

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081519\
 Data File : BF116288.D
 Acq On : 15 Aug 2019 19:49
 Operator : HP/JU
 Sample : K4356-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1

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-BF073019.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	2.246	24	27	35	rVB	33167	48606	5.25%	0.362%
2	5.439	567	570	594	rBV	463069	740827	80.09%	5.520%
3	6.457	740	743	762	rBV	560558	853839	92.31%	6.362%
4	6.592	762	766	784	rVB	849461	920806	99.55%	6.861%
5	6.816	801	804	817	rBV	394981	403275	43.60%	3.005%
6	6.975	827	831	853	rBV	591651	619100	66.93%	4.613%
7	7.380	897	900	925	rBV	372500	520104	56.23%	3.876%
8	8.098	1019	1022	1043	rBV	467622	528197	57.10%	3.936%
9	9.169	1201	1204	1227	rBV	869834	811624	87.75%	6.048%
10	9.569	1269	1272	1284	rBV	153213	151991	16.43%	1.133%
11	9.851	1316	1320	1337	rVB	661483	636360	68.80%	4.742%
12	10.639	1451	1454	1470	rBV	459250	546452	59.08%	4.072%
13	11.339	1569	1573	1584	rBV	617632	670993	72.54%	5.000%
14	11.857	1659	1661	1665	rBV	18009	22097	2.39%	0.165%
15	12.410	1753	1755	1758	rVB	12122	9952	1.08%	0.074%
16	12.910	1837	1840	1852	rVB	869100	834196	90.19%	6.216%
17	13.115	1871	1875	1876	rBV	14129	12454	1.35%	0.093%
18	13.139	1876	1879	1885	rVB	34072	34243	3.70%	0.255%
19	13.380	1917	1920	1926	rBV4	8750	10698	1.16%	0.080%
20	13.480	1933	1937	1940	rBV2	14514	15873	1.72%	0.118%
21	13.598	1954	1957	1963	rBV	26932	24020	2.60%	0.179%
22	13.804	1988	1992	2005	rBV	181990	281250	30.41%	2.096%
23	13.980	2018	2022	2034	rBV	682508	762932	82.48%	5.685%
