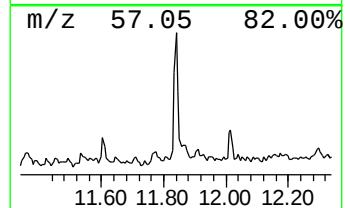
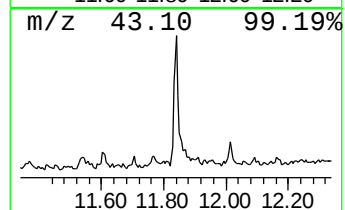
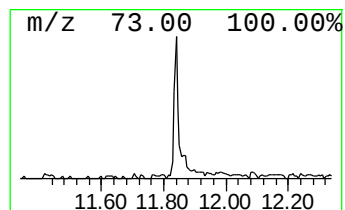
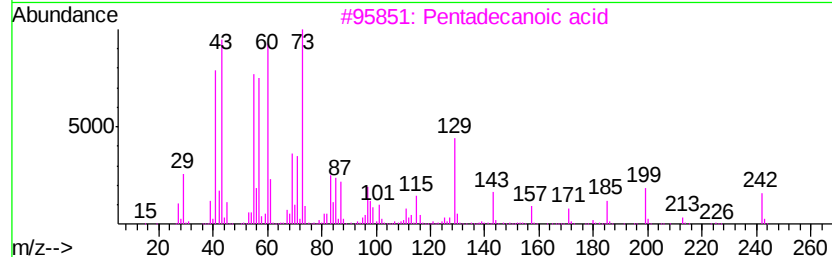
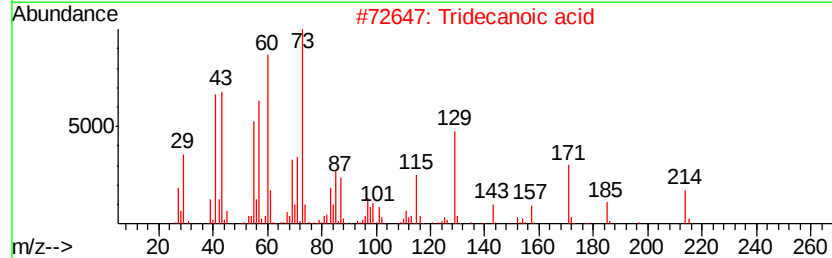
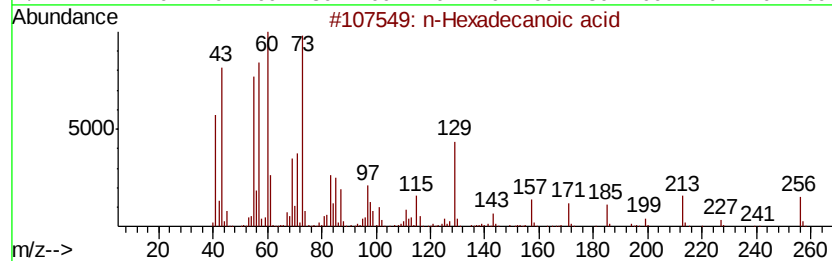
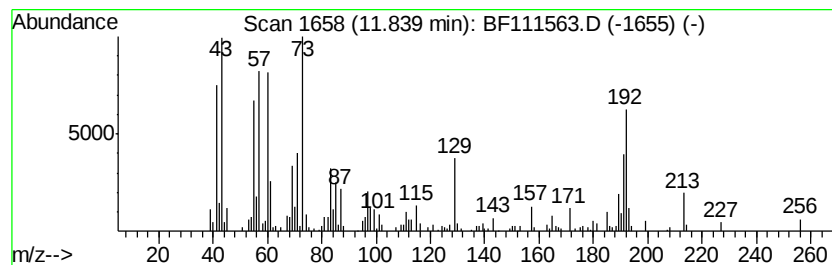
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	3.93 ng	242630	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	70
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4		Anthracene, 9-methyl-	192	C15H12	000779-02-2	56
5		Anthracene, 2-methyl-	192	C15H12	000613-12-7	25



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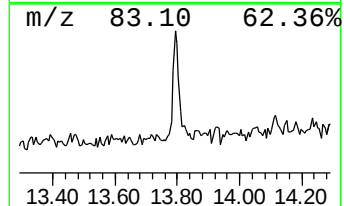
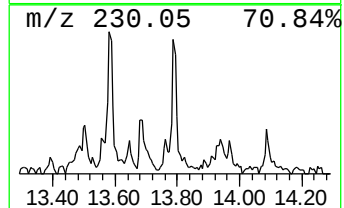
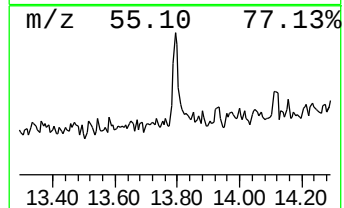
