

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
 Data File : BF117734.D
 Acq On : 8 Nov 2019 16:43
 Operator : JU
 Sample : K5722-14
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2-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-BF110619.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	2.228	19	24	30	rVB	1406219	1867498	22.19%	2.215%
2	5.151	515	521	527	rVB	1307063	1646361	19.56%	1.953%
3	5.545	582	588	591	rBV	6676772	6900362	82.00%	8.186%
4	6.545	752	758	763	rBV	6331077	7626072	90.62%	9.047%
5	6.698	779	784	787	rBV	7370449	7513405	89.28%	8.913%
6	6.928	819	823	826	rBV	2647575	2069297	24.59%	2.455%
7	7.087	846	850	853	rVB	6569217	5740718	68.22%	6.810%
8	7.486	913	918	921	rBV	4617684	4822318	57.30%	5.721%
9	8.216	1037	1042	1045	rBV	3287934	2824510	33.56%	3.351%
10	9.292	1220	1225	1228	rBV	8662278	8415361	100.00%	9.983%
11	9.686	1288	1292	1296	rBV	988589	956481	11.37%	1.135%
12	9.792	1306	1310	1313	rBV5	72021	103362	1.23%	0.123%
13	9.839	1315	1318	1321	rBV2	110121	172245	2.05%	0.204%
14	9.892	1324	1327	1331	rVB2	156042	159558	1.90%	0.189%
15	9.975	1337	1341	1345	rVB	3860547	3434174	40.81%	4.074%
16	10.233	1383	1385	1388	rBV3	134987	162237	1.93%	0.192%
17	10.298	1393	1396	1397	rBV2	92631	98353	1.17%	0.117%
18	10.392	1409	1412	1416	rBV2	195141	215172	2.56%	0.255%
19	10.633	1450	1453	1456	rVB	485895	445982	5.30%	0.529%
20	10.769	1471	1476	1479	rBV	5762347	5732943	68.12%	6.801%
21	10.898	1494	1498	1501	rBV	1938762	1845562	21.93%	2.189%
22	11.369	1575	1578	1582	rVB	1517636	1417656	16.85%	1.682%
23	11.469	1592	1595	1598	rBV	3448212	3214756	38.20%	3.814%
24	11.998	1682	1685	1688	rVB2	1091799	978563	11.63%	1.161%