24	14.121	2042	2046	2054	rBV	34492	44999	4.86%	0.335%
25	14.245	2063	2067	2074	rBV	844551	710322	76.79%	5.293%
26	14.433	2094	2099	2109	rBV2	151325	289956	31.35%	2.161%
27	14.504	2109	2111	2115	rVV2	15332	15444	1.67%	0.115%
28	14.551	2116	2119	2123	rVB3	13601	13052	1.41%	0.097%
29	14.721	2144	2148	2152	rBV	74560	81426	8.80%	0.607%
30	14.798	2158	2161	2165	rVB3	9149	10860	1.17%	0.081%
31	14.868	2168	2173	2181	rBV	349806	374678	40.51%	2.792%
32	15.051	2200	2204	2207	rBV	167735	183007	19.79%	1.364%
33	15.080	2207	2209	2215	rVB3	32248	51357	5.55%	0.383%
34	15.433	2262	2269	2285	rBV	548600	924973	100.00%	6.892%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.615	2295	2300	2307	rBV	150734	194955	21.08%	1.453%
36	15.839	2333	2338	2344	rBV	138692	204251	22.08%	1.522%
37	15.903	2344	2349	2355	rVV8	13206	33128	3.58%	0.247%
38	15.962	2355	2359	2364	rVB7	10630	18273	1.98%	0.136%
39	16.327	2415	2421	2430	rBV	52999	99941	10.80%	0.745%
40	16.609	2462	2469	2478	rBV	119968	229789	24.84%	1.712%
41	16.898	2513	2518	2524	rVB2	23177	42530	4.60%	0.317%
42	17.403	2598	2604	2610	rBV9	26385	71955	7.78%	0.536%
43	17.474	2610	2616	2629	rVB5	91284	214827	23.23%	1.601%
44	17.721	2652	2658	2667	rBV7	39328	103802	11.22%	0.773%
45	17.939	2690	2695	2699	rBV7	22068	46805	5.06%	0.349%

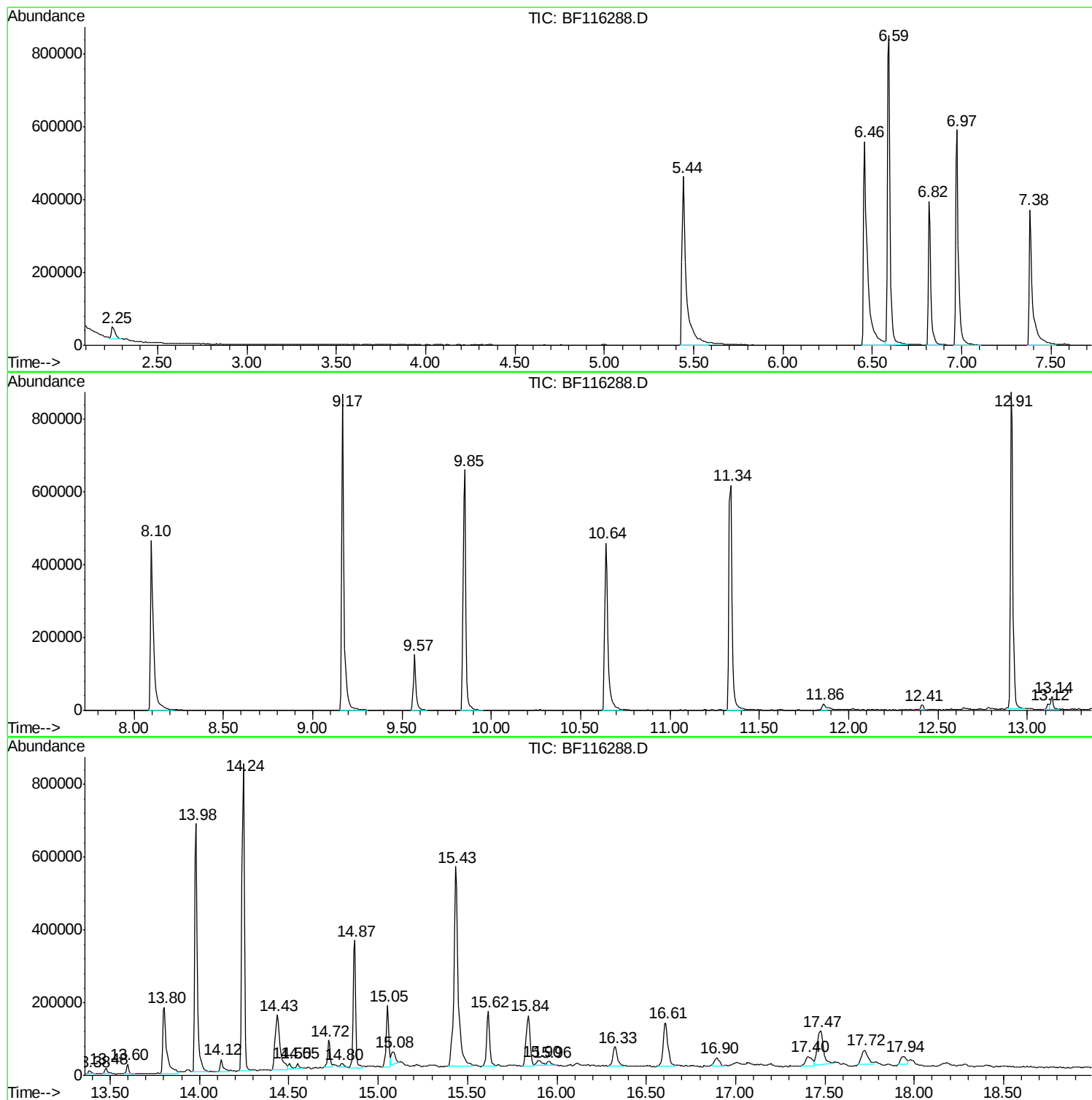
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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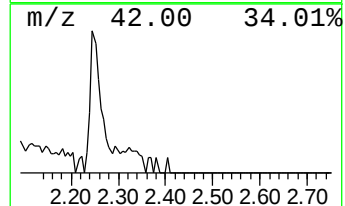
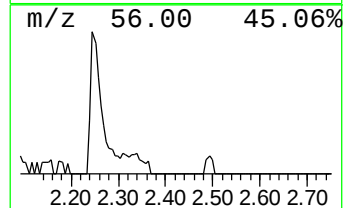
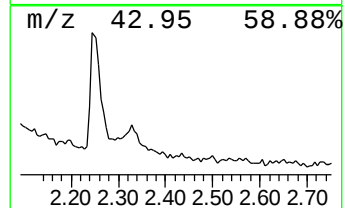
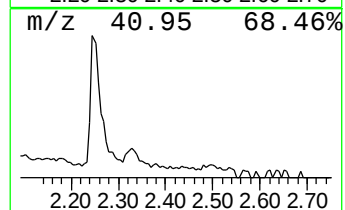