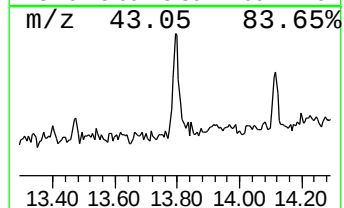
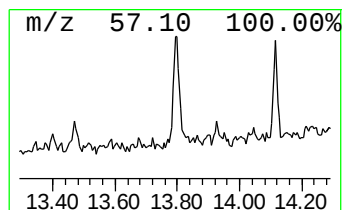
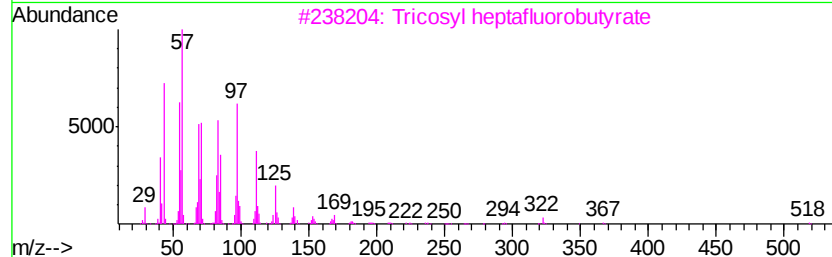
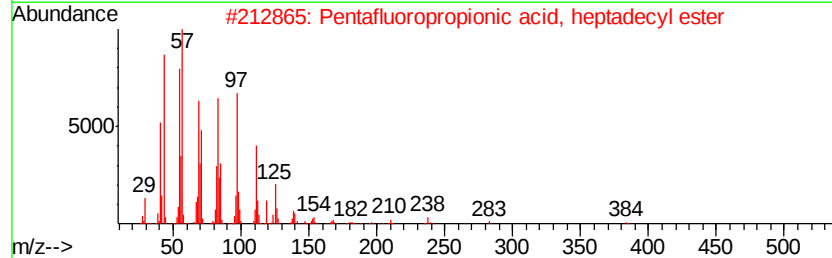
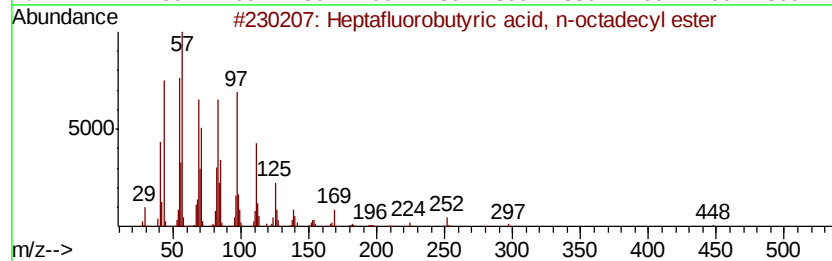
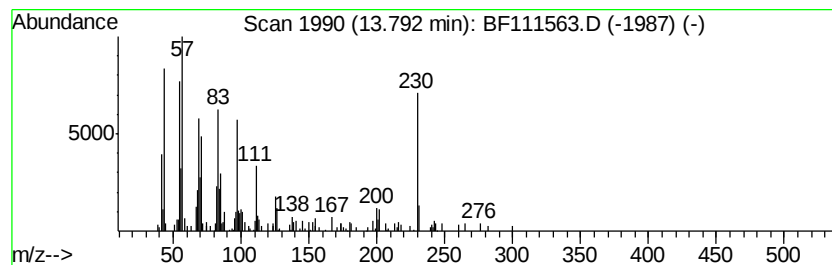
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	2.34 ng	149268	Chrysene-d12	13.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	76
2		Pentafluoropropionic acid, heptafluorobutyl ester	402	C20H35F5O2	959218-78-1	76
3		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	70
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	68
5		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	68



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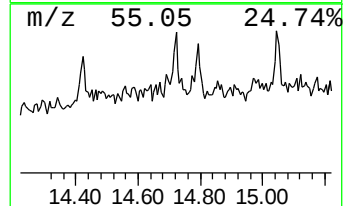