25	13.063	1862	1866	1869	rBV	6312237	6587306	78.28%	7.815%
26	13.957	2015	2018	2025	rVB2	1520041	1706649	20.28%	2.025%
27	14.115	2042	2045	2048	rVB	2249465	2289121	27.20%	2.716%
28	14.986	2190	2193	2202	rVB	394573	475406	5.65%	0.564%
29	15.174	2222	2225	2235	rVB	414096	811699	9.65%	0.963%
30	15.257	2237	2239	2242	rVB	208701	214886	2.55%	0.255%
31	15.492	2276	2279	2285	rVB	232085	291176	3.46%	0.345%
32	15.551	2287	2289	2294	rVV	164527	197430	2.35%	0.234%
33	15.621	2297	2301	2305	rVV	1733850	2226598	26.46%	2.641%
34	15.657	2305	2307	2314	rVB2	298723	422545	5.02%	0.501%

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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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 >
Peak separation: 5

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35	16.121	2382	2386	2391	rBV	178207	267769	3.18%	0.318%
36	16.656	2474	2477	2488	rVB3	130201	244064	2.90%	0.290%
37	17.139	2555	2559	2565	rVB2	103848	196462	2.33%	0.233%

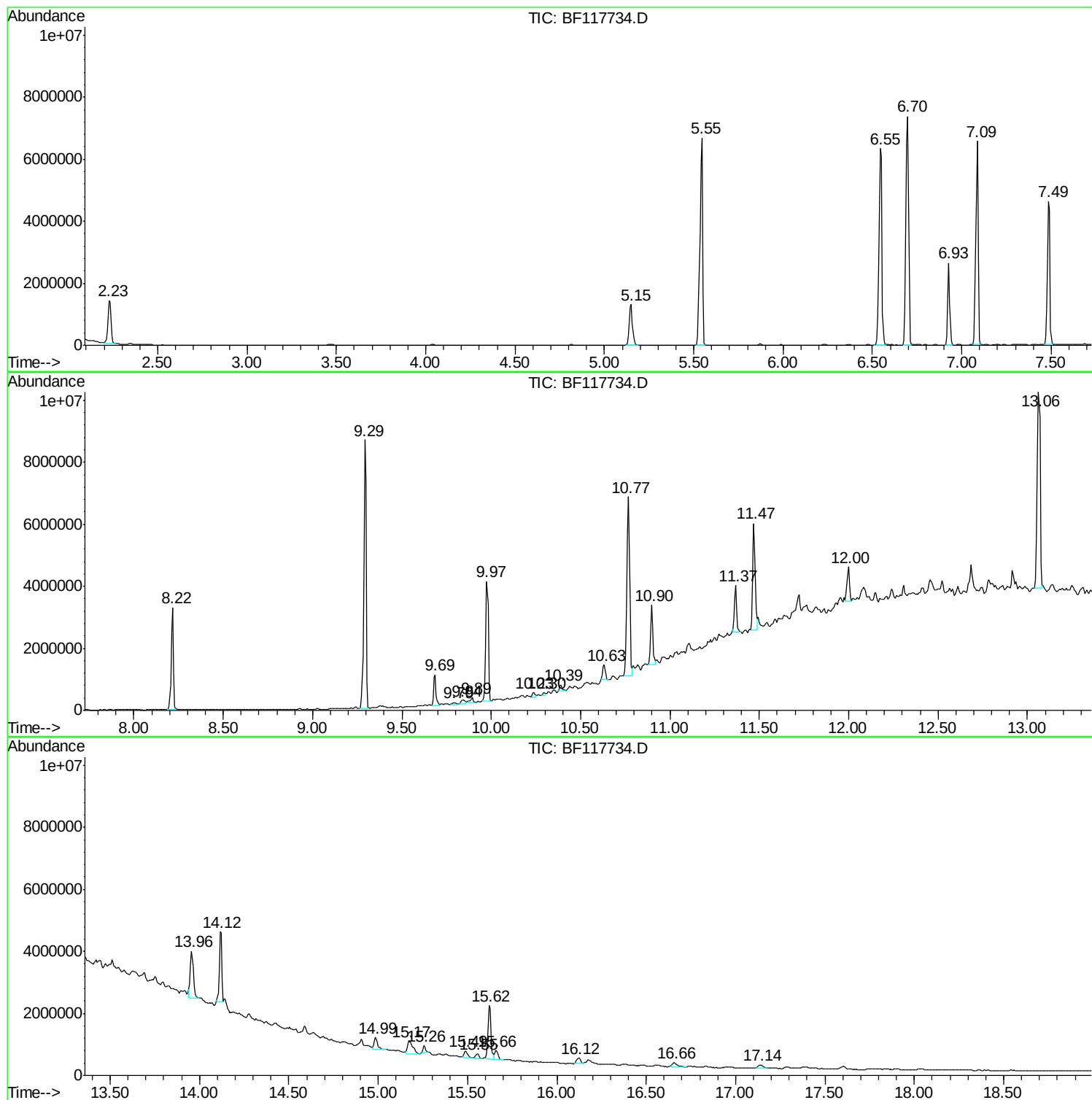
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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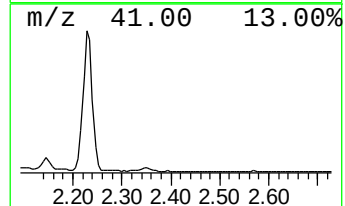
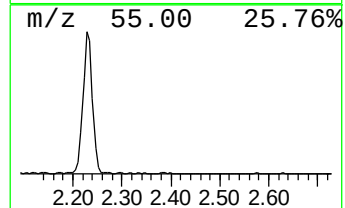
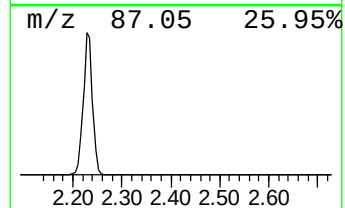
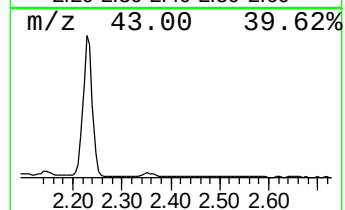
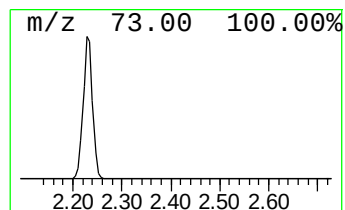
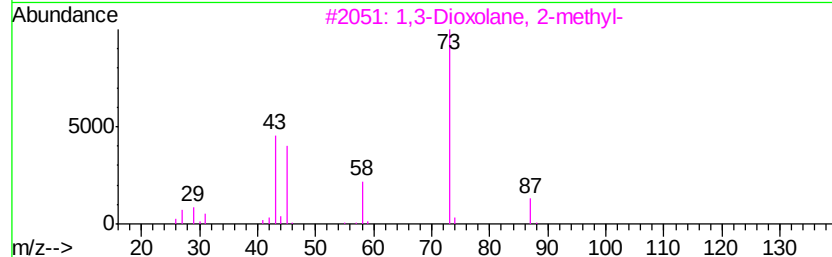
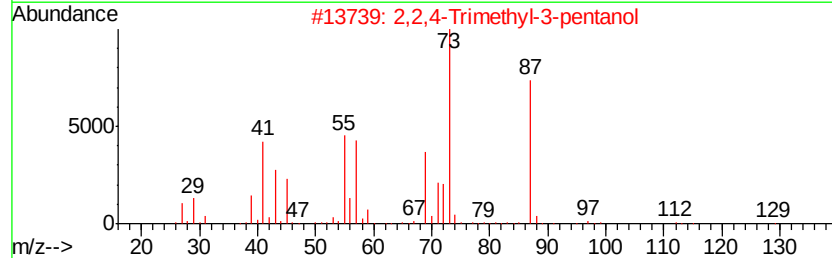
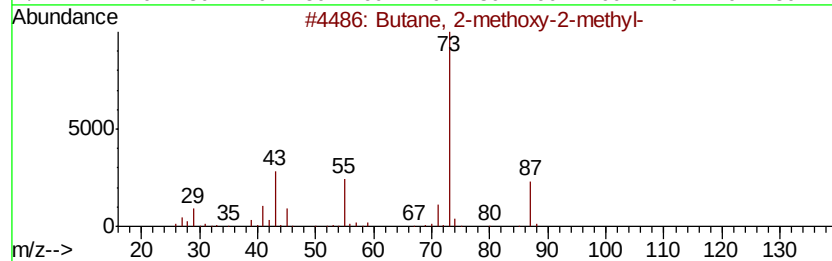
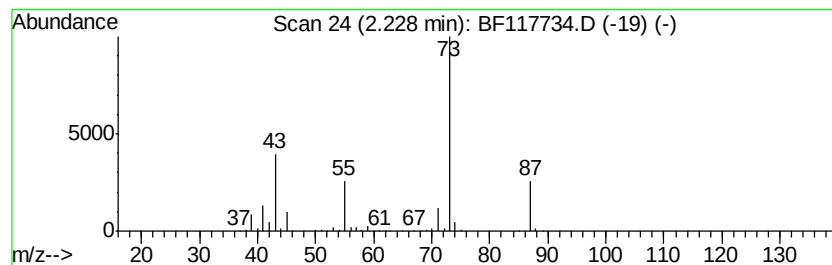
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	18.05 ng	1867500	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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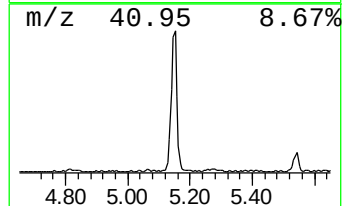