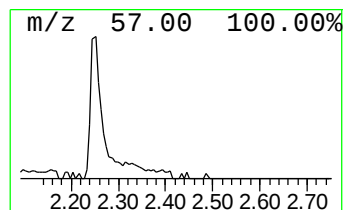
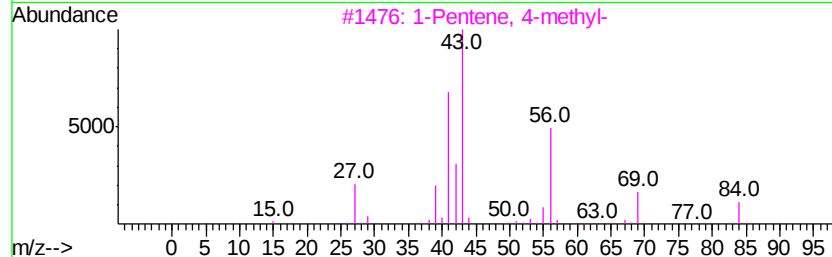
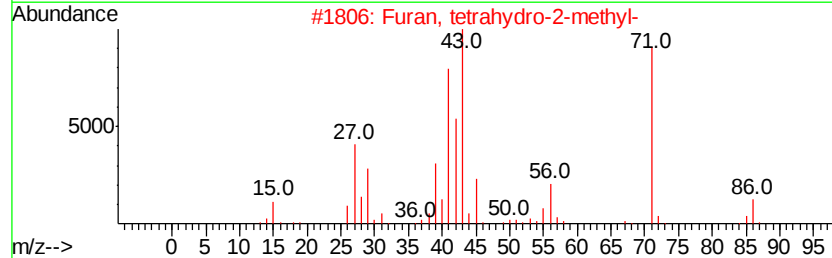
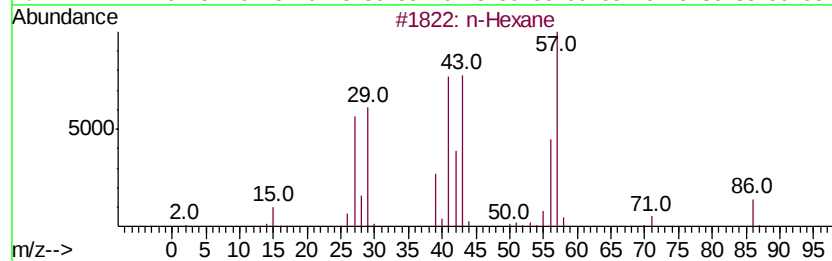
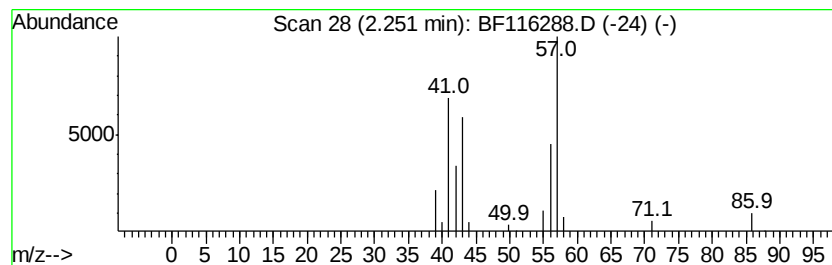
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	2.41 ng	48606	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	78
2		Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	47
3		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	36
4		Butanal, 2-methyl-	86	C5H10O	000096-17-3	12
5		Oxetane, 2,2-dimethyl-	86	C5H10O	006245-99-4	9



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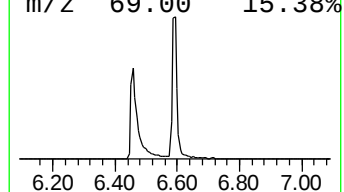
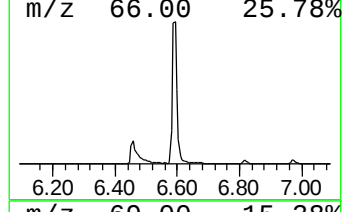
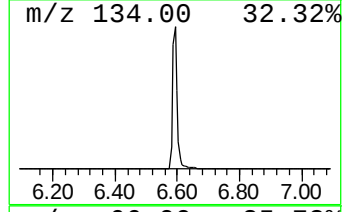
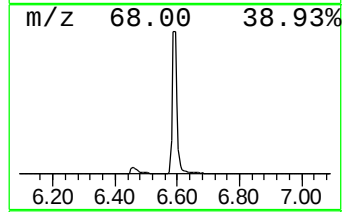
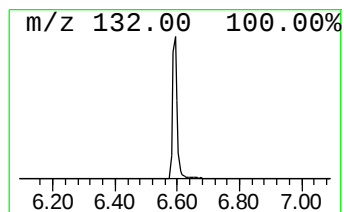
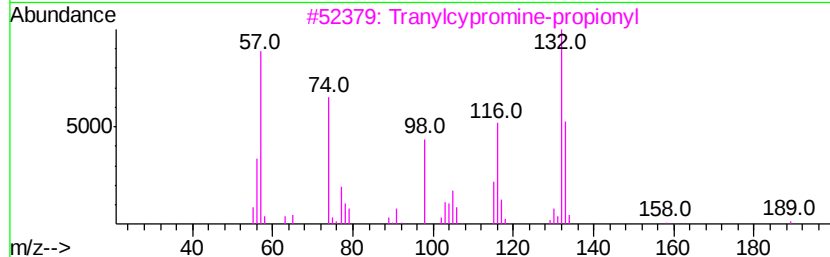
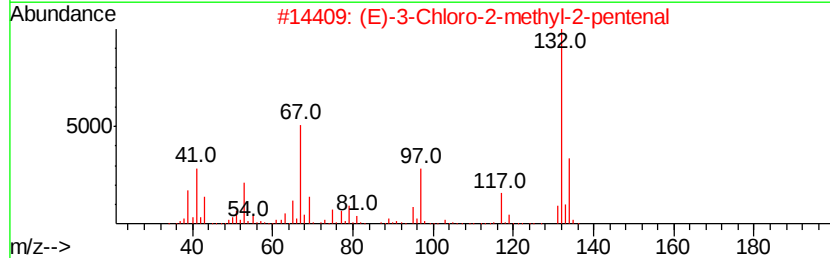
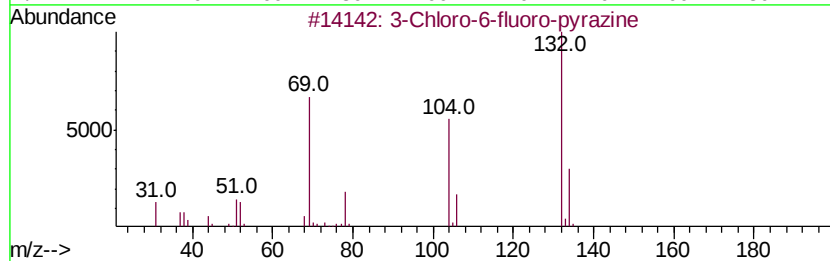
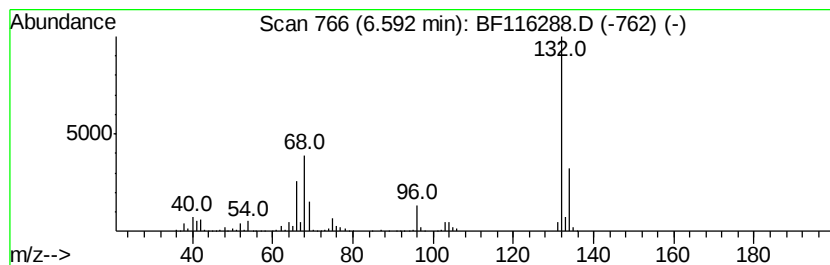
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Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	45.67 ng	920806	1,4-Dichlorobenzene-d4	6.82

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	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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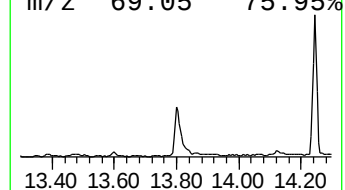
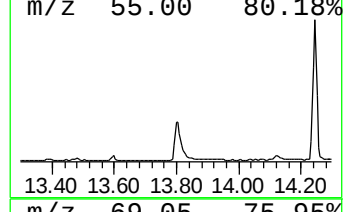
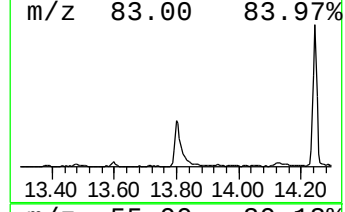
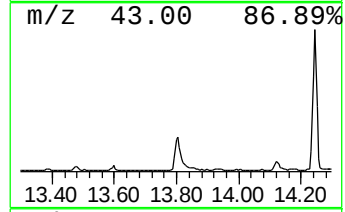
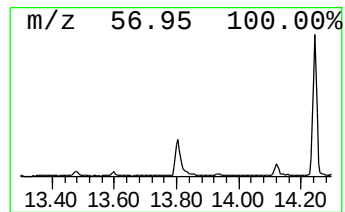
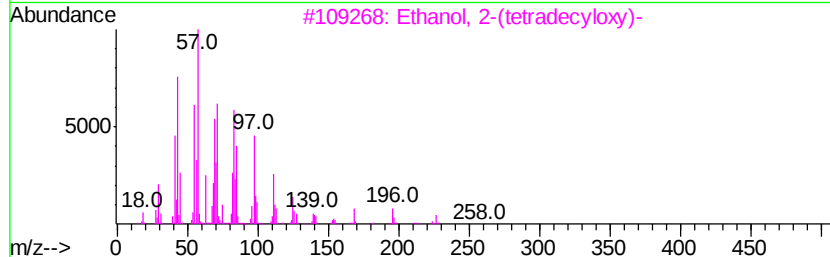
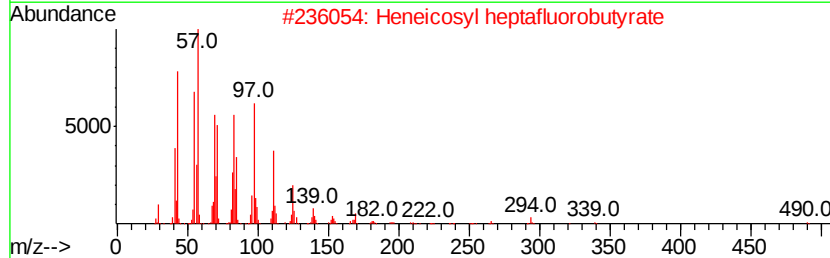
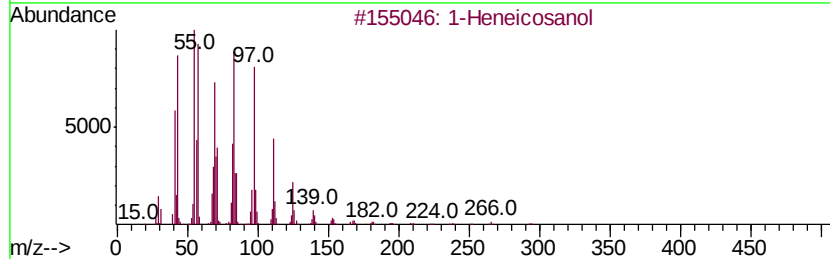