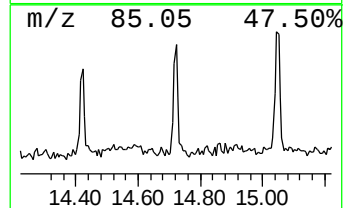
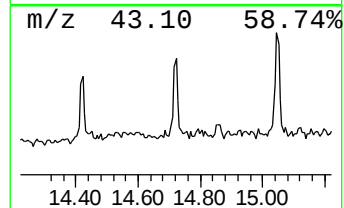
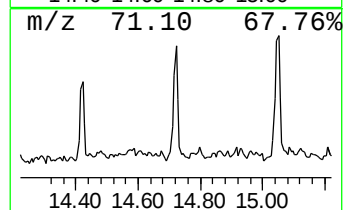
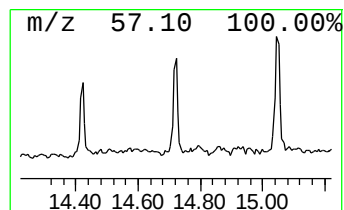
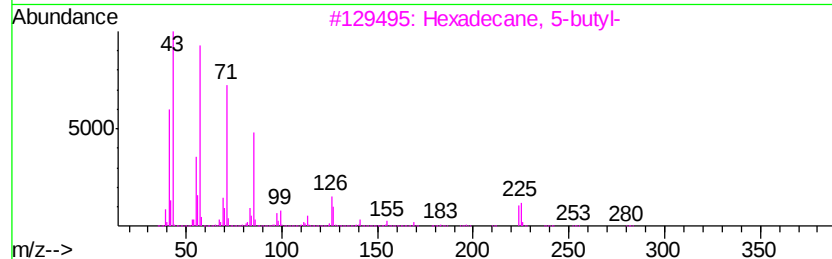
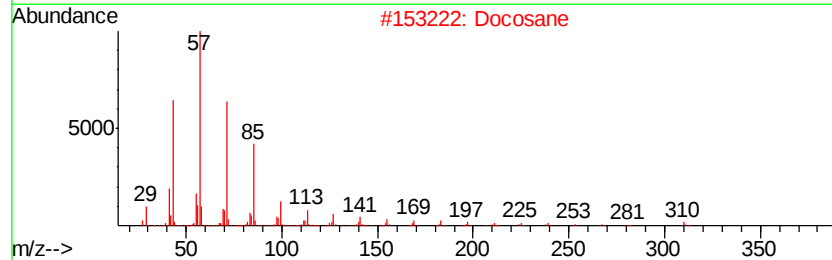
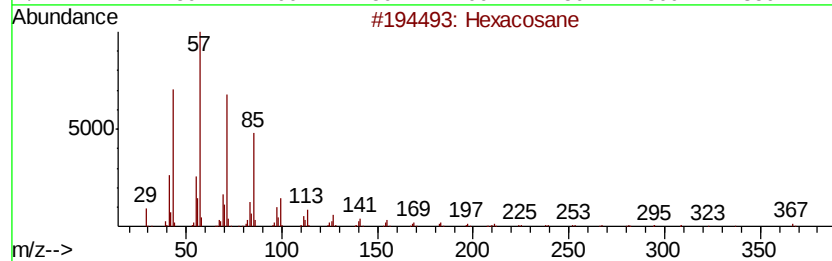
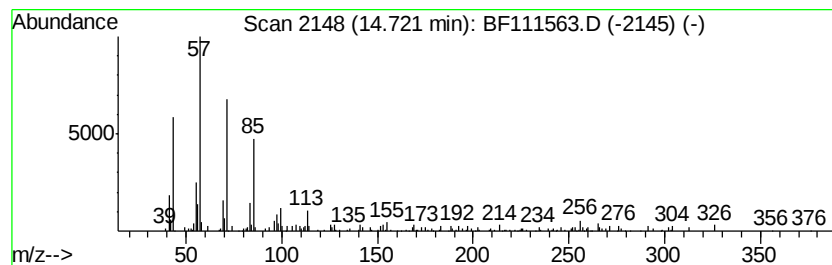
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.14 ng	90105	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	83
2		Docosane	310	C22H46	000629-97-0	80
3		Hexadecane, 5-butyl-	282	C20H42	006912-07-8	80
4		Undecane, 3-methyl-	170	C12H26	001002-43-3	72
5		Octadecane	254	C18H38	000593-45-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111563.D
Acq On : 18 Dec 2018 2:26
Operator : JU/SJ
Sample : J6403-49