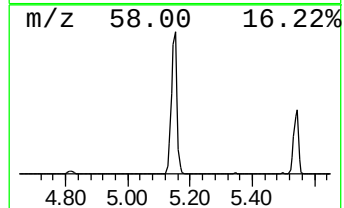
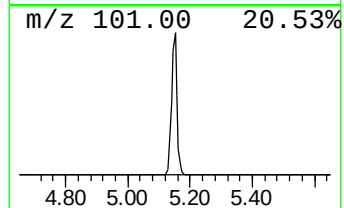
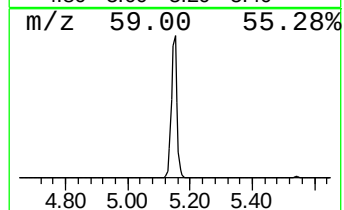
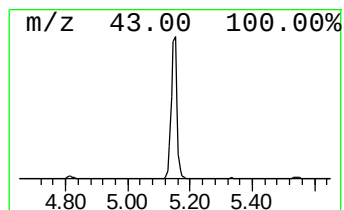
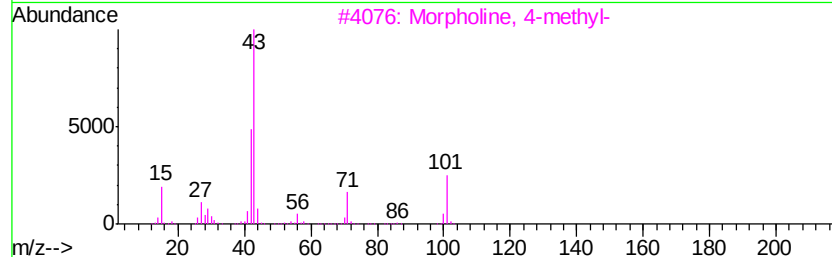
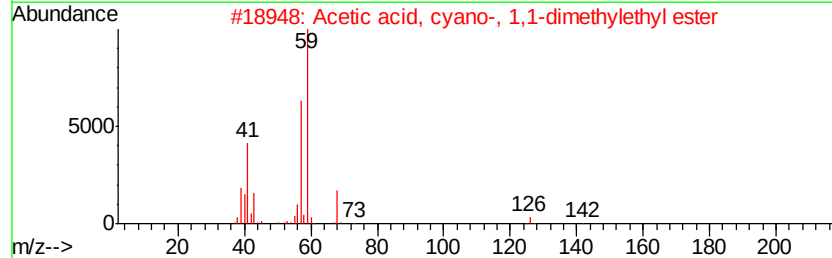
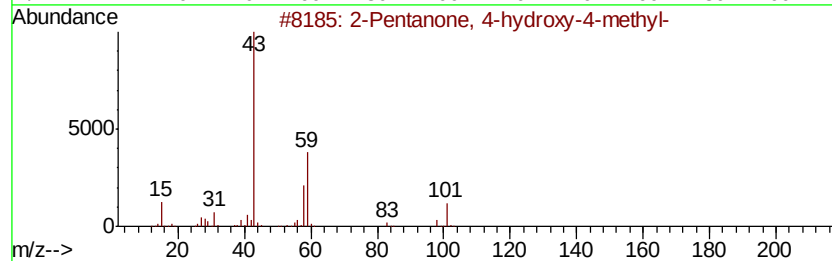
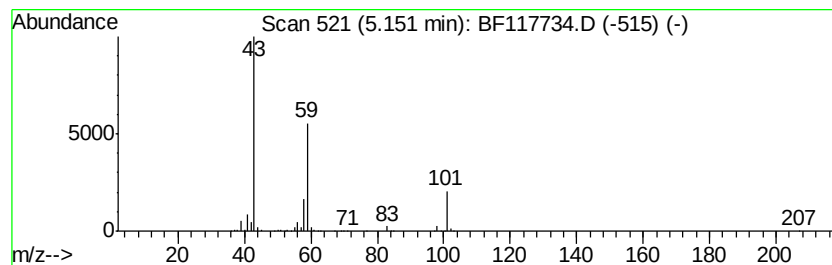
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	15.91 ng	1646360	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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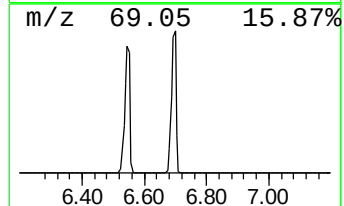
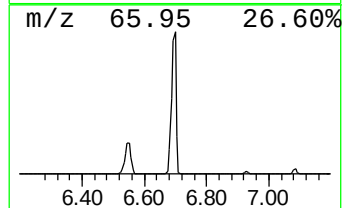
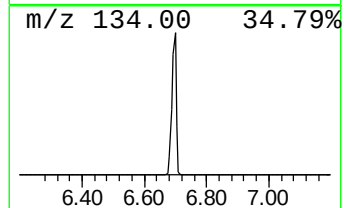
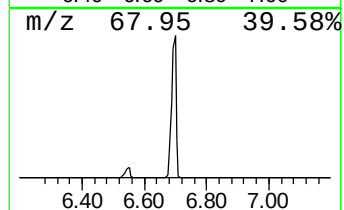
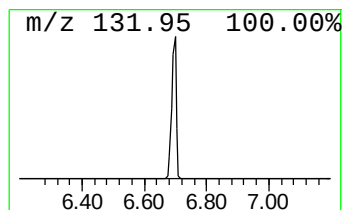
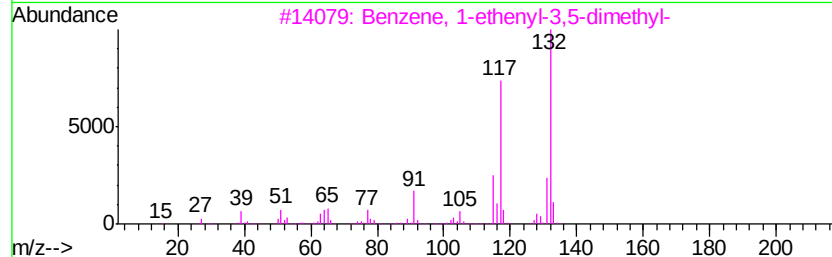
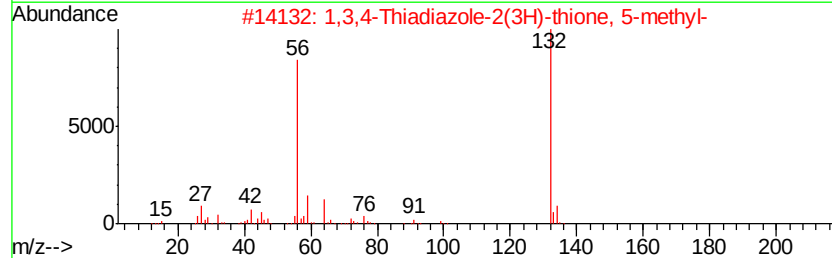
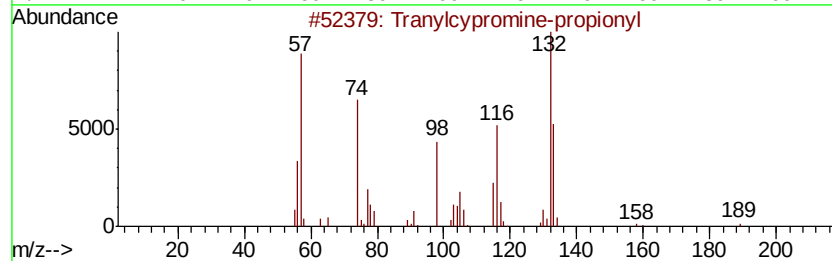
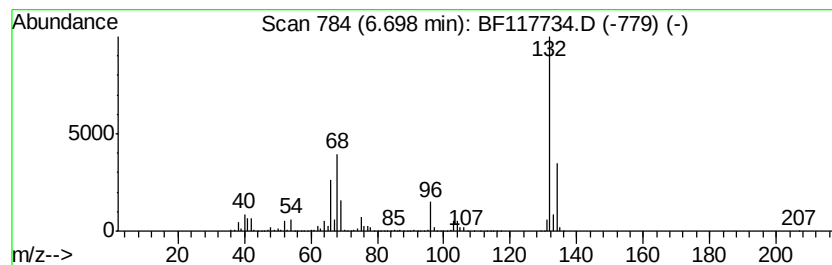
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	72.62 ng	7513410	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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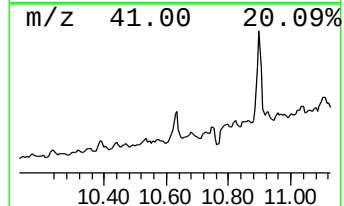
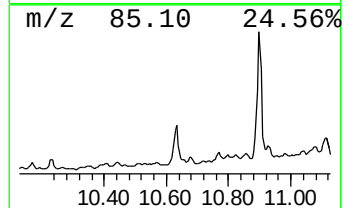
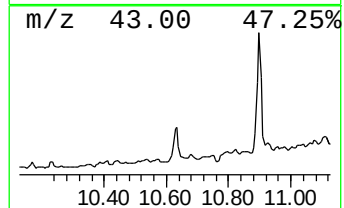
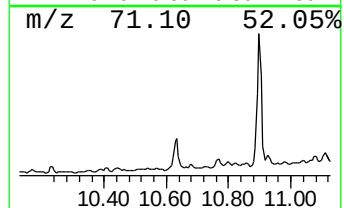
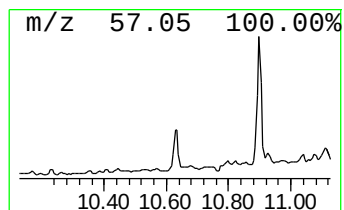
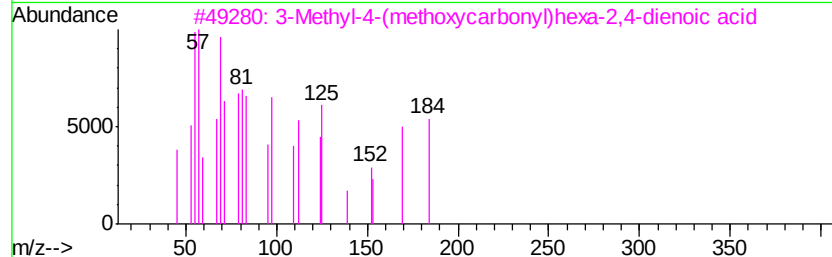
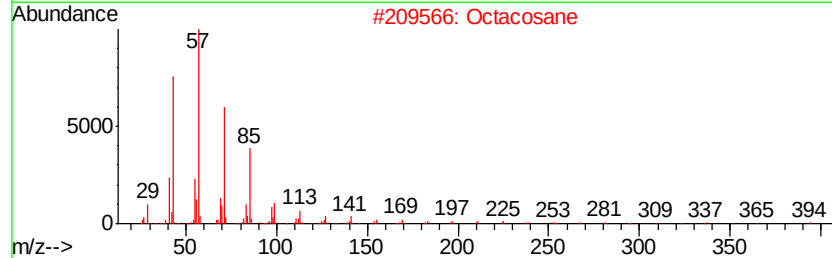
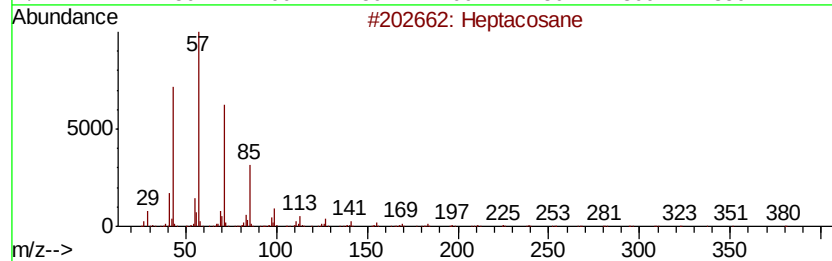
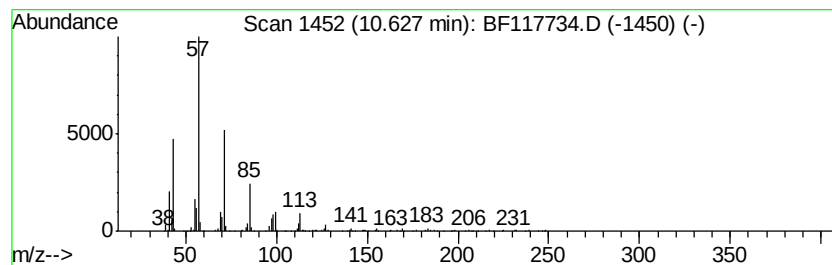
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.60 ng	445982	Acenaphthene-d10	9.97
