

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
 Data File : BF118152.D
 Acq On : 9 Dec 2019 18:53
 Operator : JU
 Sample : K6162-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP2

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-BF120619.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	2.122	3	6	13	rVB	228562	275464	11.65%	1.191%
2	5.075	503	508	518	rVB	335025	379085	16.04%	1.640%
3	5.487	573	578	581	rBV	1847069	1833698	77.57%	7.931%
4	6.498	745	750	763	rBV	2125656	1964551	83.10%	8.497%
5	6.639	769	774	777	rBV	2440272	2153178	91.08%	9.313%
6	6.869	809	813	816	rBV	735449	586937	24.83%	2.539%
7	7.022	836	839	843	rBV	1941582	1702606	72.02%	7.364%
8	7.428	904	908	918	rBV	1258318	1259807	53.29%	5.449%
9	8.151	1028	1031	1046	rBV	788694	750197	31.73%	3.245%
10	9.233	1211	1215	1218	rBV	2641413	2364013	100.00%	10.225%
11	9.627	1278	1282	1291	rVB	156701	145205	6.14%	0.628%
12	9.916	1327	1331	1343	rVB	982744	848710	35.90%	3.671%
13	10.704	1461	1465	1481	rBV	1657362	1528478	64.66%	6.611%
14	11.404	1581	1584	1587	rBV	855934	781774	33.07%	3.381%
15	11.427	1587	1588	1593	rVV	143252	111864	4.73%	0.484%
16	11.480	1593	1597	1601	rVB3	26379	29813	1.26%	0.129%
17	11.927	1666	1673	1681	rBV3	199691	244331	10.34%	1.057%