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7-A

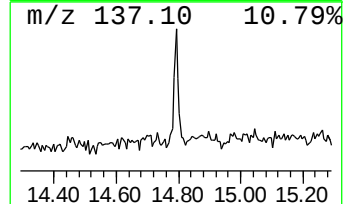
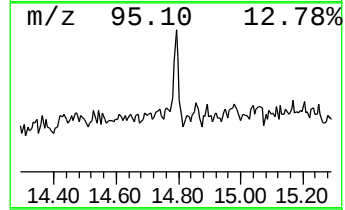
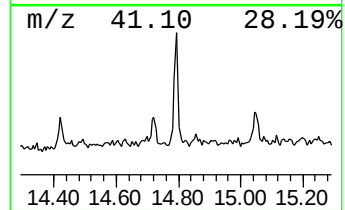
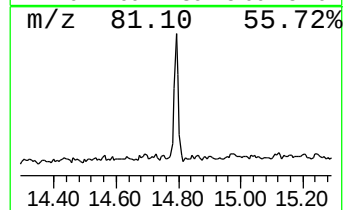
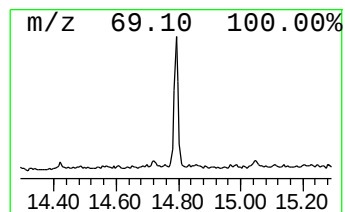
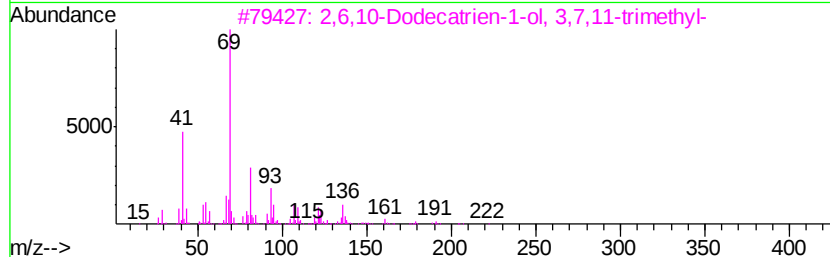
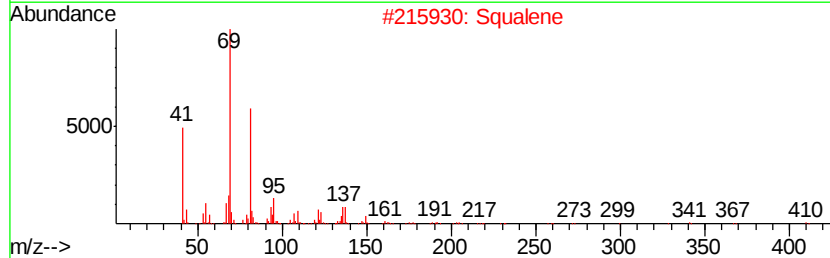
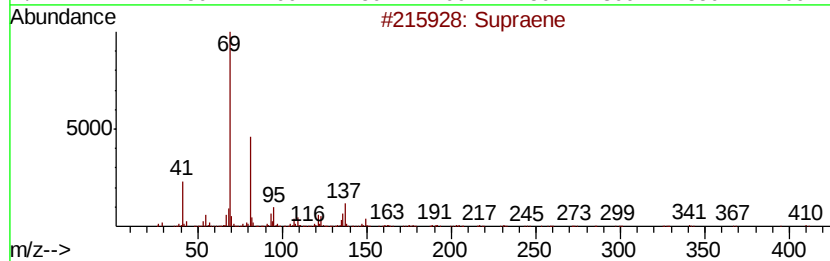
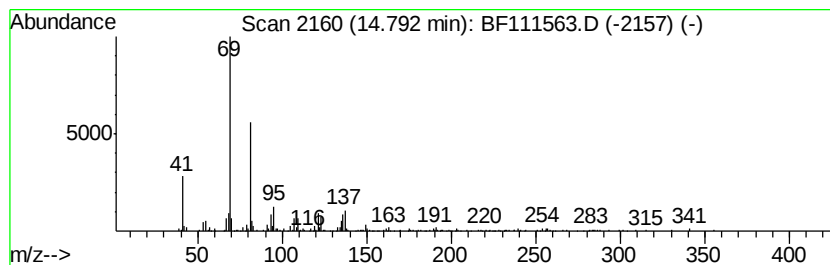
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	4.79 ng	202074	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	90
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	80
4		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58
5		1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111563.D
Acq On : 18 Dec 2018 2:26