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane		380 C27H56	000593-49-7 91
2	Octacosane		394 C28H58	000630-02-4 87
3	3-Methyl-4-(methoxycarbonyl)hexa...		184 C9H12O4	1000104-10-8 86
4	Octadecane		254 C18H38	000593-45-3 86
5	Hexadecane		226 C16H34	000544-76-3 86



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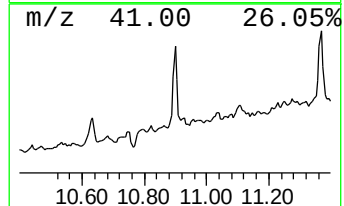
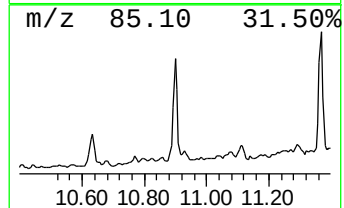
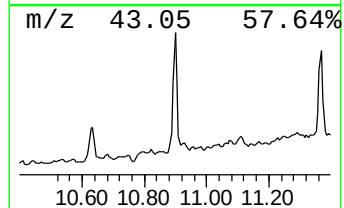
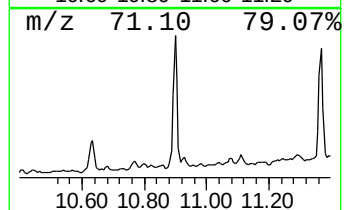
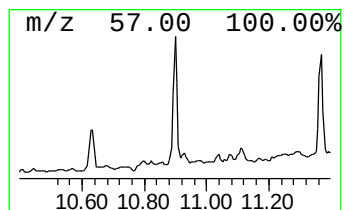
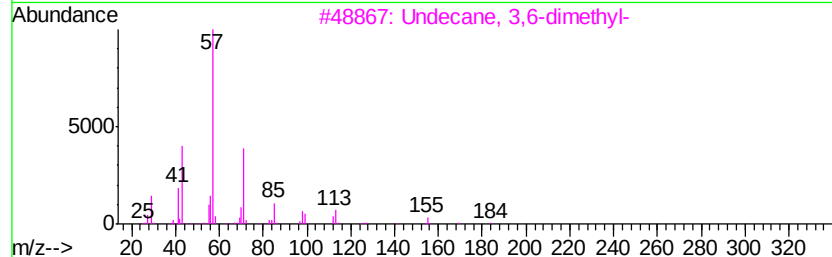
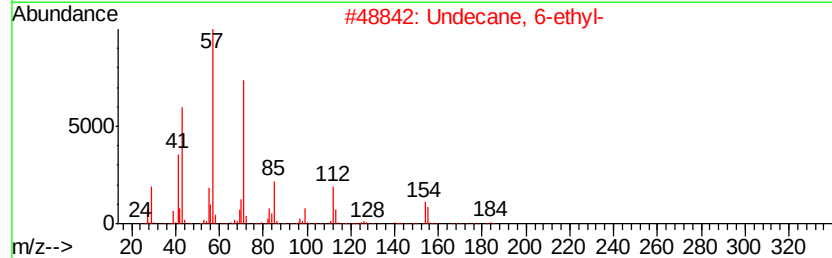
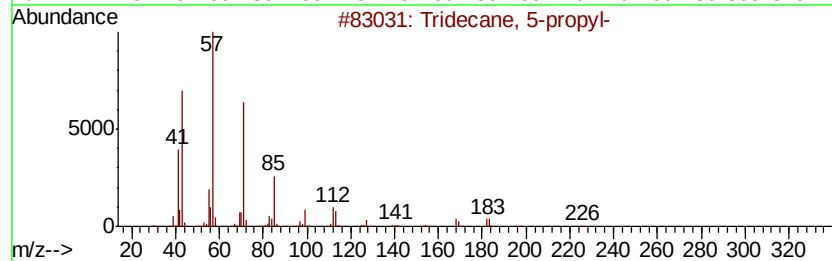
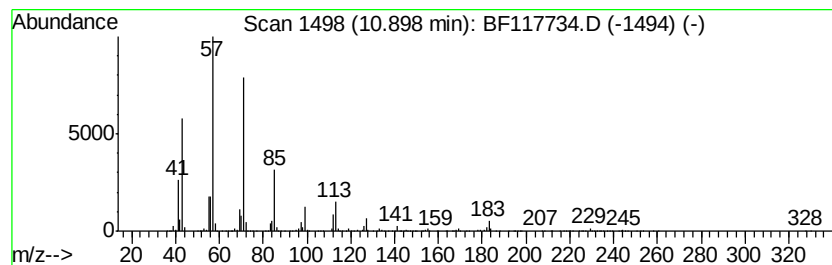
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tridecane, 5-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.90	11.48 ng	1845560	Phenanthrene-d10		11.47	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane,	5-propyl-	226	C16H34	055045-11-9	90
2	Undecane,	6-ethyl-	184	C13H28	017312-60-6	83
3	Undecane,	3,6-dimethyl-	184	C13H28	017301-28-9	81
4	Nonane,	3,7-dimethyl-	156	C11H24	017302-32-8	81
5	Dodecane,	2,7,10-trimethyl-	212	C15H32	074645-98-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
Data File : BF117734.D
Acq On : 8 Nov 2019 16:43
Operator : JU
Sample : K5722-14
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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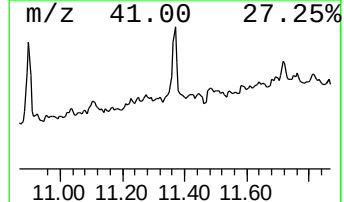
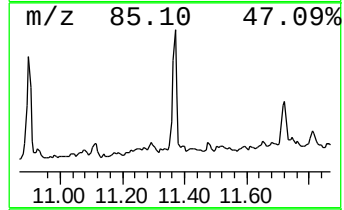
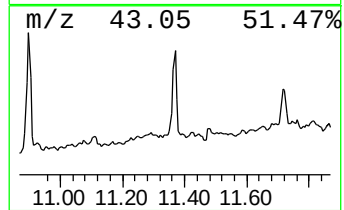
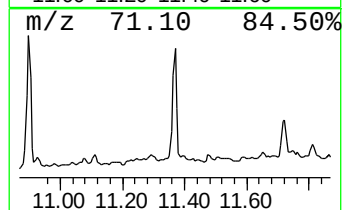
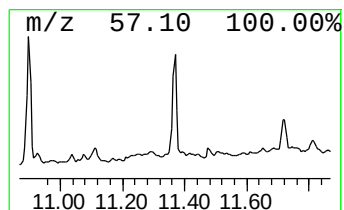
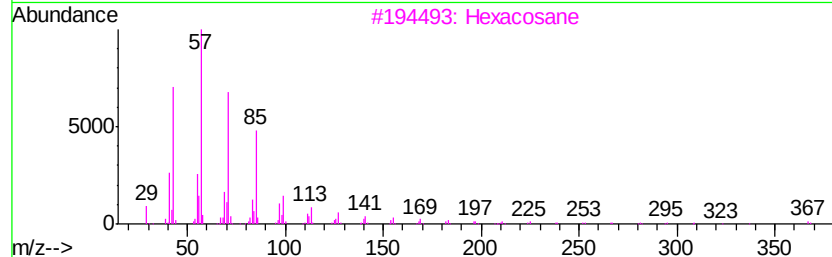