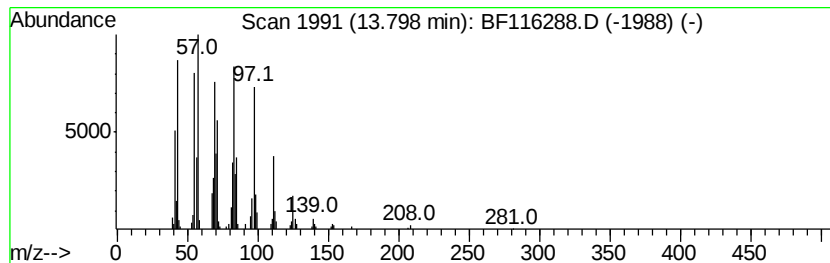
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.80	7.37 ng	281250	Chrysene-d12		13.98		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
3			Ethanol, 2-(tetradecyl)-	258	C16H34O2	002136-70-1	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



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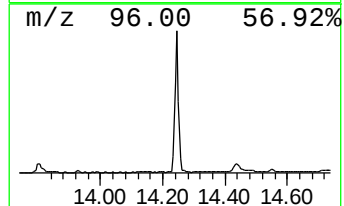
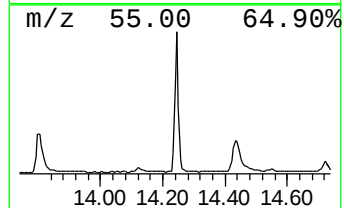
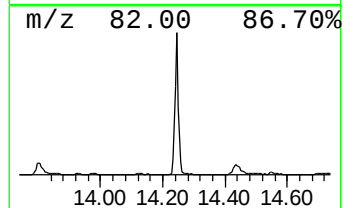
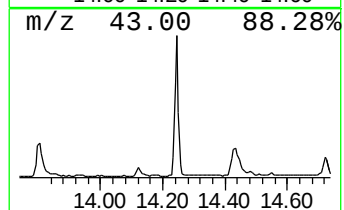
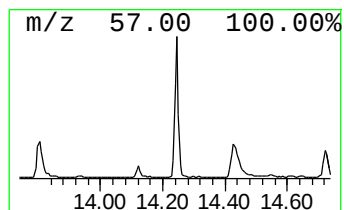
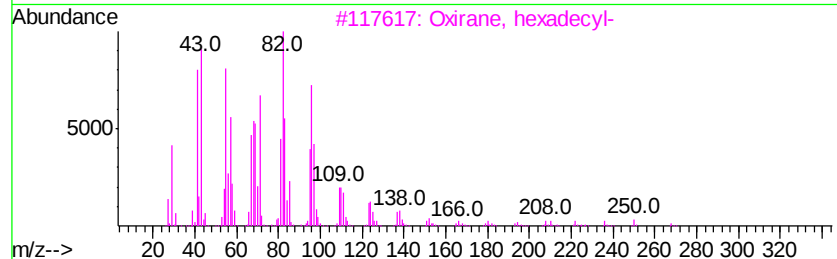
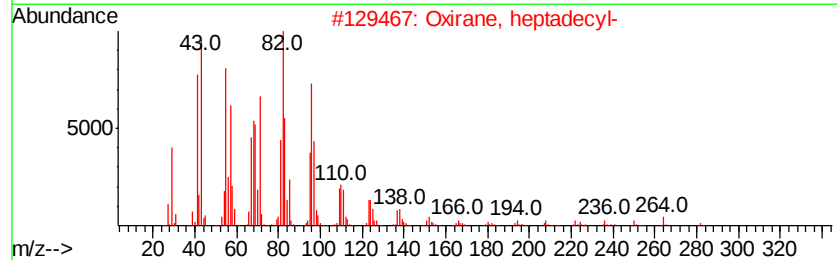
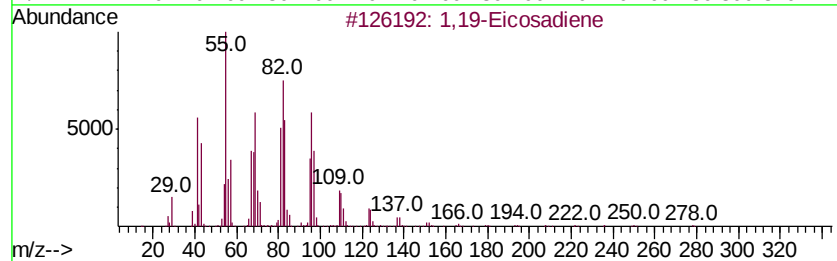
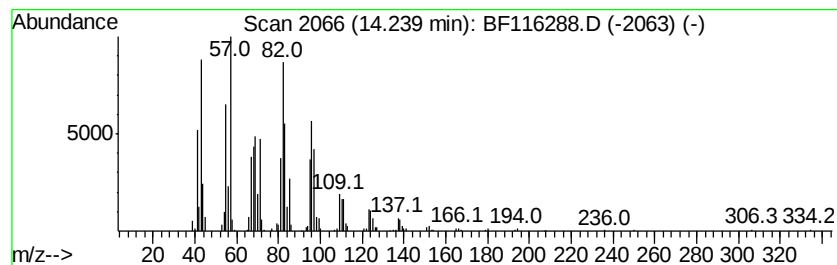
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,19-Eicosadiene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.24	18.62 ng	710322	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	95
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
4	Octadecanal	268	C18H36O	000638-66-4	91
5	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	91



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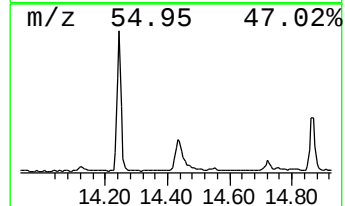
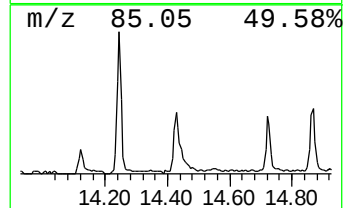
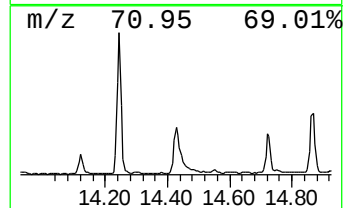
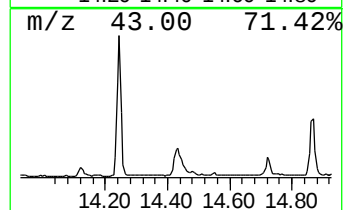
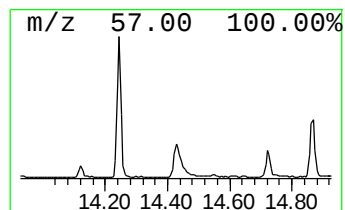
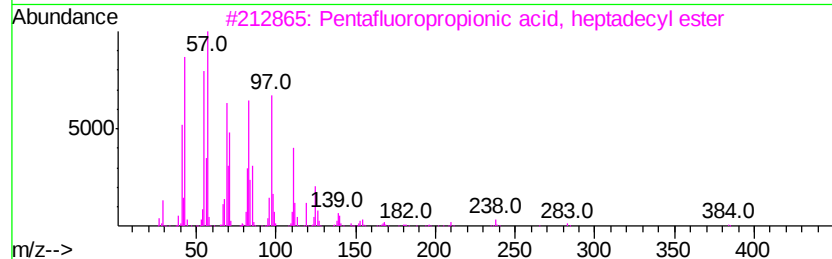
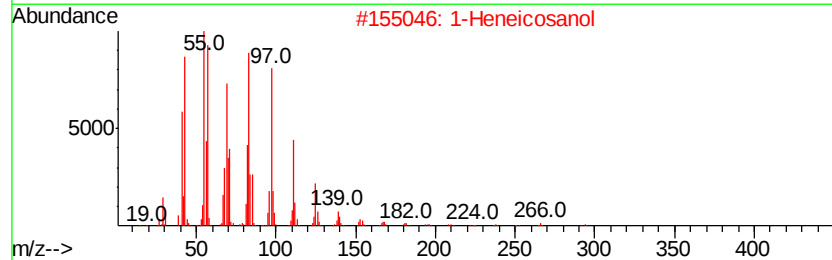
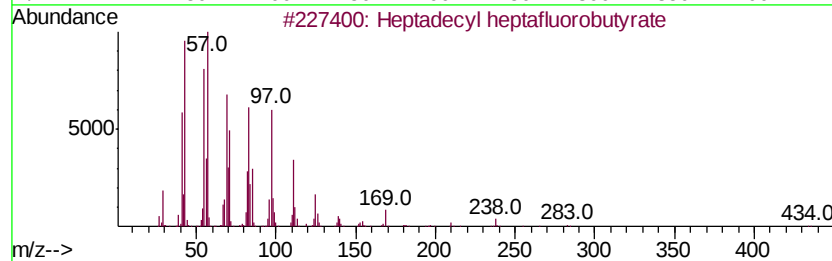
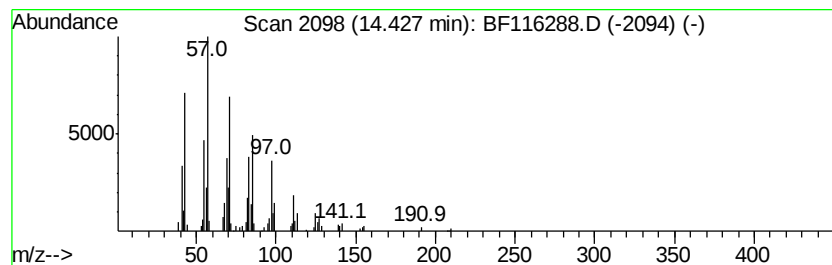
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	7.60 ng	289956	Chrysene-d12	13.98