18	12.021	1686	1689	1692	rBV2	24793	28019	1.19%	0.121%
19	12.621	1788	1791	1797	rBV	251495	244162	10.33%	1.056%
20	12.716	1805	1807	1815	rBV2	58457	71559	3.03%	0.310%
21	12.857	1825	1831	1836	rBV	231314	246084	10.41%	1.064%
22	12.998	1850	1855	1858	rBV	2139152	1894035	80.12%	8.192%
23	13.286	1900	1904	1907	rBV2	25731	27423	1.16%	0.119%
24	13.568	1947	1952	1955	rBV6	20547	28639	1.21%	0.124%
25	13.698	1966	1974	1977	rBV	25120	38352	1.62%	0.166%
26	13.810	1989	1993	1995	rBV2	21597	26598	1.13%	0.115%
27	13.892	2003	2007	2015	rVB3	204173	273113	11.55%	1.181%
28	14.057	2027	2035	2038	rBV2	759894	817726	34.59%	3.537%
29	14.080	2038	2039	2048	rVB	133769	126573	5.35%	0.547%
30	14.215	2058	2062	2066	rBV2	48064	56588	2.39%	0.245%
31	14.521	2110	2114	2119	rBV3	79312	105629	4.47%	0.457%
32	14.827	2163	2166	2170	rBV	83190	87537	3.70%	0.379%
33	15.110	2210	2214	2222	rBV2	114418	231814	9.81%	1.003%
34	15.174	2222	2225	2229	rVV	101417	116501	4.93%	0.504%

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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	15.221	2230	2233	2235	rVB	24130	27370	1.16%	0.118%
36	15.415	2263	2266	2273	rVB	66487	88085	3.73%	0.381%
37	15.480	2273	2277	2283	rVB	110356	138592	5.86%	0.599%