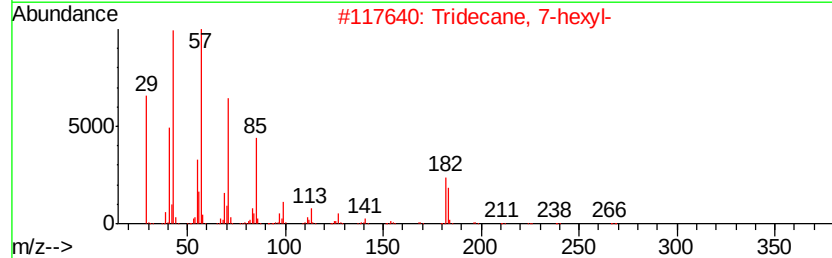
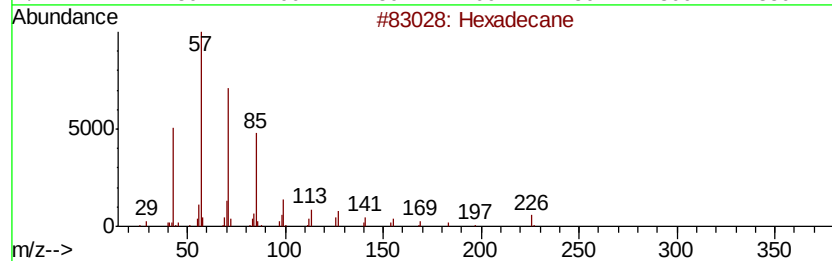
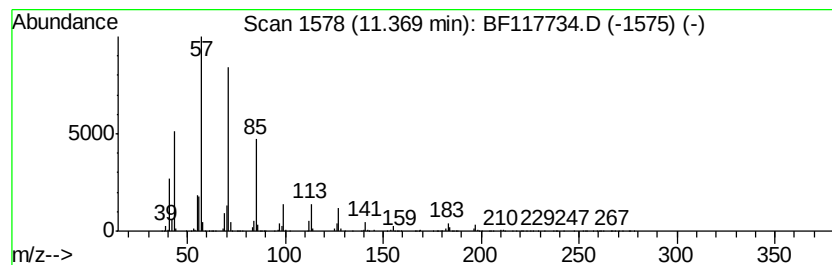
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.37	8.82 ng	1417660	Phenanthrene-d10	11.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	91
2		Tridecane, 7-hexyl-	268	C19H40	007225-66-3	90
3		Hexacosane	366	C26H54	000630-01-3	90
4		Pentadecane	212	C15H32	000629-62-9	87
5		Tridecane	184	C13H28	000629-50-5	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
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Acq On : 8 Nov 2019 16:43
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ALS Vial : 7 Sample Multiplier: 1

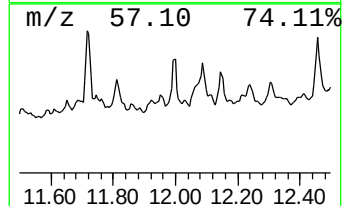
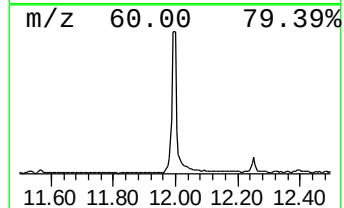
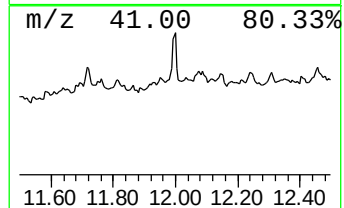
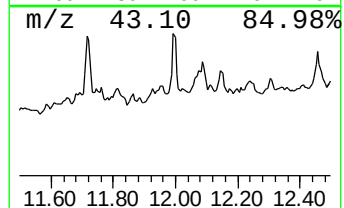
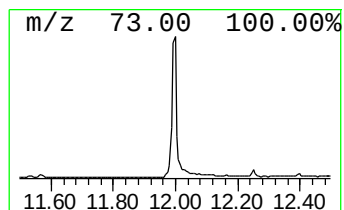
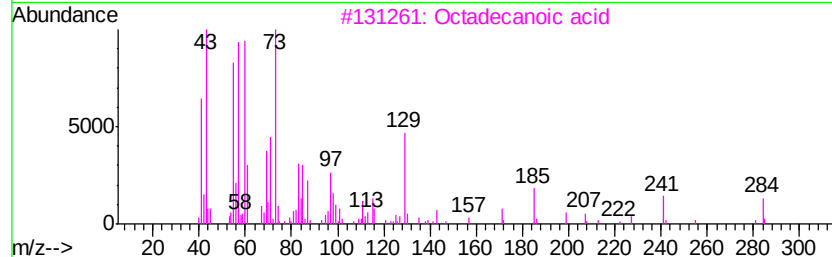
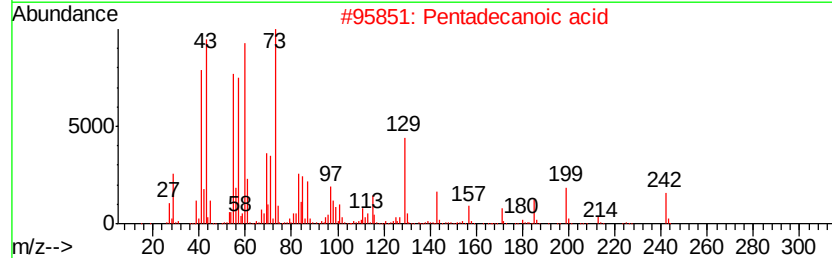
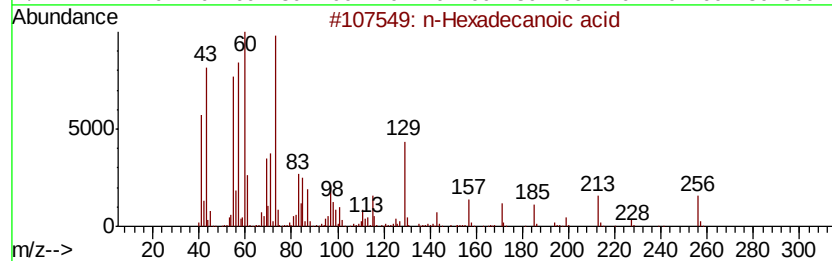
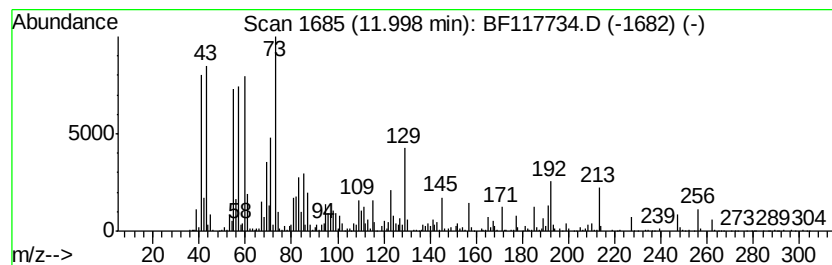
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.00	6.09 ng	978563	Phenanthrene-d10	11.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Octadecanoic acid	284	C18H36O2	000057-11-4	62
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Benzamide, 4-butoxy-N-[2-(2-thie...	303	C17H21NO2S	1000319-87-5	41



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
Data File : BF117734.D
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Sample : K5722-14
Misc :
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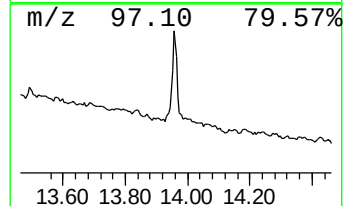
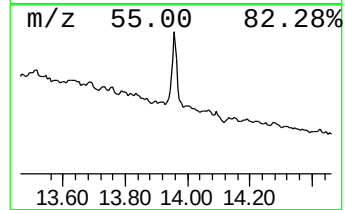