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081519\
Data File : BF116288.D
Acq On : 15 Aug 2019 19:49
Operator : HP/JU
Sample : K4356-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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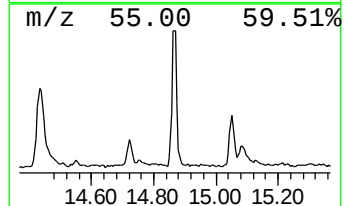
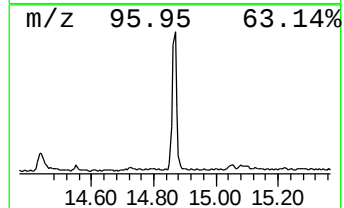
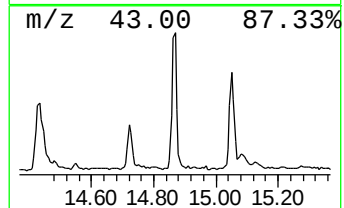
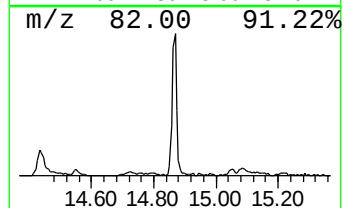
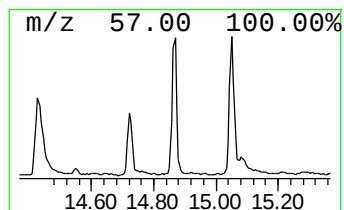
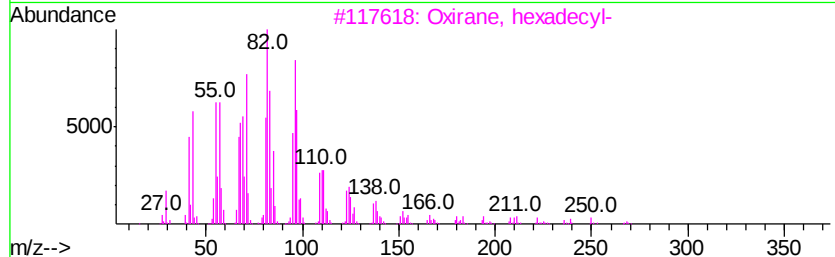
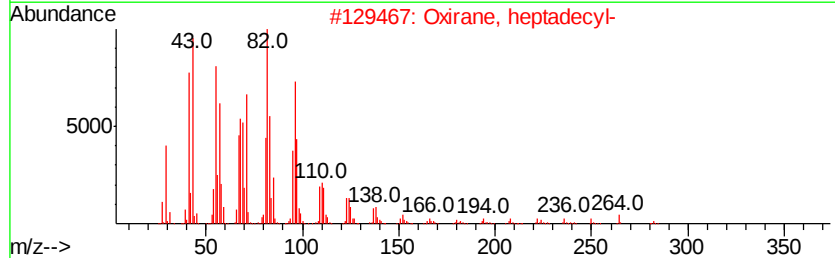
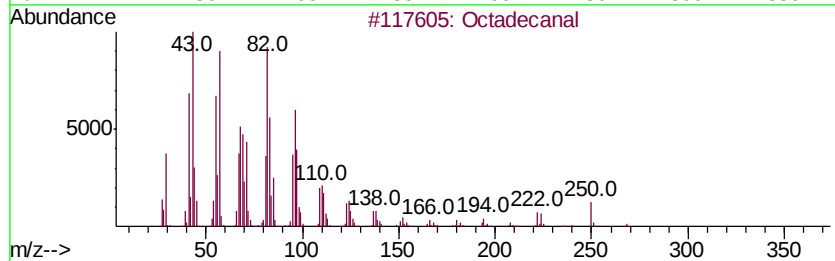
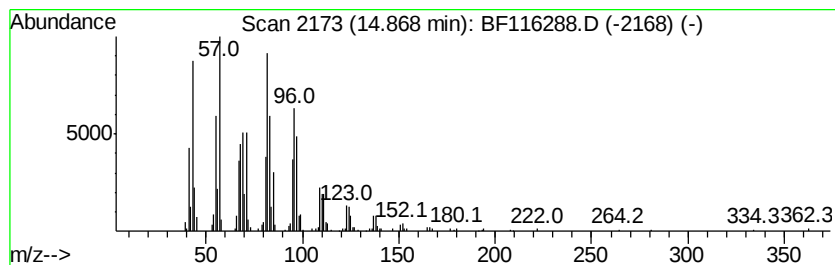
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	8.10 ng	374678	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	91
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4		Tetracosanal	352	C24H48O	057866-08-7	91
5		Heptadecanal	254	C17H34O	1000376-70-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081519\
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Acq On : 15 Aug 2019 19:49
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Misc :
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ClientSampleId :
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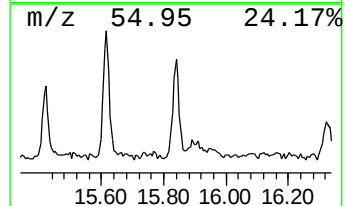
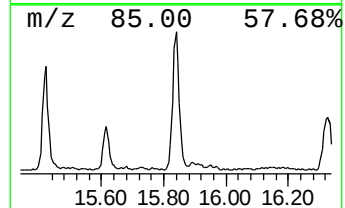
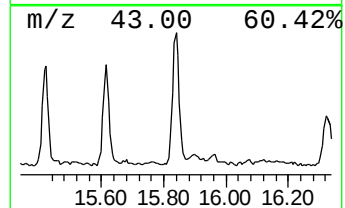
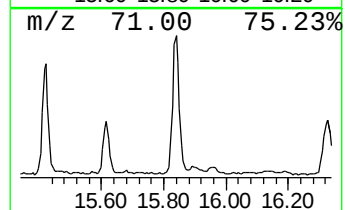
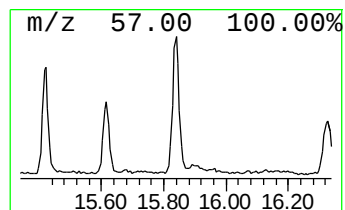
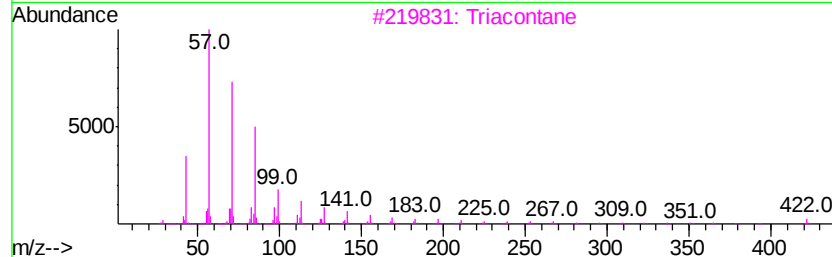
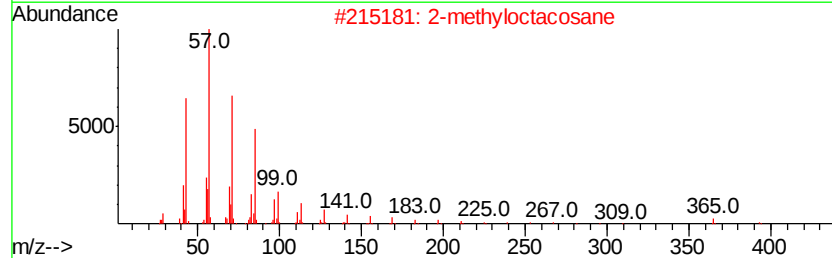
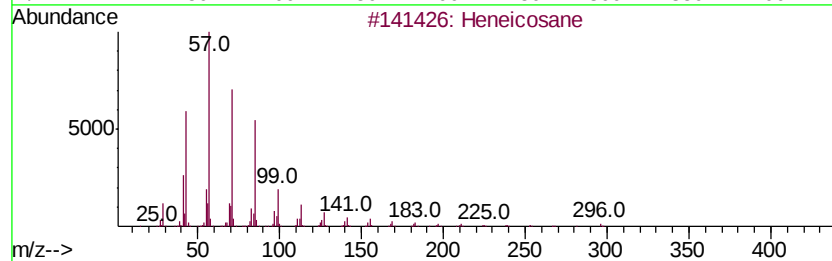
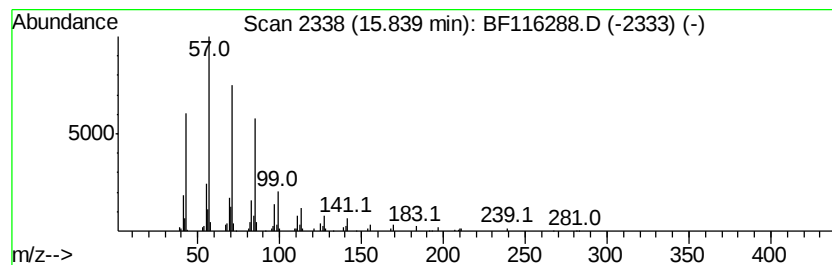