38	15.551	2283	2289	2303	rBV	578726	913173	38.63%	3.950%
39	16.015	2362	2368	2372	rBV	83749	135449	5.73%	0.586%
40	16.074	2374	2378	2385	rVB7	29598	64048	2.71%	0.277%
41	16.527	2450	2455	2469	rBV4	52068	124103	5.25%	0.537%
42	17.051	2538	2544	2551	rBV3	50860	101282	4.28%	0.438%
43	17.139	2557	2559	2566	rVB4	29511	42930	1.82%	0.186%
44	17.245	2571	2577	2579	rVV7	14753	27531	1.16%	0.119%
45	17.503	2616	2621	2629	rVB	38171	77812	3.29%	0.337%

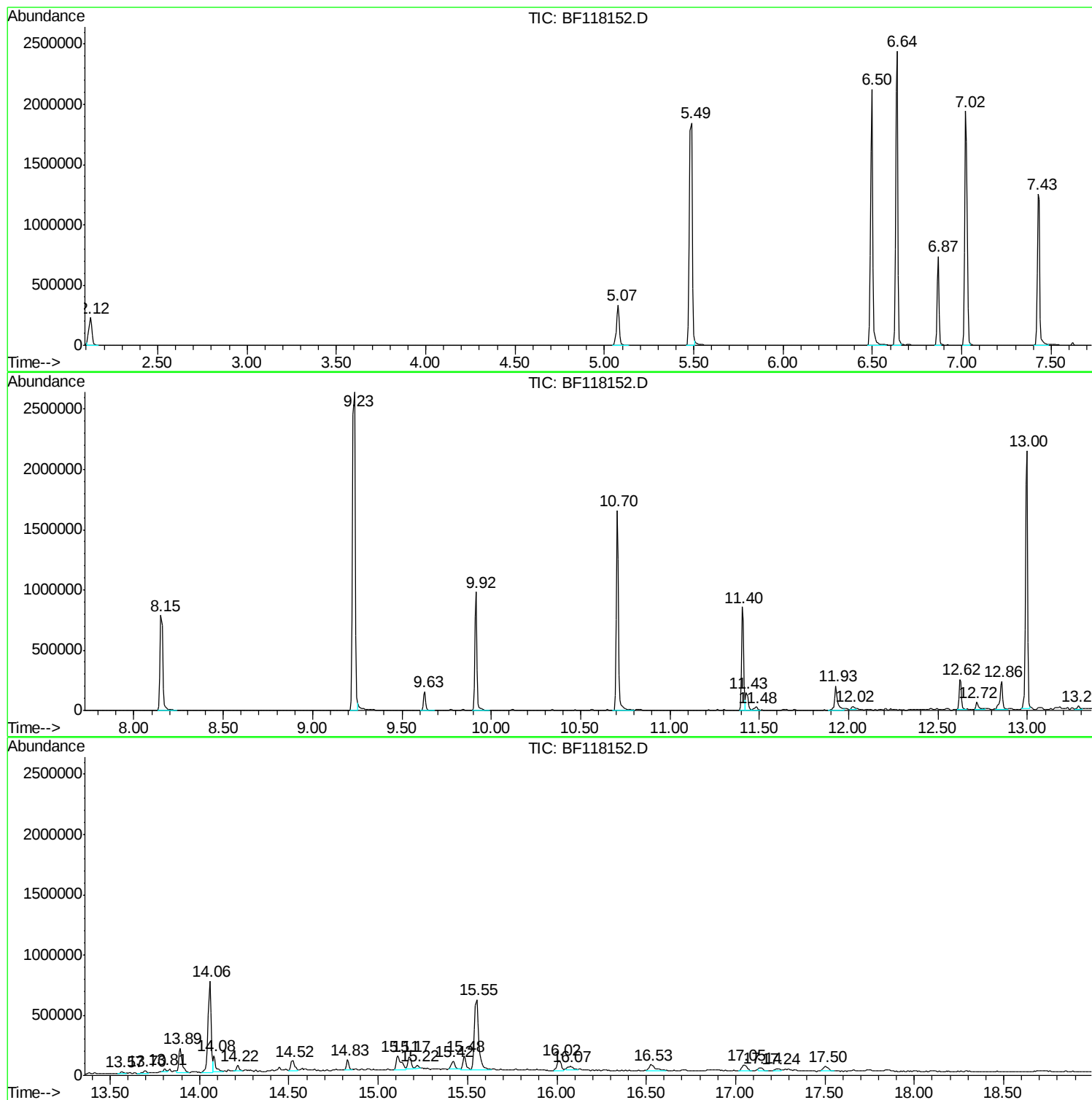
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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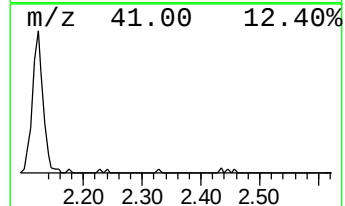
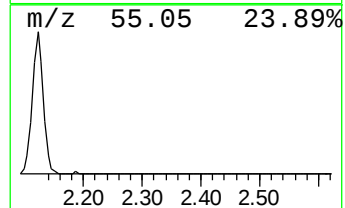
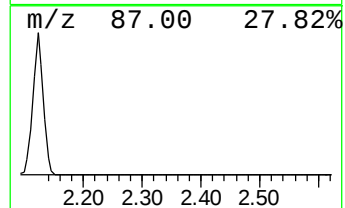
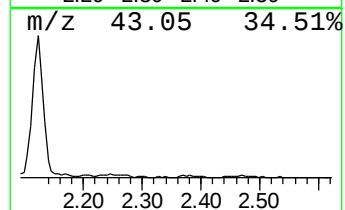
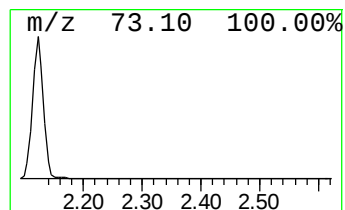
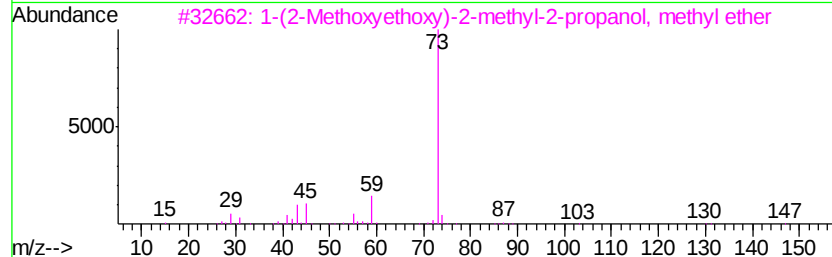
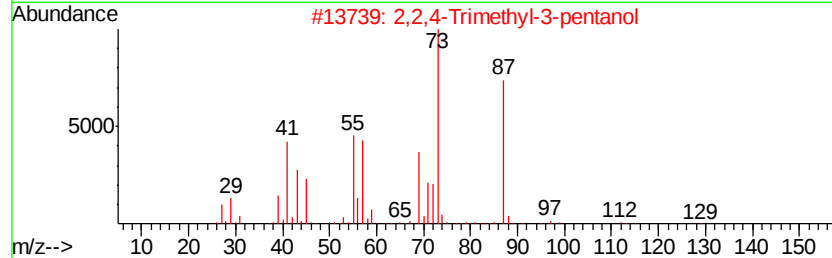
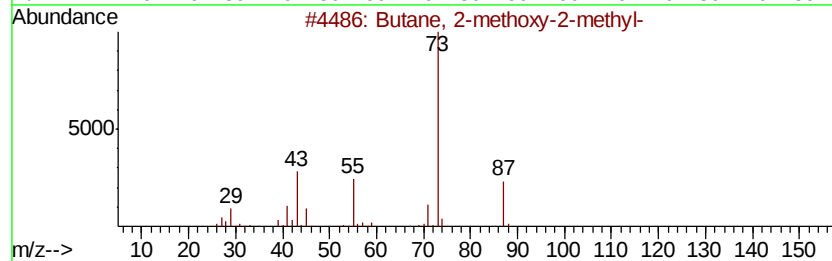
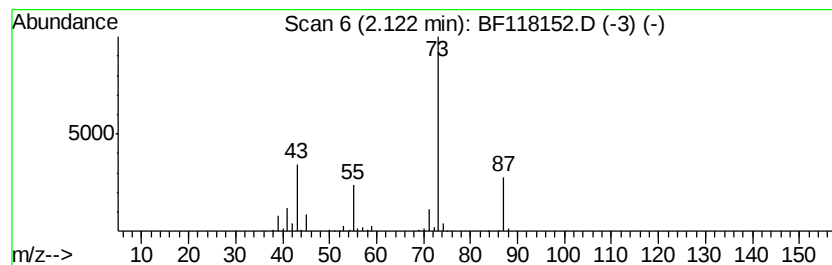
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	9.39 ng	275464	1,4-Dichlorobenzene-d4	6.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1-(2-Methoxyethoxy)-2-methyl-2-propanol	162	C8H18O3	1000364-24-4	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12