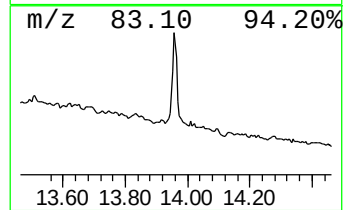
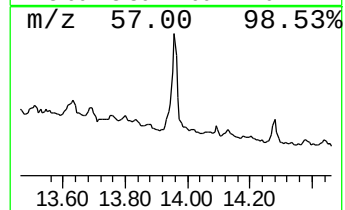
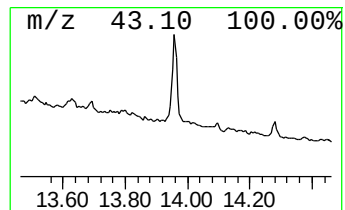
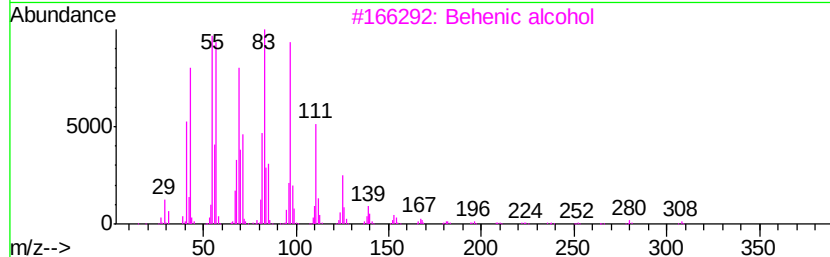
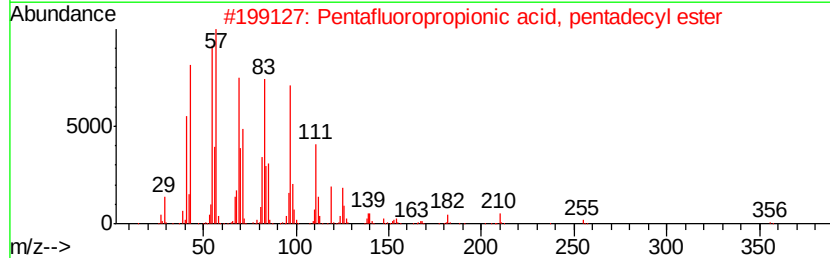
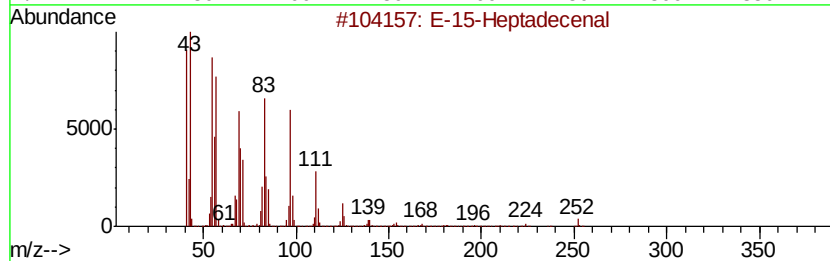
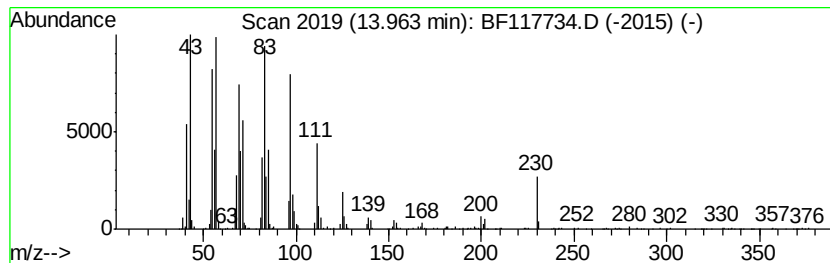
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	14.91 ng	1706650	Chrysene-d12	14.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	E-15-Heptadecenal	252 C17H32O	1000130-97-9	97
2	Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1	94
3	Behenic alcohol	326 C22H46O	000661-19-8	94
4	Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5	94
5	1-Heneicosanol	312 C21H44O	015594-90-8	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
Data File : BF117734.D
Acq On : 8 Nov 2019 16:43
Operator : JU
Sample : K5722-14
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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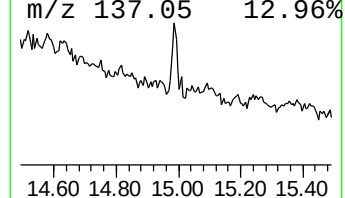
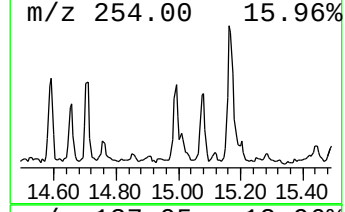
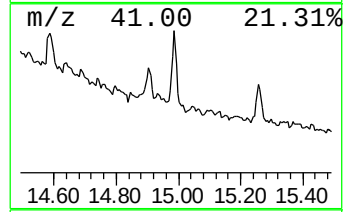
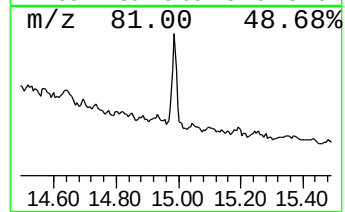
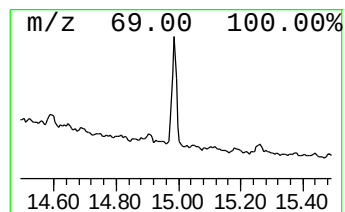
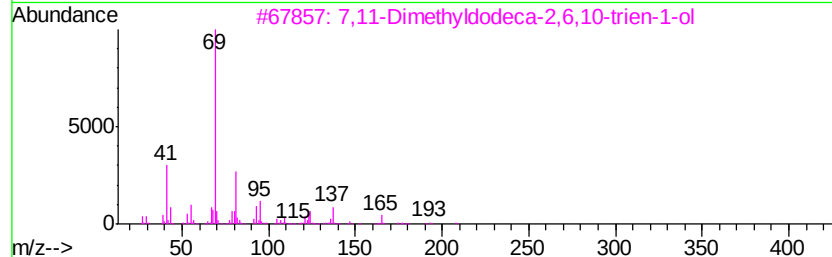
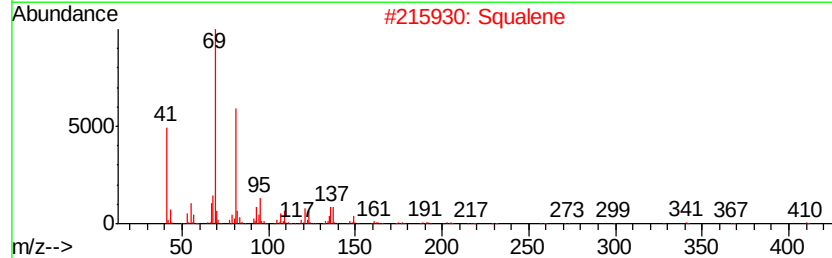
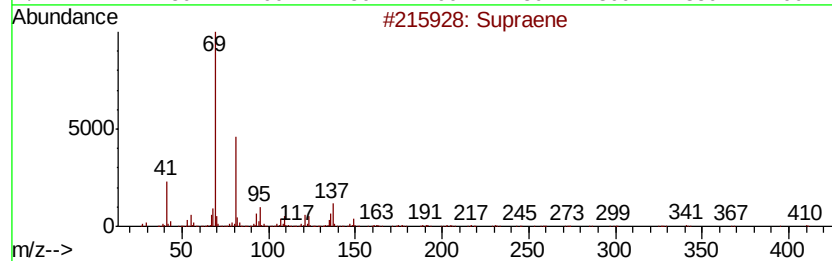
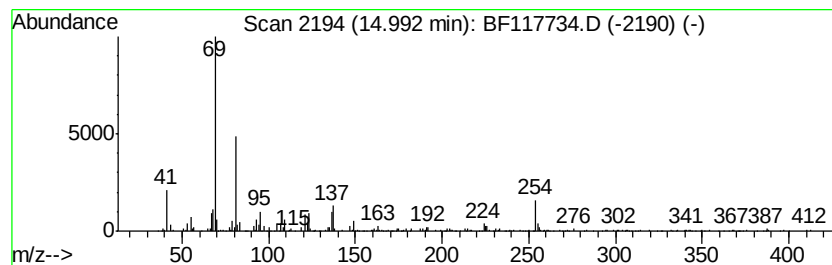
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	4.27 ng	475406	Perylene-d12	15.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	98
2		Squalene	410	C30H50	000111-02-4	92
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4		6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	72
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