Operator : JU/SJ
Sample : J6403-49
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7-A

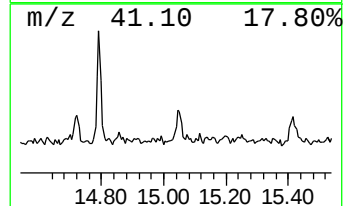
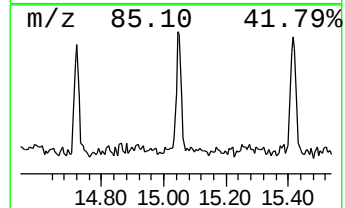
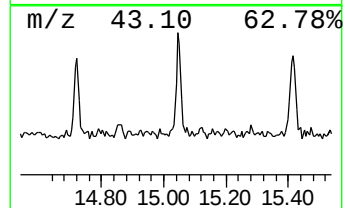
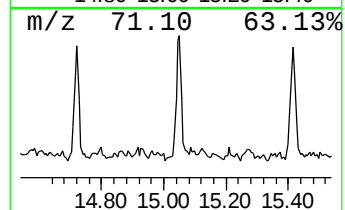
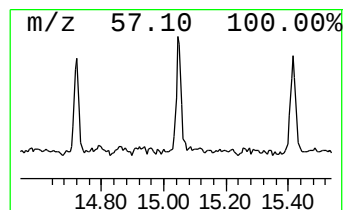
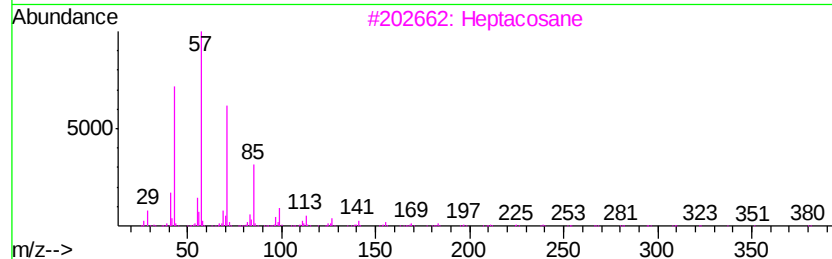
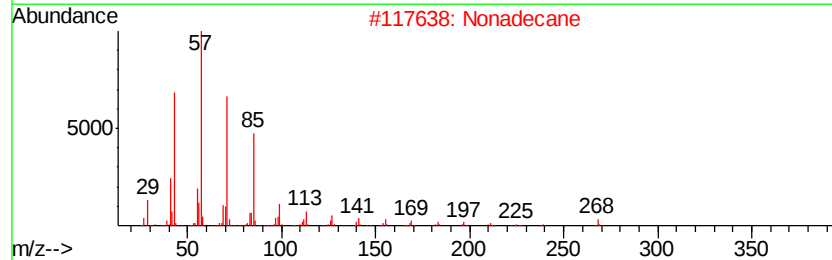
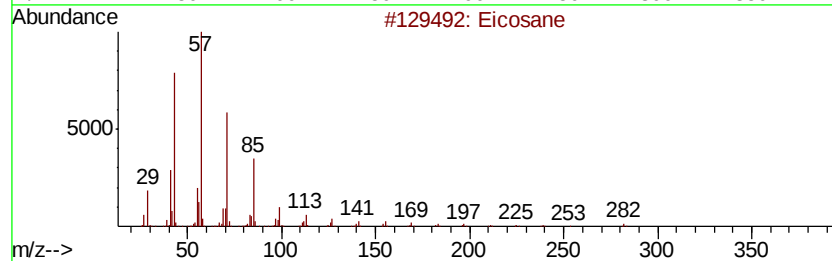
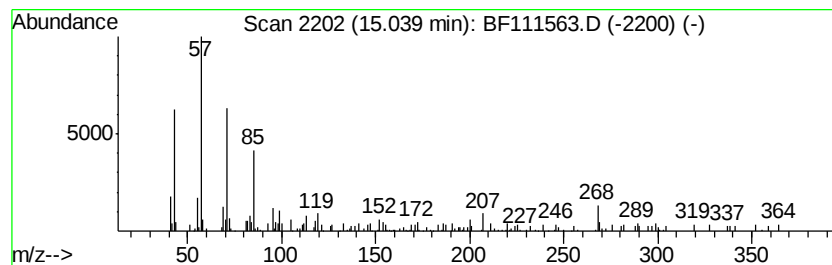
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	2.82 ng	118990	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	90
2		Nonadecane	268	C19H40	000629-92-5	78
3		Heptacosane	380	C27H56	000593-49-7	74
4		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	72