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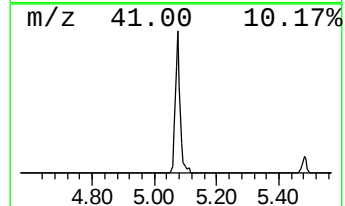
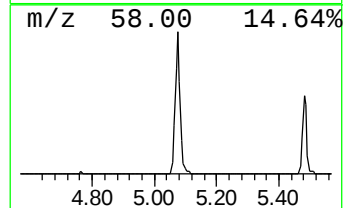
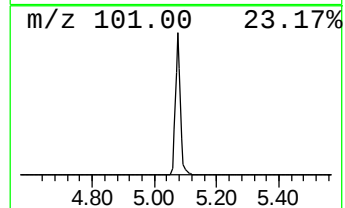
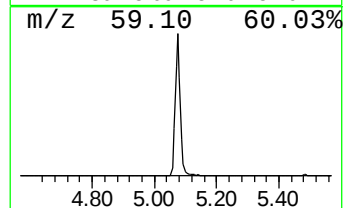
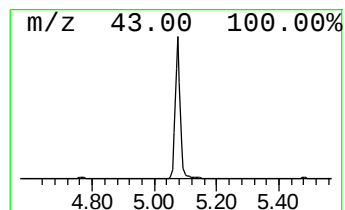
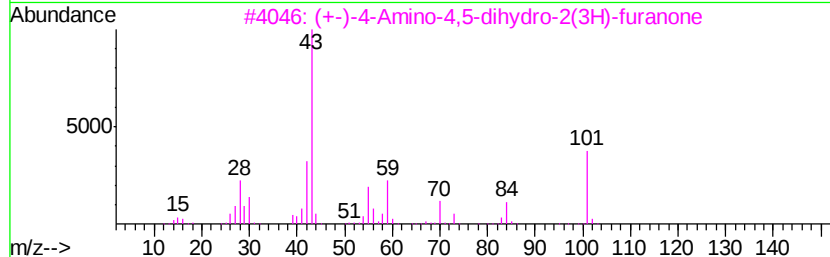
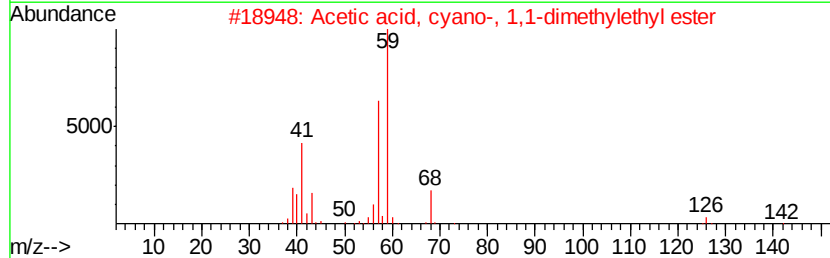
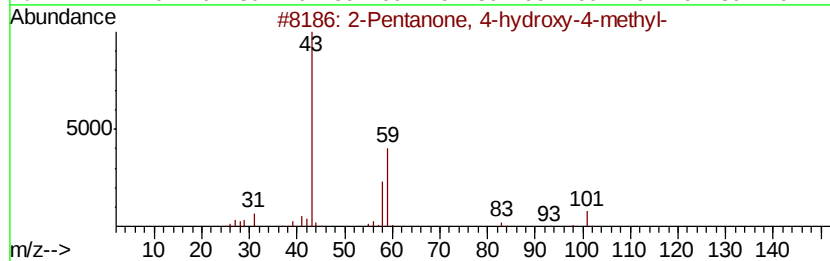
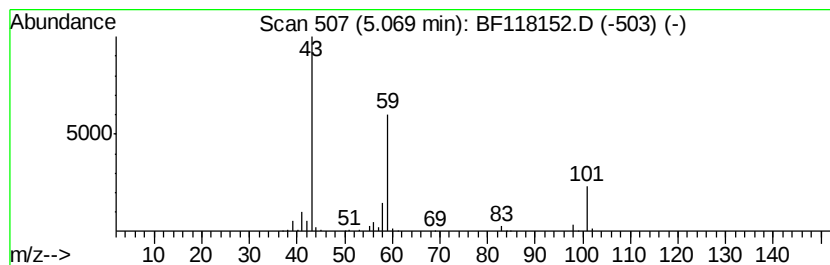
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	12.92 ng	379085	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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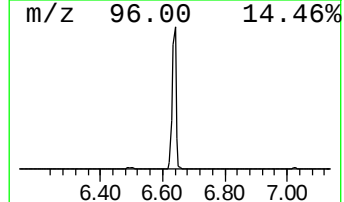
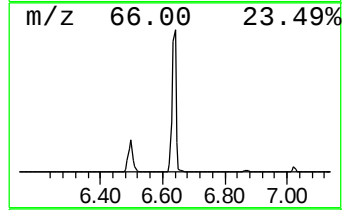
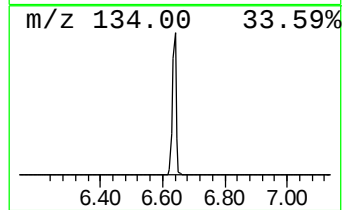
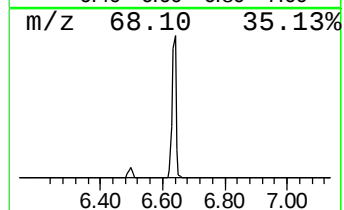
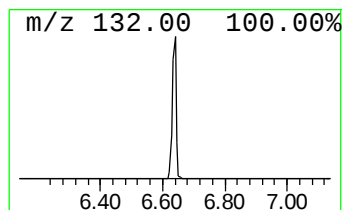
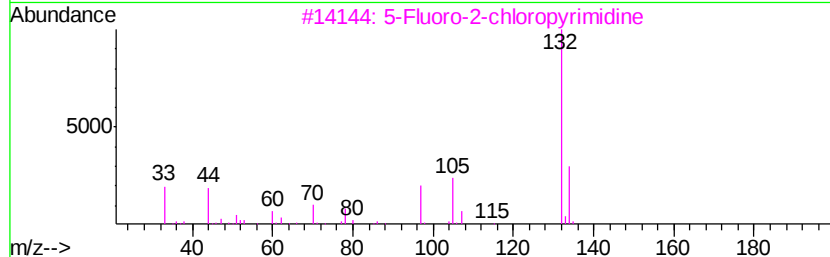
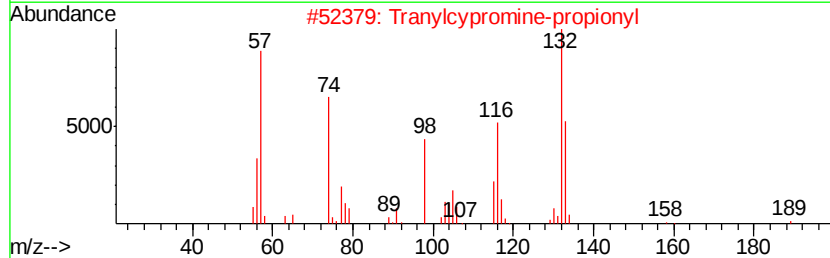
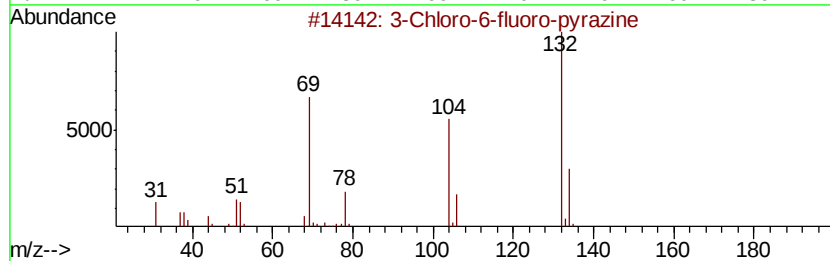
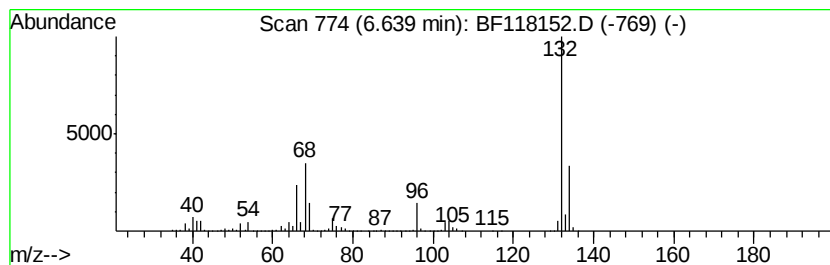
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	73.37 ng	2153180	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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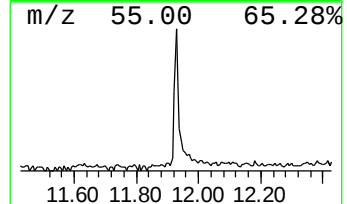
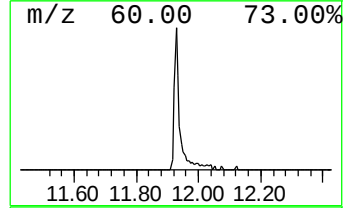
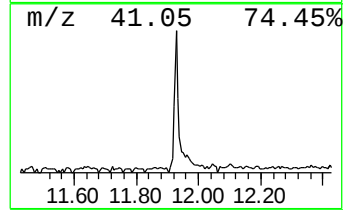