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	4.42 ng	204251	Perylene-d12	15.43

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Octadecane, 2-methyl-	268	C19H40	001560-88-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081519\
Data File : BF116288.D
Acq On : 15 Aug 2019 19:49
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Sample : K4356-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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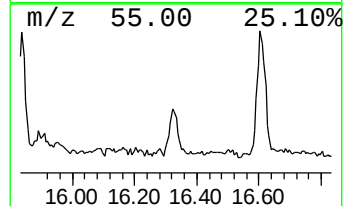
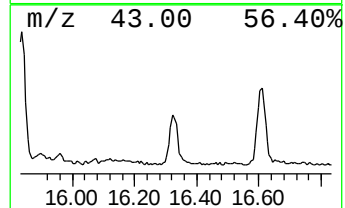
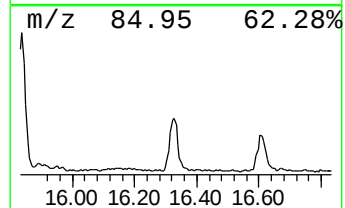
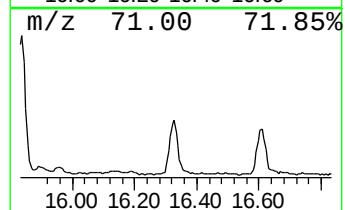
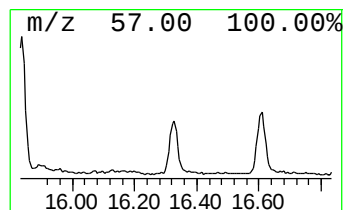
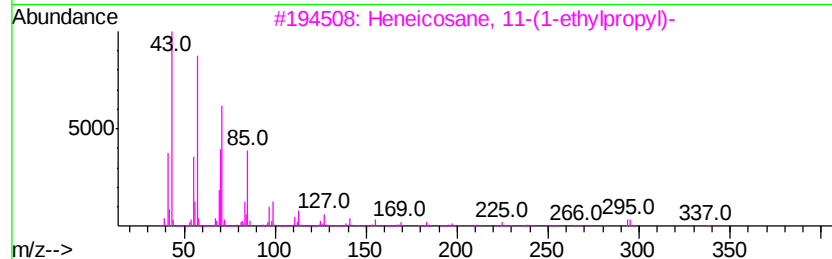
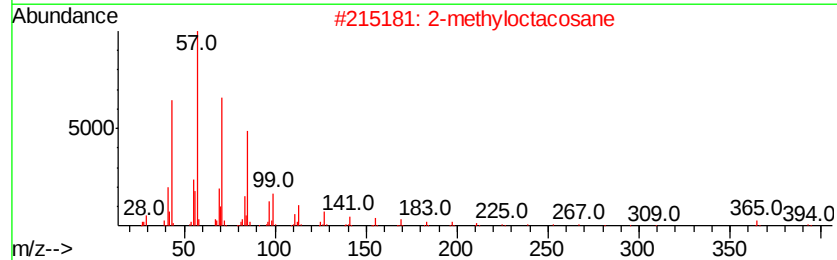
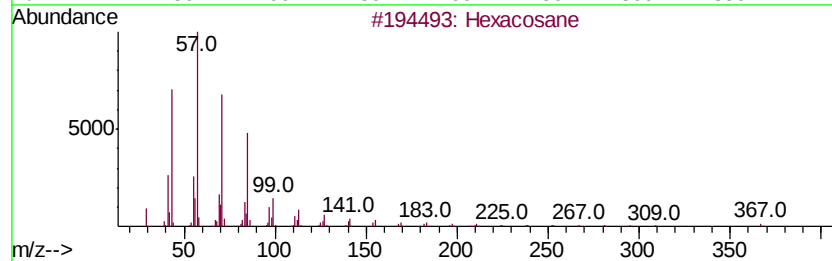
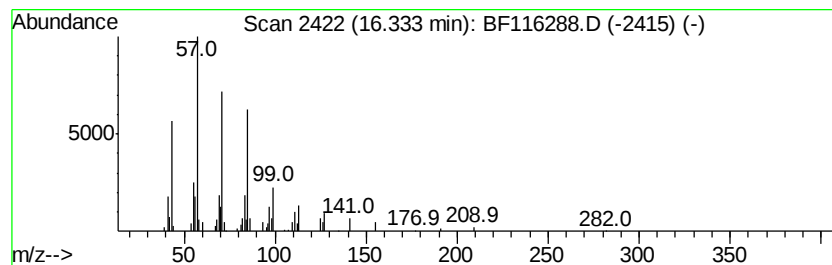
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	2.16 ng	99941	Perylene-d12	15.43

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4			Heptacosane	380	C27H56	000593-49-7	87
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081519\
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Sample : K4356-01
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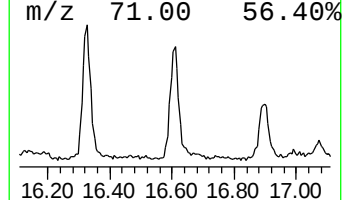
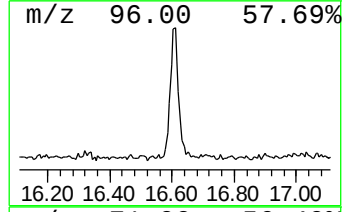
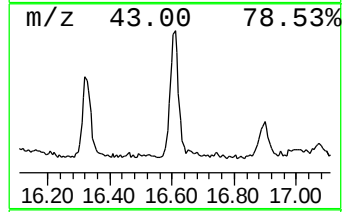
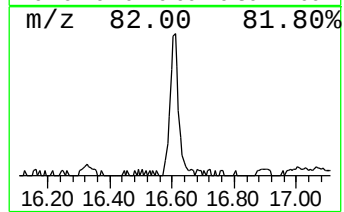
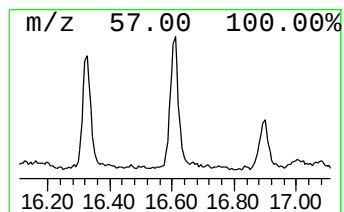
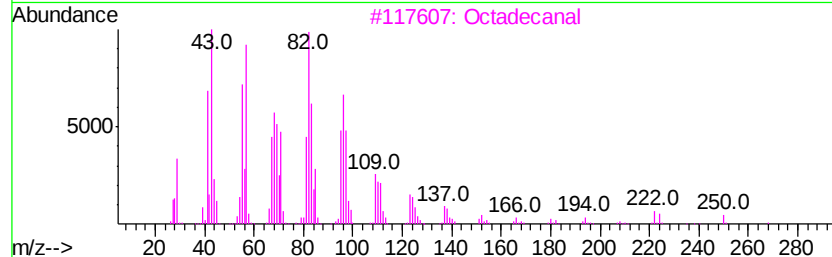
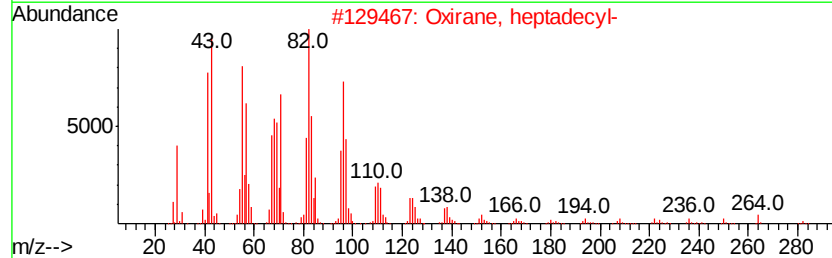
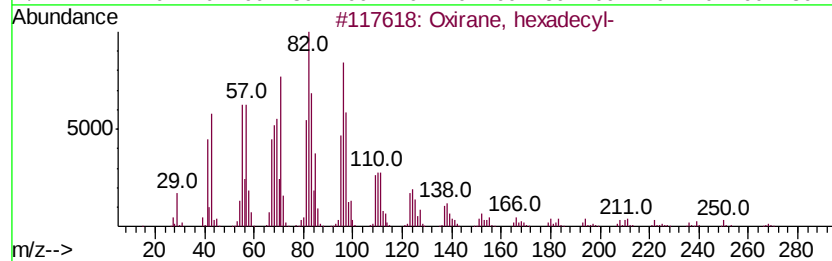
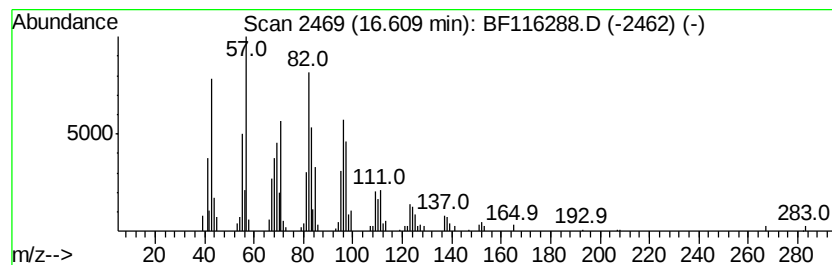
