

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091119\
 Data File : BF116954.D
 Acq On : 11 Sep 2019 18:54
 Operator : HP/JU
 Sample : K4786-03
 Misc :
 ALS Vial : 5 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-BF083019.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	497	500	509	rVB	30182	36063	1.77%	0.207%
2	5.440	566	570	573	rBV	1459074	1314363	64.40%	7.527%
3	6.110	681	684	686	rBV	38753	33876	1.66%	0.194%
4	6.451	738	742	752	rBV	1383443	1489380	72.98%	8.530%
5	6.528	752	755	759	rVB	50721	42147	2.07%	0.241%
6	6.592	762	766	769	rBV	1770091	1506142	73.80%	8.626%
7	6.822	801	805	815	rBV	543531	437698	21.45%	2.507%
8	6.981	828	832	835	rBV	1332703	1135697	55.65%	6.504%
9	7.381	895	900	903	rBV	1005621	871021	42.68%	4.988%
10	8.104	1019	1023	1043	rBV	594719	593757	29.09%	3.400%
11	9.175	1201	1205	1215	rBV	2149814	1847429	90.52%	10.580%
12	9.563	1268	1271	1279	rBV	147820	141826	6.95%	0.812%
13	9.851	1317	1320	1330	rVB	829995	707636	34.67%	4.053%
14	10.639	1450	1454	1466	rBV	1126863	1037143	50.82%	5.940%
15	11.333	1568	1572	1580	rBV	760659	737929	36.16%	4.226%
16	11.863	1656	1662	1671	rBV	136757	197908	9.70%	1.133%