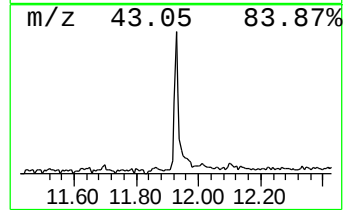
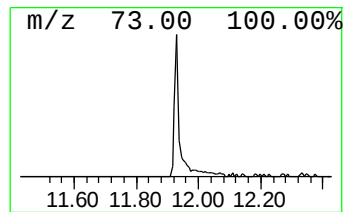
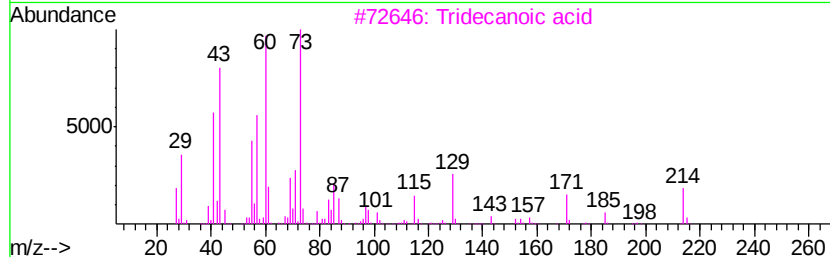
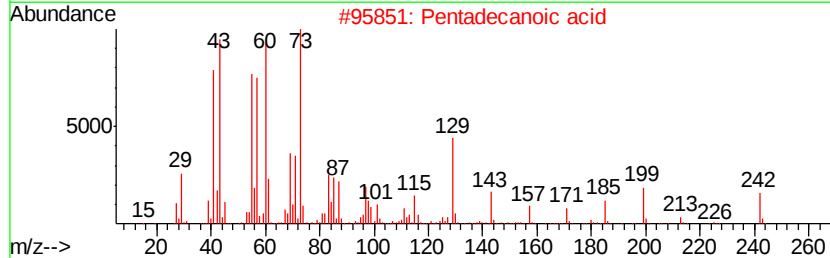
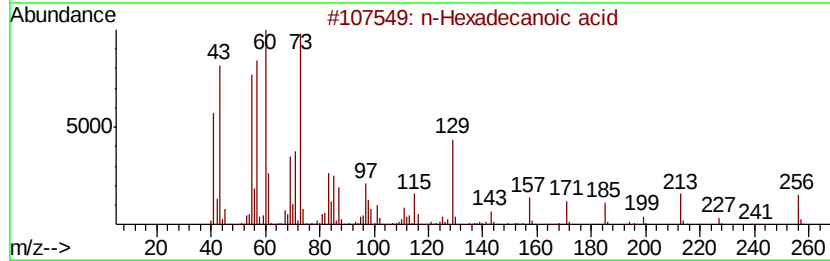
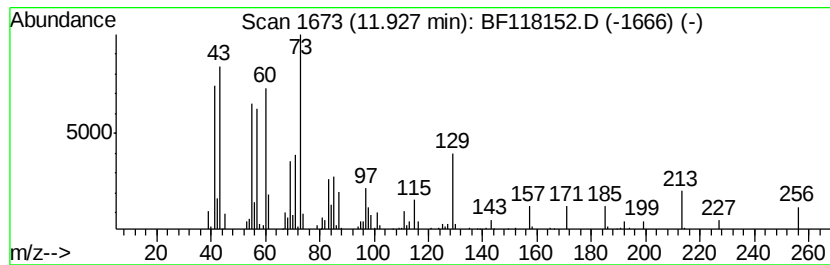
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.93	6.25 ng	244331	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	25



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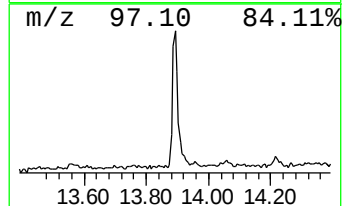
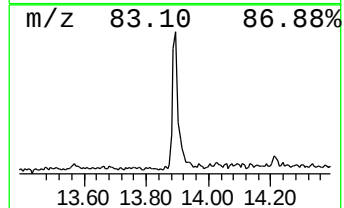
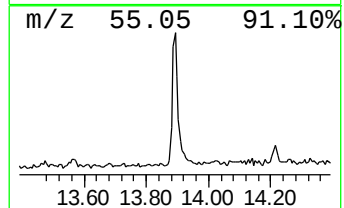
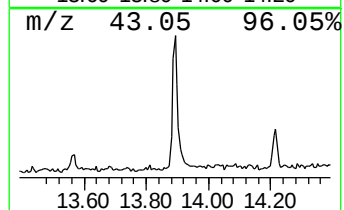
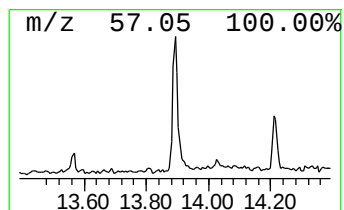
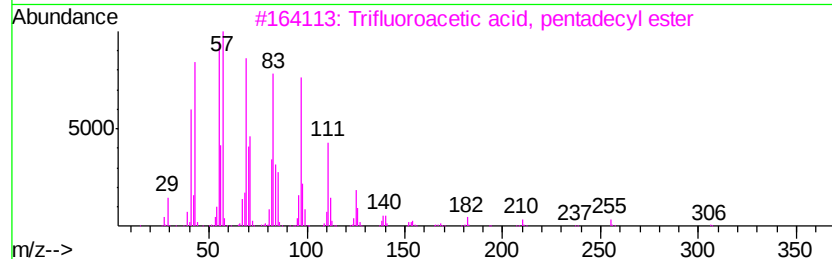
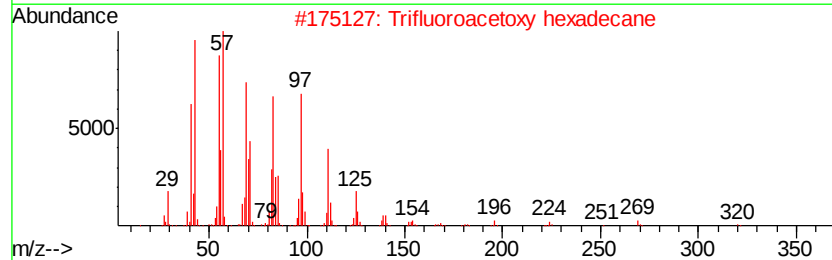
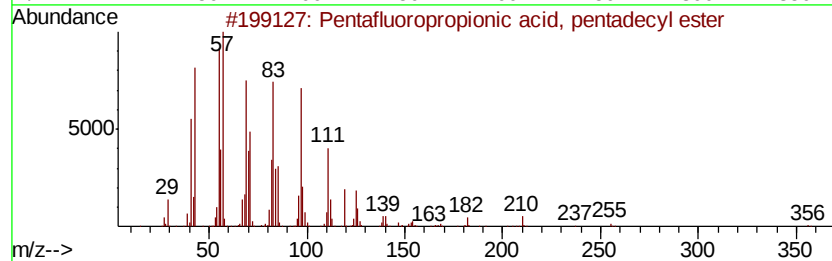
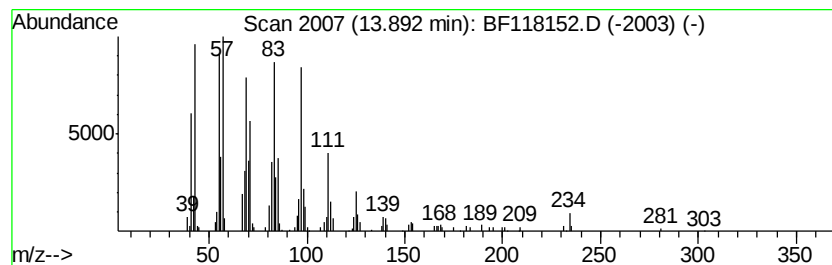
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	6.68 ng	273113	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118152.D
Acq On : 9 Dec 2019 18:53
Operator : JU
Sample : K6162-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

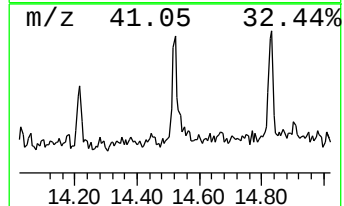
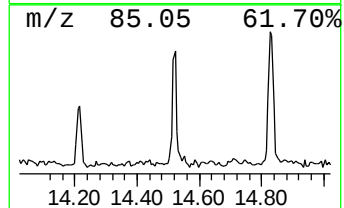
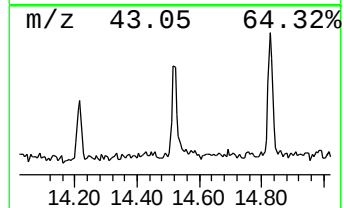
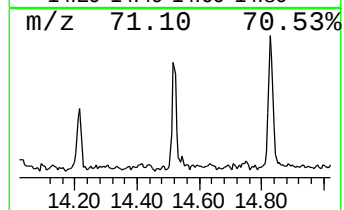
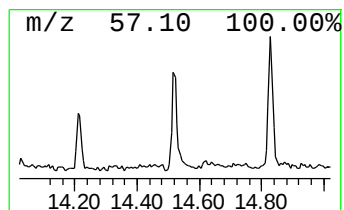