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Oxirane, hexadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.61	4.97 ng	229789	Perylene-d12		15.43
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3	Octadecanal	268	C18H36O	000638-66-4	74
4	Hexadecanal	240	C16H32O	000629-80-1	58
5	1-Heptacosanol	396	C27H56O	002004-39-9	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081519\
Data File : BF116288.D
Acq On : 15 Aug 2019 19:49
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Instrument :
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ClientSampleId :
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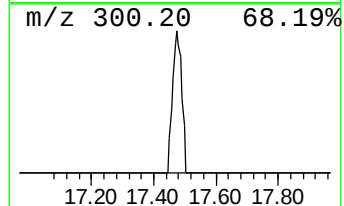
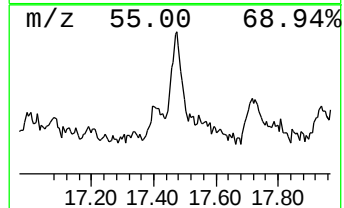
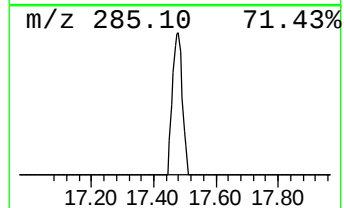
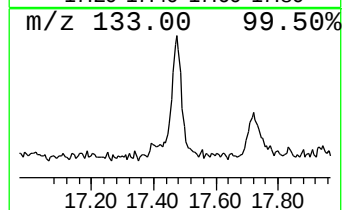
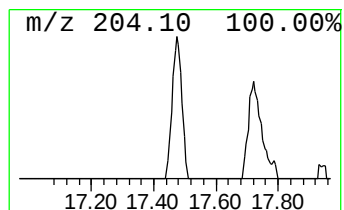
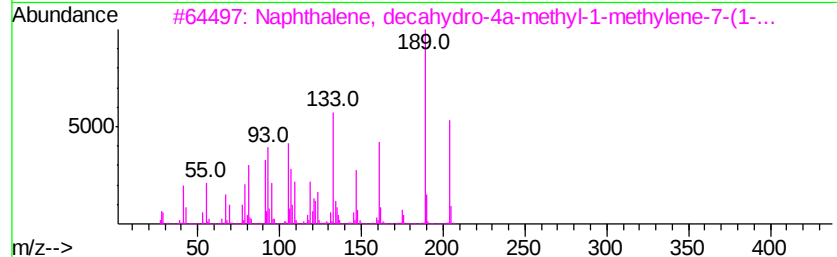
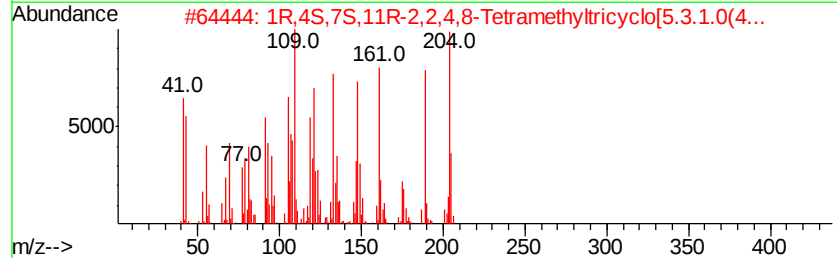
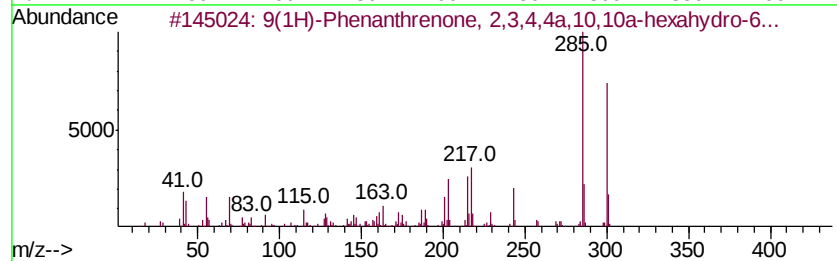
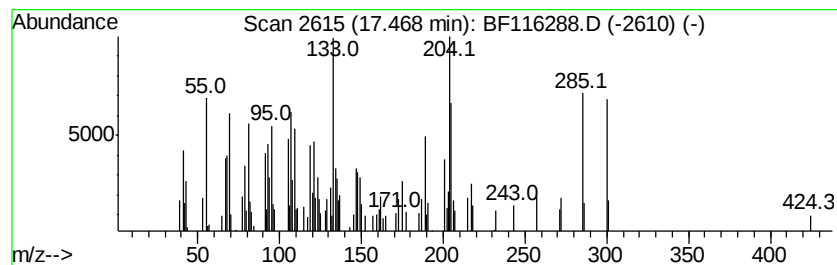
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 9(1H)-Phenanthrenone, 2,3,4... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	4.65 ng	214827	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9(1H)-Phenanthrenone, 2,3,4,4a,1...	300	C20H28O2	000511-05-7	59
2		1R,4S,7S,11R-2,2,4,8-Tetramethyl...	204	C15H24	1000140-07-6	49
3		Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	43
4		1H-Cycloprop[elazulene, 1a,2,3,4...	204	C15H24	000489-40-7	38
5		1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081519\
Data File : BF116288.D