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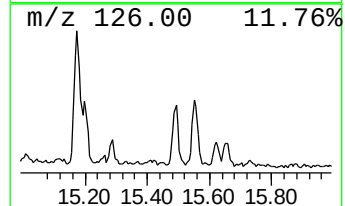
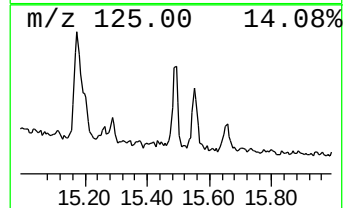
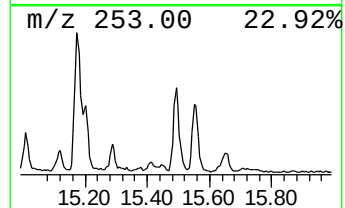
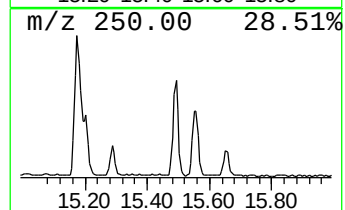
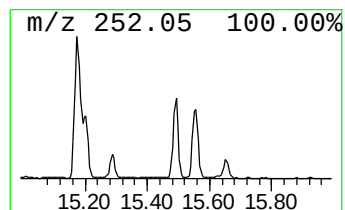
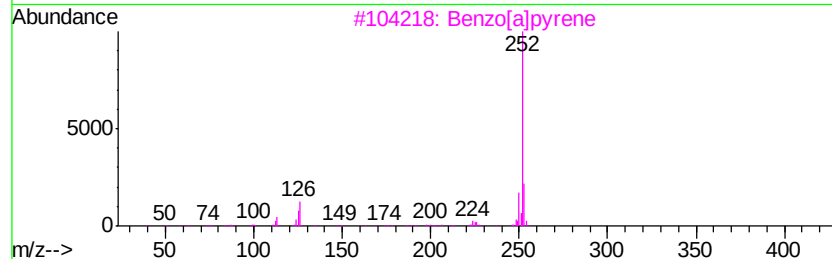
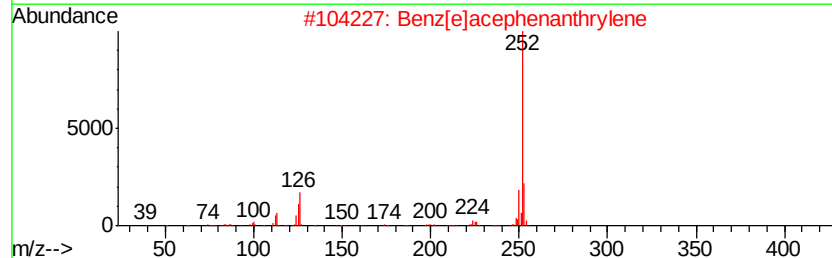
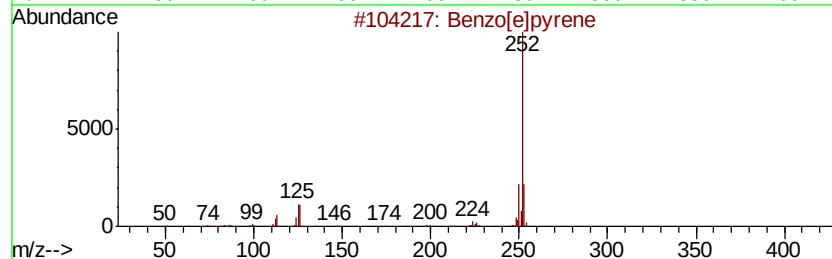
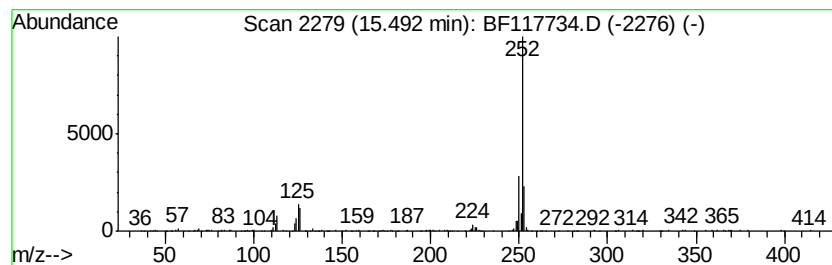
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.49	2.62 ng	291176	Perylene-d12	15.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[el]pyrene	252	C20H12	000192-97-2	98
2	Benzo[el]acephenanthrylene	252	C20H12	000205-99-2	96
3	Benzo[al]pyrene	252	C20H12	000050-32-8	95
4	Benzo[i]lfluoranthene	252	C20H12	000205-82-3	93
5	Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
Data File : BF117734.D
Acq On : 8 Nov 2019 16:43
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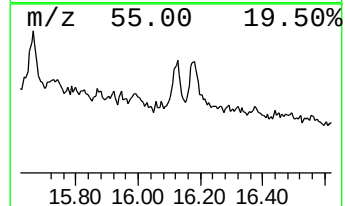
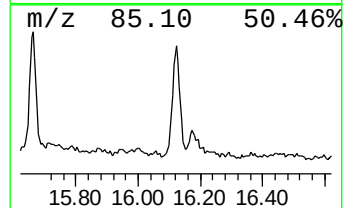
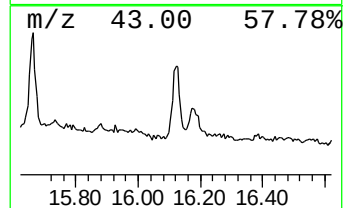
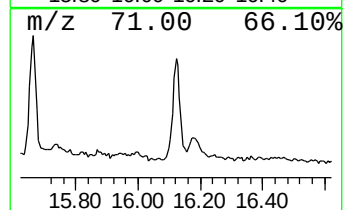
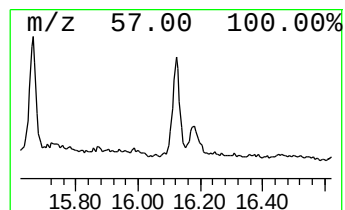
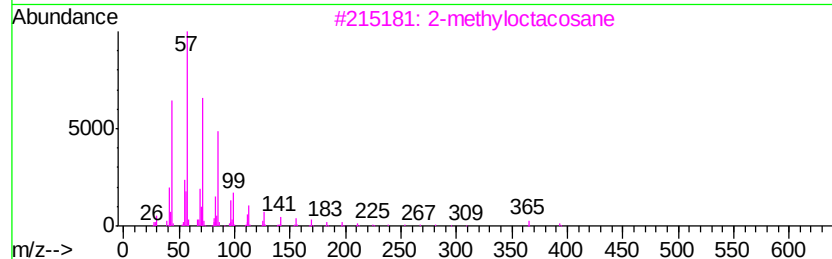
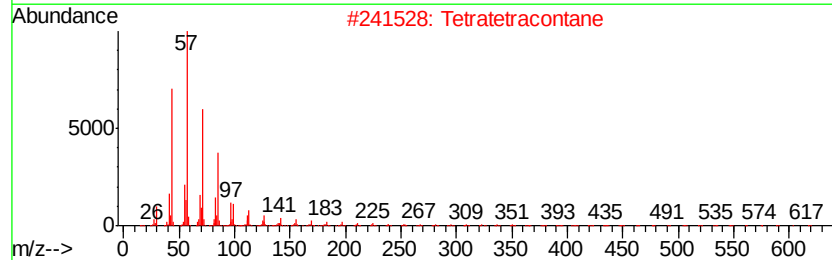
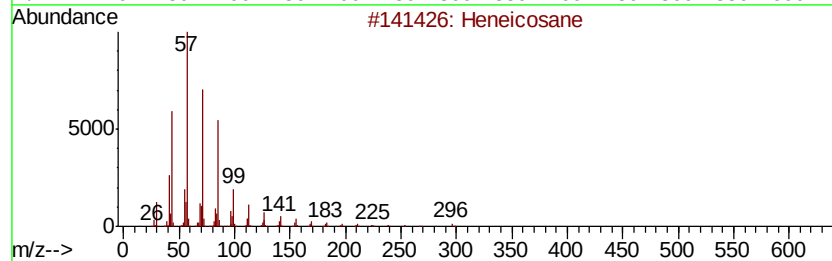
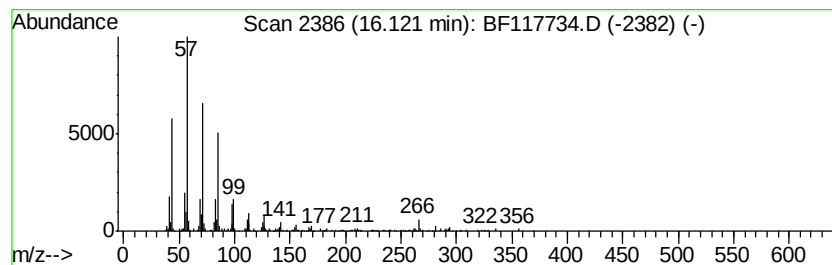
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	2.41 ng	267769	Perylene-d12	15.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	87
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		2-methyloctacosane	408	C29H60	1000376-72-8	87
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	87
5		Tridecane, 6-propyl-	226	C16H34	055045-10-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