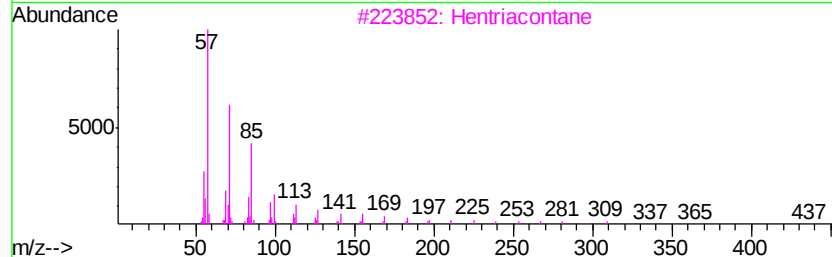
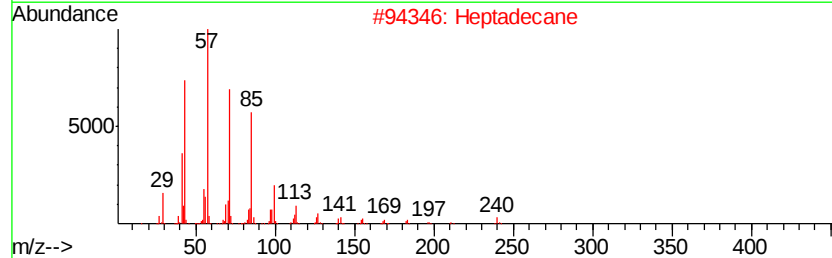
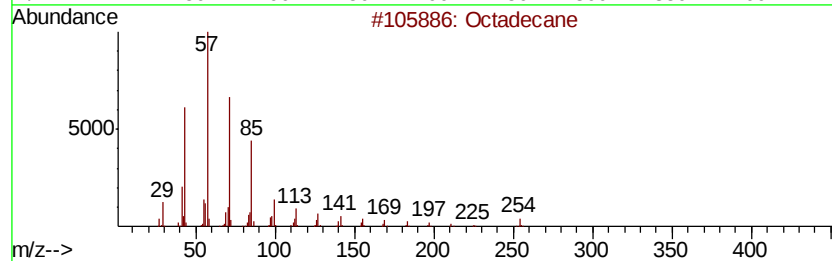
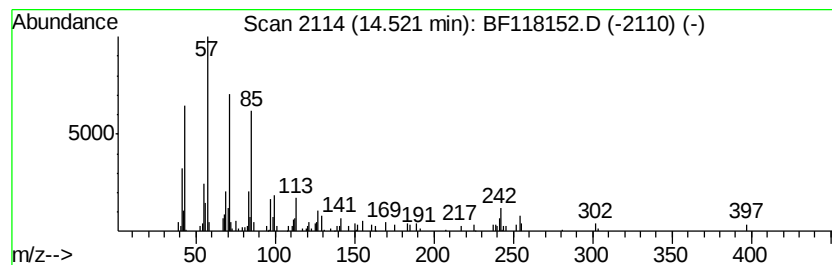
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.58 ng	105629	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	96
2		Heptadecane	240	C17H36	000629-78-7	96
3		Hentriacontane	437	C31H64	000630-04-6	76
4		Tetracosane	338	C24H50	000646-31-1	76
5		2-methyloctacosane	408	C29H60	1000376-72-8	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118152.D
Acq On : 9 Dec 2019 18:53
Operator : JU
Sample : K6162-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

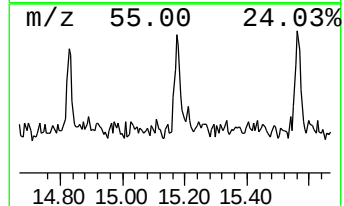
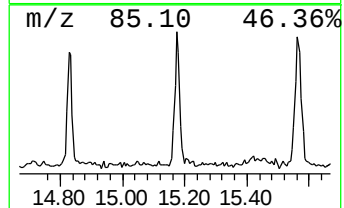
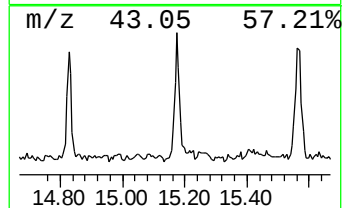
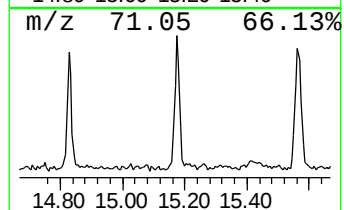
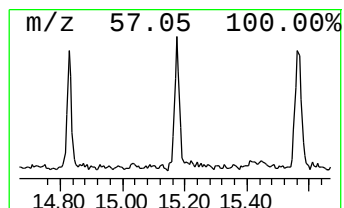
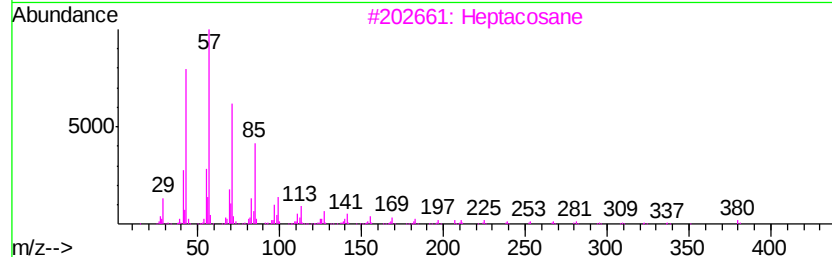
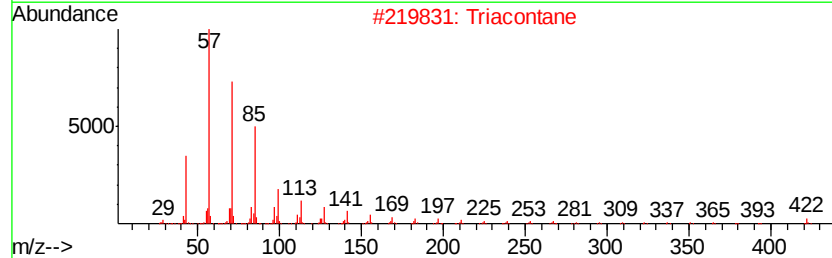
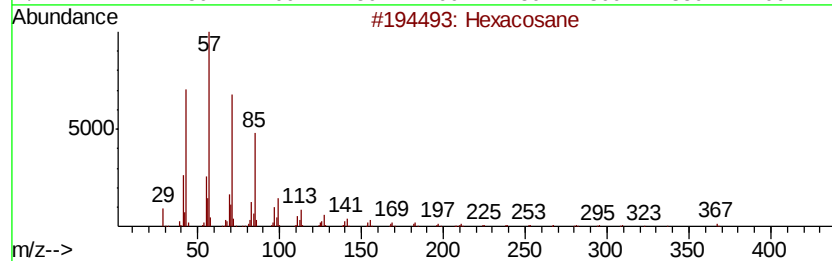
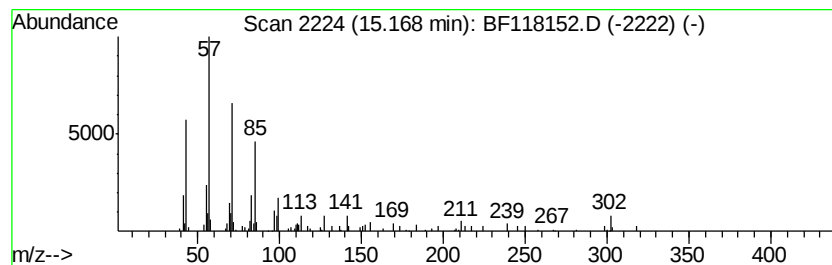
Instrument :
BNA_F
ClientSampleId :
TP2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
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 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.55 ng	116501	Perylene-d12	15.55