17	12.569	1775	1782	1784	rBV3	28861	47740	2.34%	0.273%
18	12.645	1790	1795	1807	rBV	198129	269875	13.22%	1.546%
19	12.916	1837	1841	1844	rBV	2234458	2040827	100.00%	11.688%
20	13.145	1877	1880	1890	rVB6	16235	24260	1.19%	0.139%
21	13.416	1923	1926	1929	rVB	125727	104681	5.13%	0.600%
22	13.821	1989	1995	2011	rBV3	115207	294486	14.43%	1.687%
23	13.968	2015	2020	2028	rVB	743946	726527	35.60%	4.161%
24	14.127	2042	2047	2050	rBV	34688	32169	1.58%	0.184%
25	14.433	2094	2099	2101	rBV	68024	61890	3.03%	0.354%
26	14.733	2146	2150	2154	rVB	98839	90508	4.43%	0.518%
27	14.804	2159	2162	2166	rVB	39393	42038	2.06%	0.241%
28	15.062	2201	2206	2210	rBV	137476	151324	7.41%	0.867%
29	15.415	2260	2266	2275	rVB	498533	778376	38.14%	4.458%
30	15.857	2336	2341	2348	rBV	104314	156643	7.68%	0.897%
31	15.968	2350	2360	2369	rVV	15532	62511	3.06%	0.358%
32	16.345	2418	2424	2430	rBV2	43056	78234	3.83%	0.448%
33	16.921	2517	2522	2527	rBV6	21623	43138	2.11%	0.247%
34	17.180	2561	2566	2571	rVB7	11961	25605	1.25%	0.147%

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ClientSampleId :