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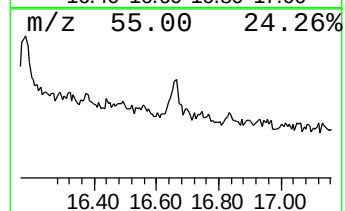
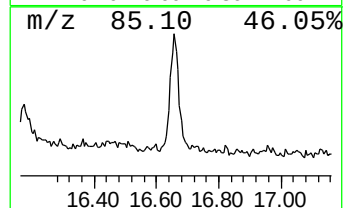
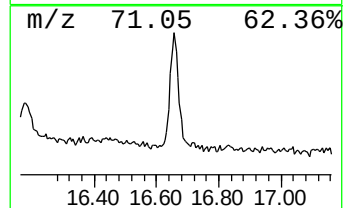
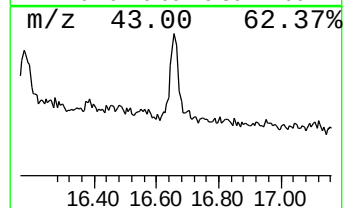
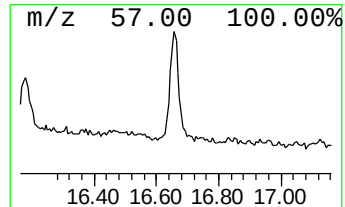
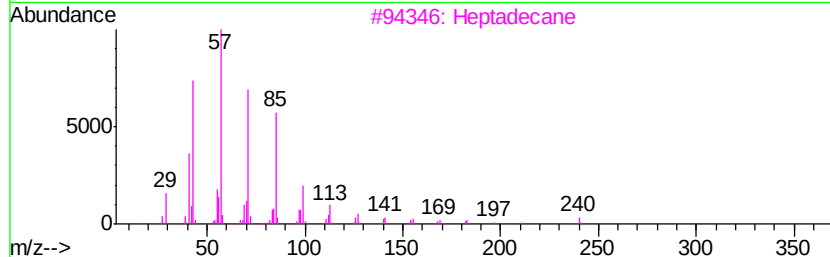
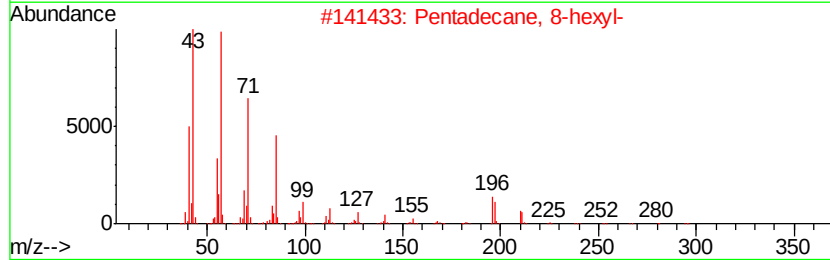
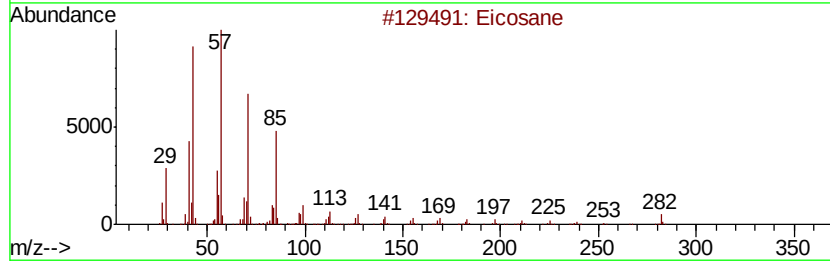
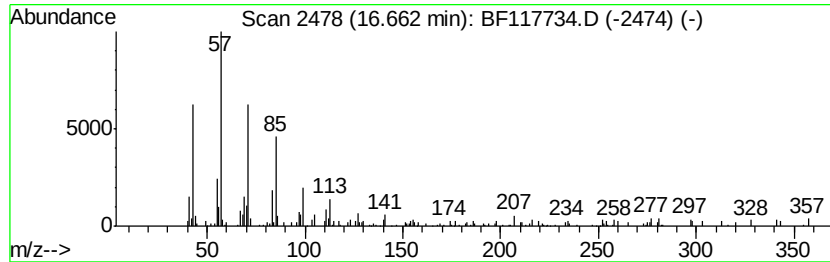
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.66	2.19 ng	244064	Perylene-d12	15.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
3	Heptadecane	240	C17H36	000629-78-7	91
4	Nonadecane	268	C19H40	000629-92-5	91
5	Octadecane	254	C18H38	000593-45-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110819\
 Data File : BF117734.D
 Acq On : 8 Nov 2019 16:43
 Operator : JU
 Sample : K5722-14
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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...	2.23	18.1	ng	1867500	1	6.93	2069300	20.0
2-Pentanone, 4-hy...	5.15	15.9	ng	1646360	1	6.93	2069300	20.0
unknown6.70	6.70	72.6	ng	7513410	1	6.93	2069300	20.0
Heptacosane	10.63	2.6	ng	445982	3	9.97	3434170	20.0
Tridecane, 5-propyl-	10.90	11.5	ng	1845560	4	11.47	3214760	20.0
Hexadecane	11.37	8.8	ng	1417660	4	11.47	3214760	20.0
n-Hexadecanoic acid	12.00	6.1	ng	978563	4	11.47	3214760	20.0
E-15-Heptadecenal	13.96	14.9	ng	1706650	5	14.12	2289120	20.0
Supraene	14.99	4.3	ng	475406	6	15.62	2226600	20.0
Benzo[e]pyrene	15.49	2.6	ng	291176	6	15.62	2226600	20.0
Heneicosane	16.12	2.4	ng	267769	6	15.62	2226600	20.0
Eicosane	16.66	2.2	ng	244064	6	15.62	2226600	20.0