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	90
2	triacontane	422 C30H62	000638-68-6	90
3	Heptacosane	380 C27H56	000593-49-7	90
4	2-methyloctacosane	408 C29H60	1000376-72-8	90
5	Pentadecane, 8-hexyl-	296 C21H44	013475-75-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118152.D
Acq On : 9 Dec 2019 18:53
Operator : JU
Sample : K6162-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

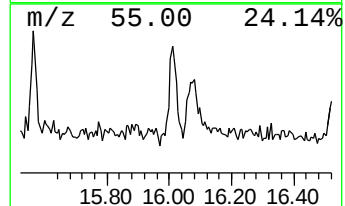
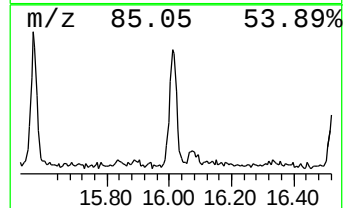
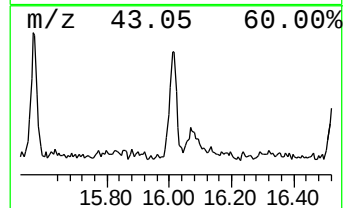
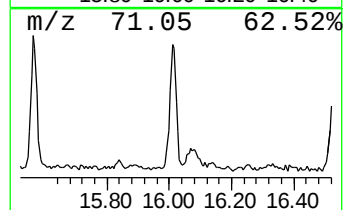
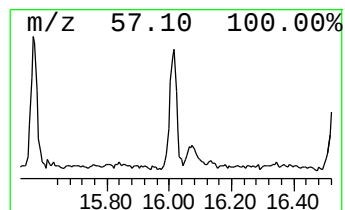
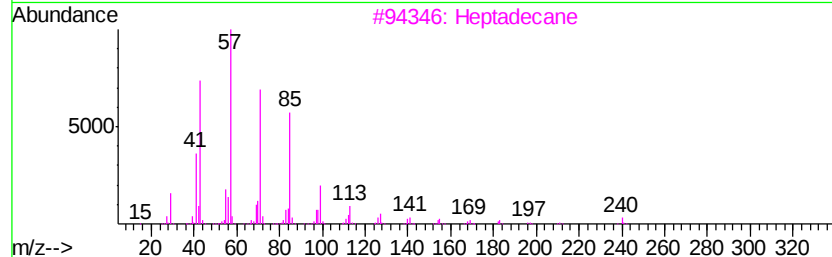
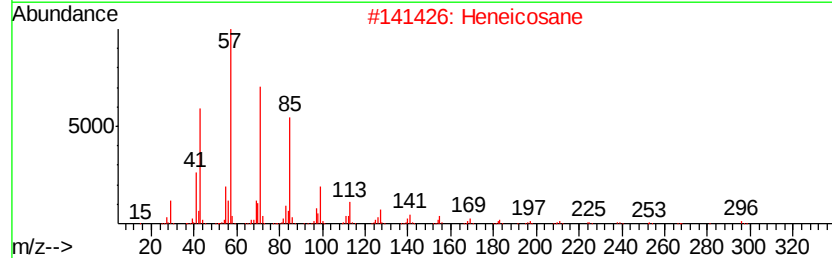
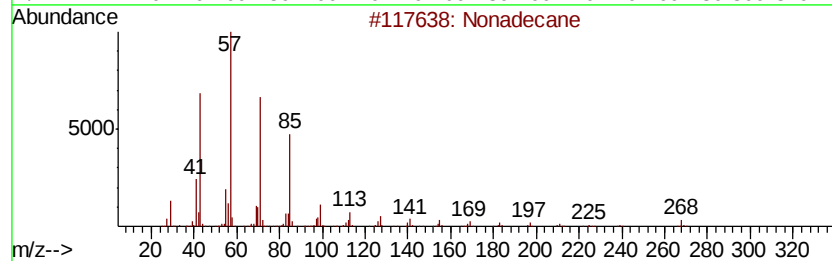
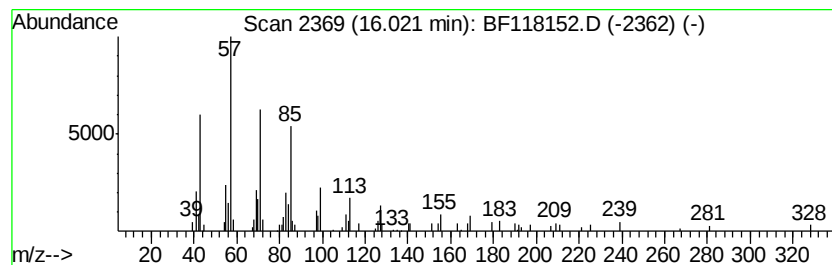
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.97 ng	135449	Perylene-d12	15.55
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	Heptadecane	240 C17H36	000629-78-7	91
4	Hexacosane	366 C26H54	000630-01-3	91
5	Octacosane	394 C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118152.D
Acq On : 9 Dec 2019 18:53
Operator : JU
Sample : K6162-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

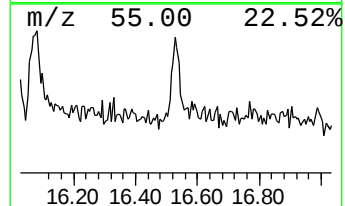
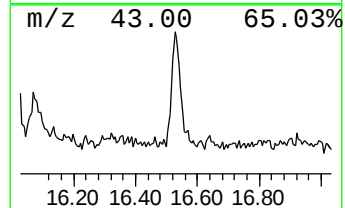