5		Undecane, 3-methyl-	170	C12H26	001002-43-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
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Operator : JU/SJ
Sample : J6403-49
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7-A

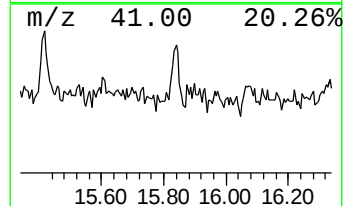
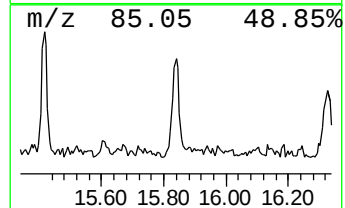
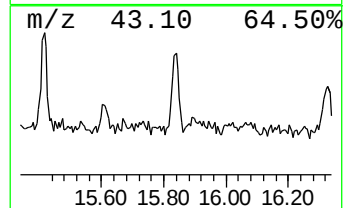
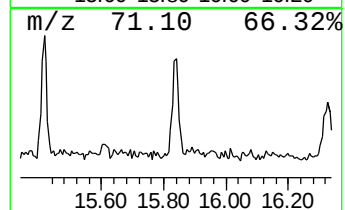
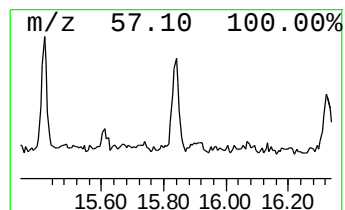
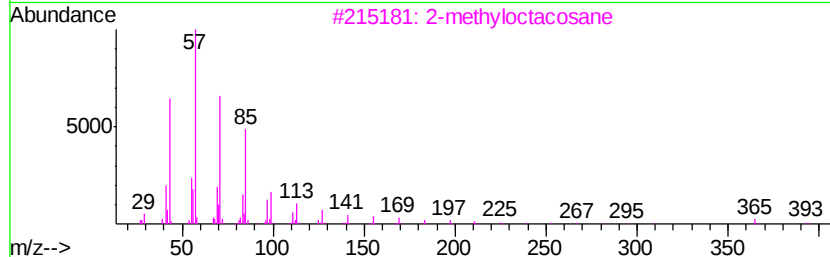
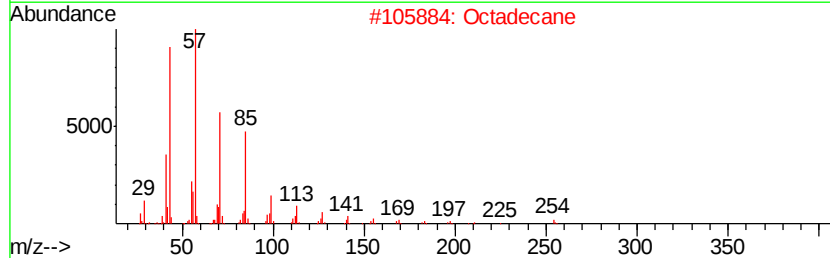
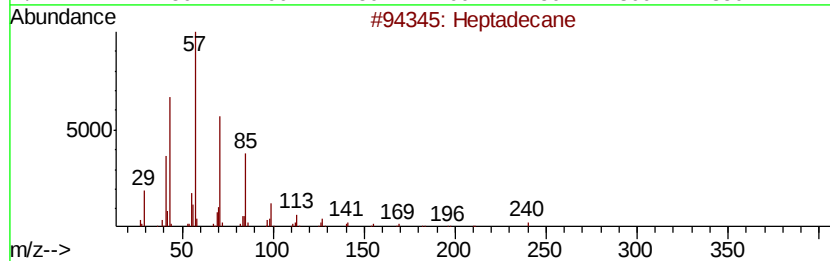
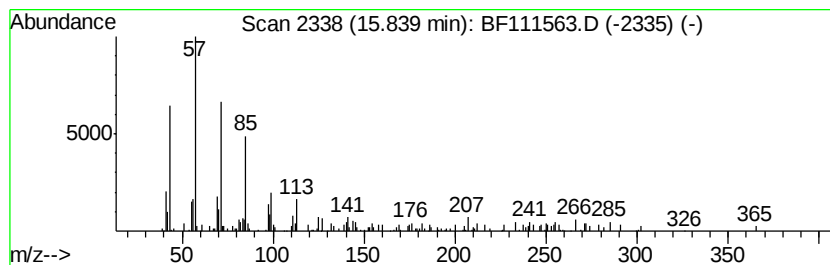
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.86 ng	120394	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	91
2		Octadecane	254	C18H38	000593-45-3	89
3		2-methyloctacosane	408	C29H60	1000376-72-8	68
4		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	64
5		Tetracosane	338	C24H50	000646-31-1	64



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Sample : J6403-49
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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...	4.99	4.1 ng		165516	1	6.79	815844	20.0
unknown6.56	6.56	74.0 ng		3016470	1	6.79	815844	20.0
n-Hexadecanoic acid	11.84	3.9 ng		242630	4	11.30	1233230	20.0
Heptafluorobutyri...	13.79	2.3 ng		149268	5	13.94	1276340	20.0
Hexacosane	14.72	2.1 ng		90105	6	15.39	843375	20.0
Supraene	14.79	4.8 ng		202074	6	15.39	843375	20.0
Eicosane	15.04	2.8 ng		118990	6	15.39	843375	20.0
Heptadecane	15.84	2.9 ng		120394	6	15.39	843375	20.0