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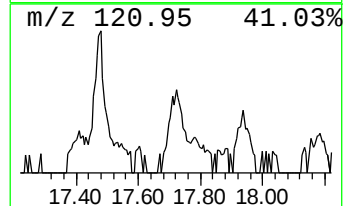
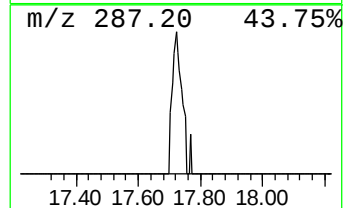
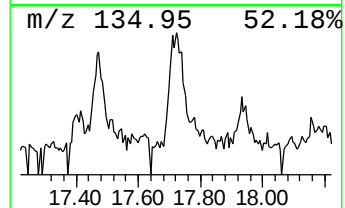
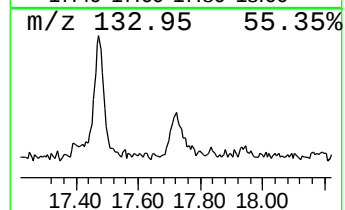
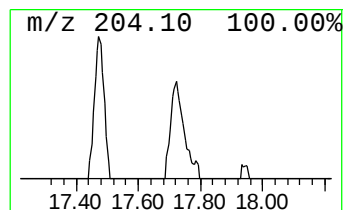
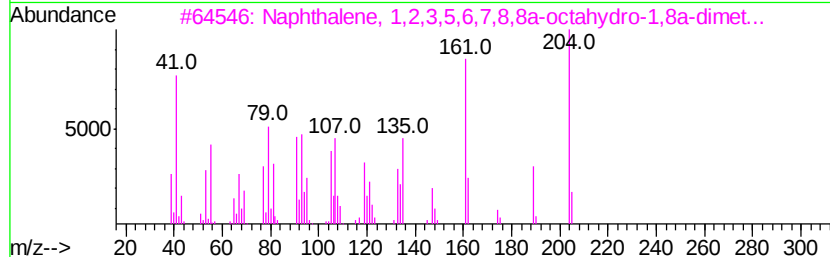
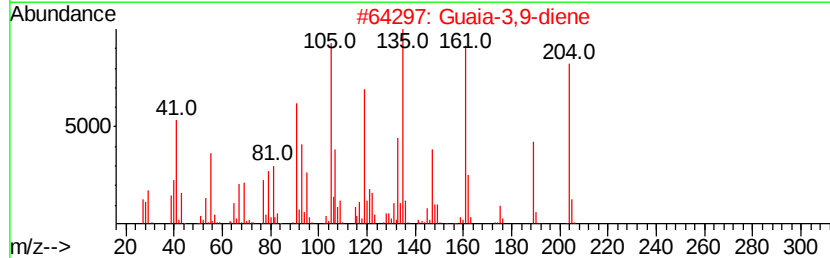
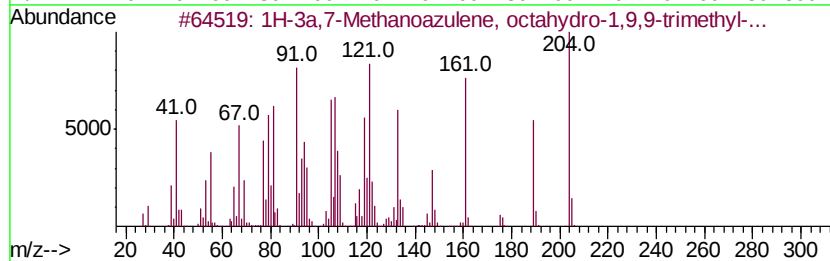
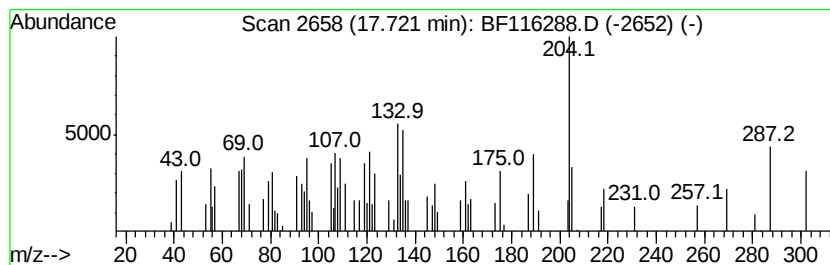
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1H-3a,7-Methanoazulene, oct... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.72	2.24 ng	103802	Perylene-d12	15.43

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	64
2			Guaia-3,9-diene	204	C15H24	000489-83-8	49
3			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	47
4			2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H200	124957-09-1	45
5			1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081519\
Data File : BF116288.D
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Sample : K4356-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.59	6.59	45.7	ng	920806	1	6.82	403275	20.0
1-Heneicosanol	13.80	7.4	ng	281250	5	13.98	762932	20.0
1,19-Eicosadiene	14.24	18.6	ng	710322	5	13.98	762932	20.0
Heptadecyl heptaf...	14.43	7.6	ng	289956	5	13.98	762932	20.0
Octadecanal	14.87	8.1	ng	374678	6	15.43	924973	20.0
Heneicosane	15.84	4.4	ng	204251	6	15.43	924973	20.0
Hexacosane	16.33	2.2	ng	99941	6	15.43	924973	20.0
Oxirane, hexadecyl-	16.61	5.0	ng	229789	6	15.43	924973	20.0
9(1H)-Phenanthren...	17.47	4.7	ng	214827	6	15.43	924973	20.0
1H-3a,7-Methanoaz...	17.72	2.2	ng	103802	6	15.43	924973	20.0