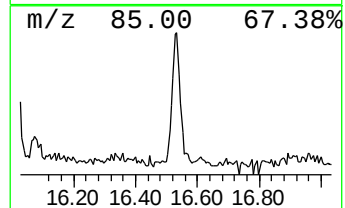
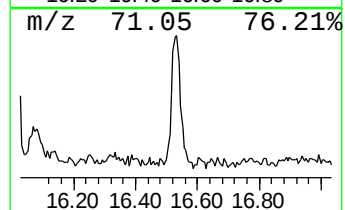
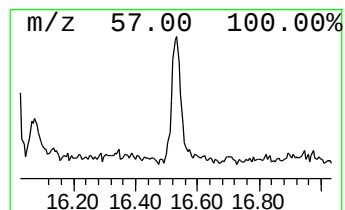
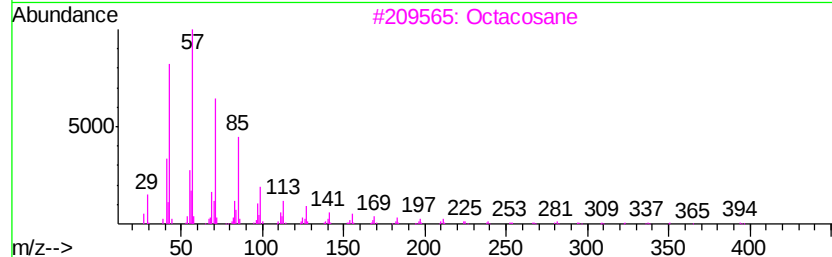
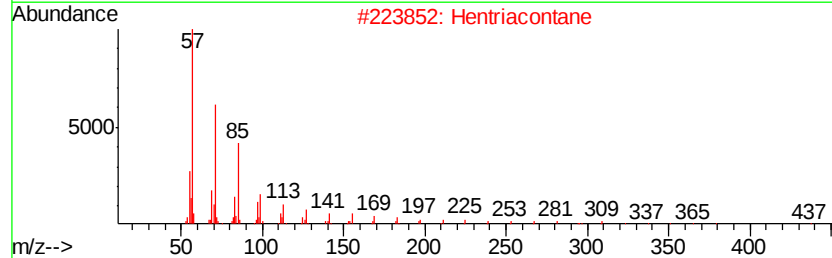
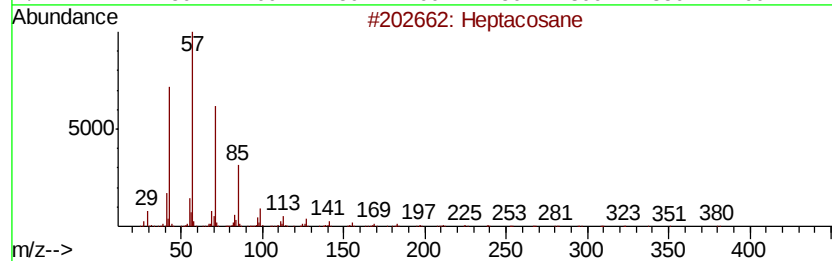
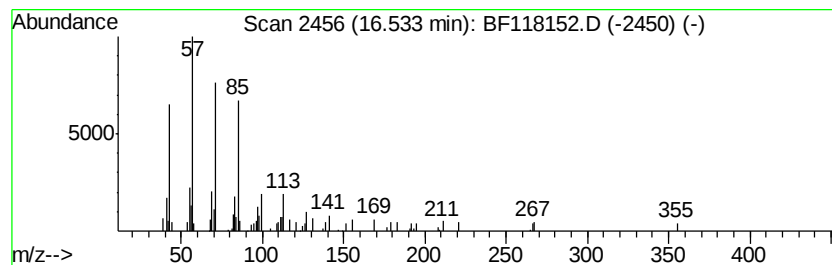
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.72 ng	124103	Perylene-d12	15.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	90
2		Hentriacontane	437	C31H64	000630-04-6	87
3		Octacosane	394	C28H58	000630-02-4	86
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120919\
Data File : BF118152.D
Acq On : 9 Dec 2019 18:53
Operator : JU
Sample : K6162-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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...	2.12	9.4	ng	275464	1	6.87	586937	20.0
2-Pentanone, 4-hy...	5.07	12.9	ng	379085	1	6.87	586937	20.0
unknown6.64	6.64	73.4	ng	2153180	1	6.87	586937	20.0
n-Hexadecanoic acid	11.93	6.3	ng	244331	4	11.40	781774	20.0
Pentafluoropropio...	13.89	6.7	ng	273113	5	14.06	817726	20.0
Octadecane	14.52	2.6	ng	105629	5	14.06	817726	20.0
Hexacosane	15.17	2.5	ng	116501	6	15.55	913173	20.0
Nonadecane	16.02	3.0	ng	135449	6	15.55	913173	20.0
Hentriacontane	16.53	2.7	ng	124103	6	15.55	913173	20.0