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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.980	2693	2702	2712	rBV7	64849	155937	7.64%	0.893%
36	18.392	2762	2772	2773	rBV6	32698	79997	3.92%	0.458%
37	18.668	2813	2819	2832	rVB6	21968	64226	3.15%	0.368%

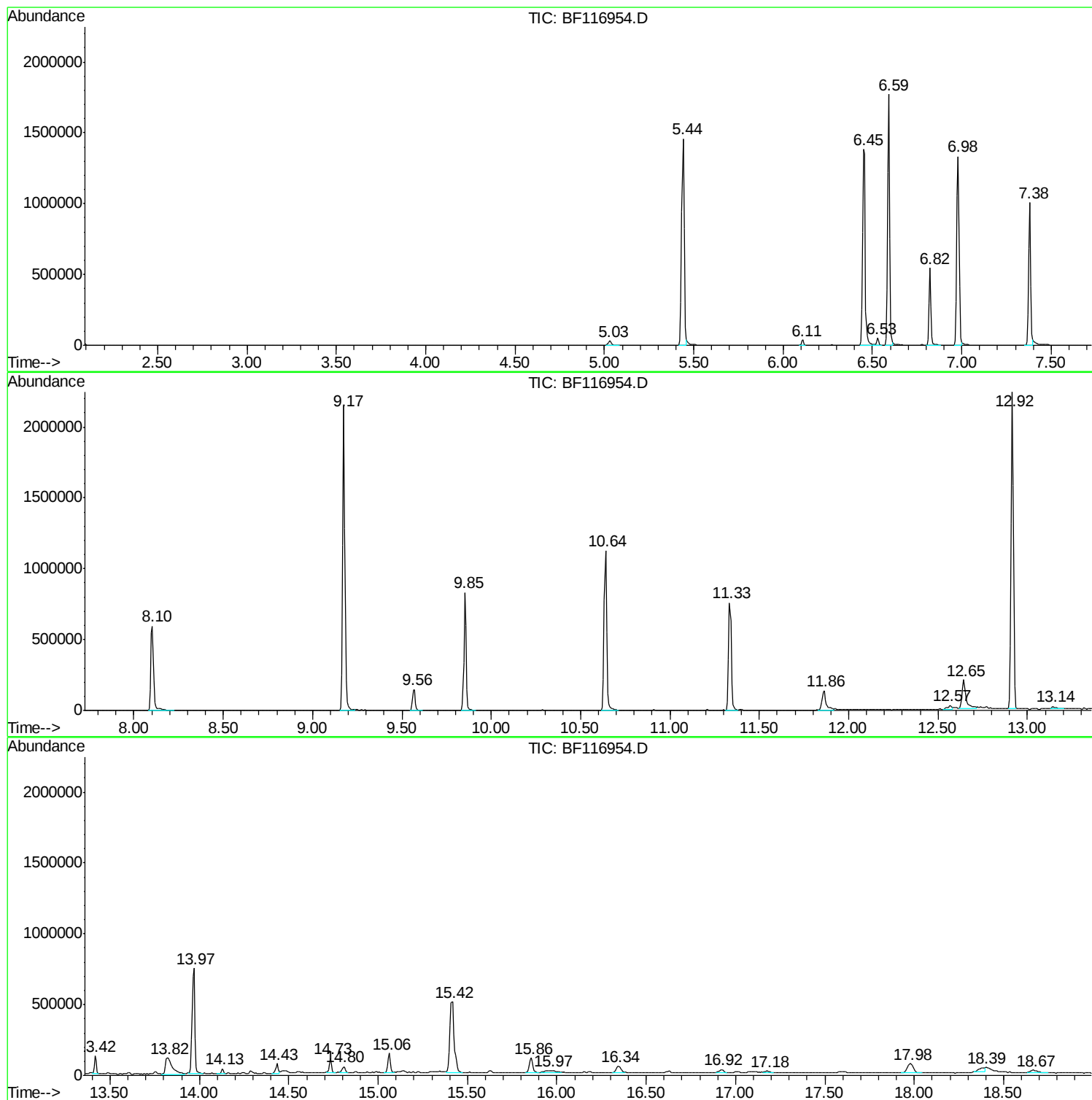
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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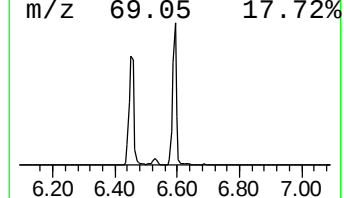
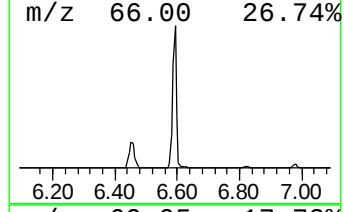
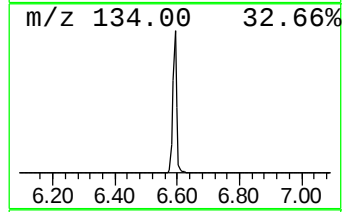
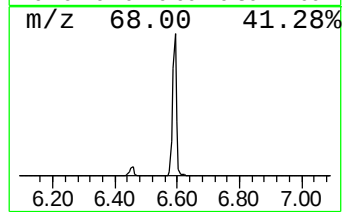
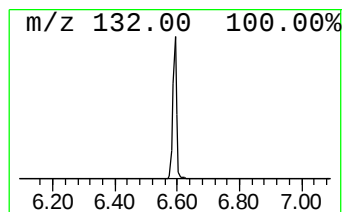
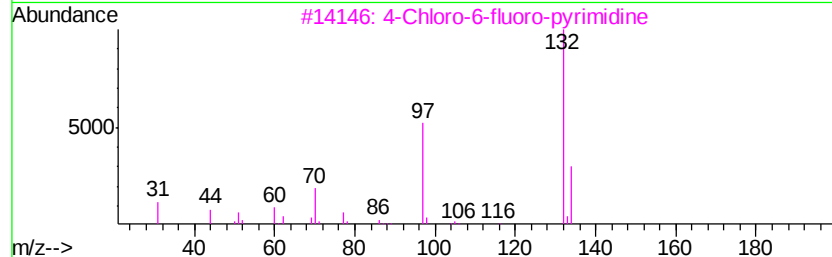
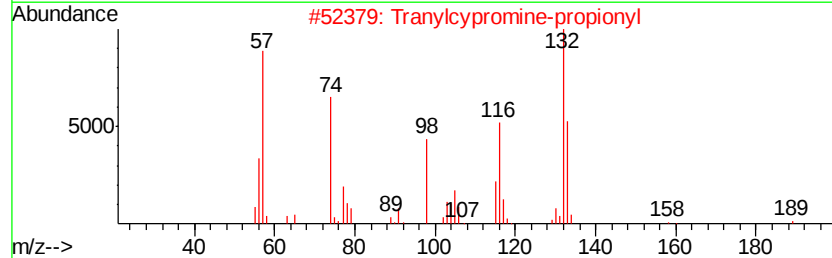
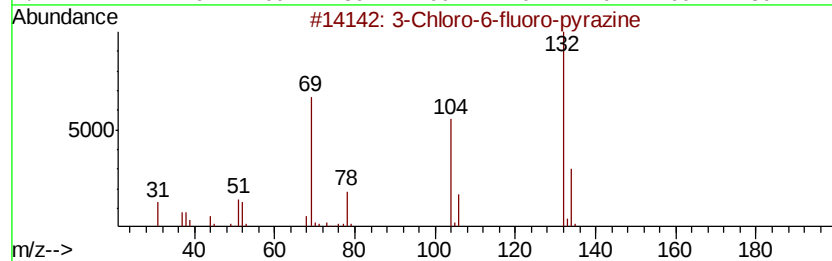
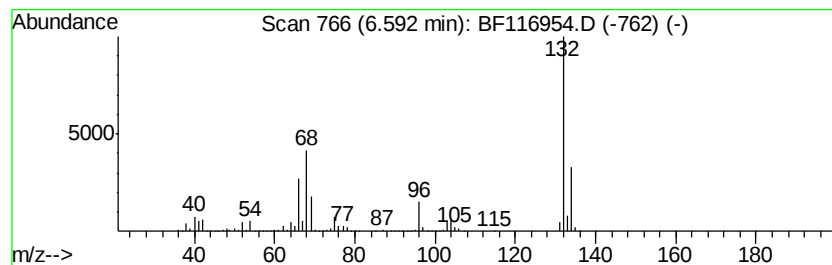
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	68.82 ng	1506140	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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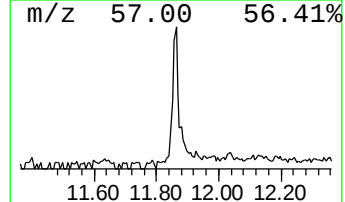
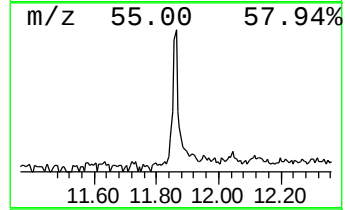
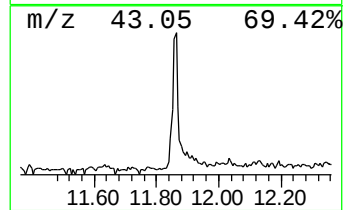
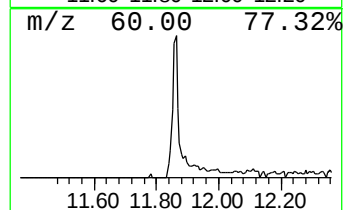
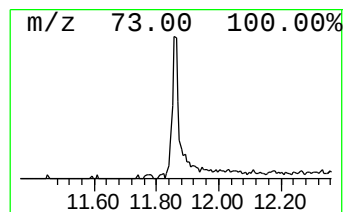
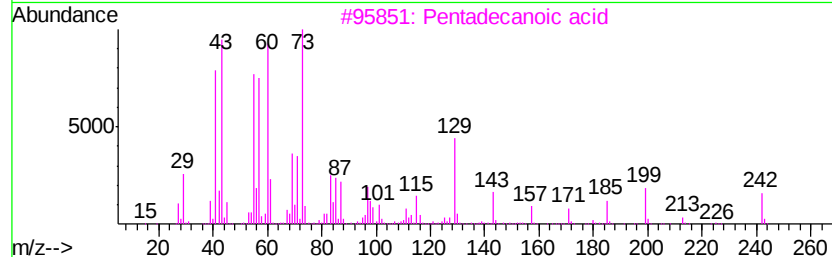
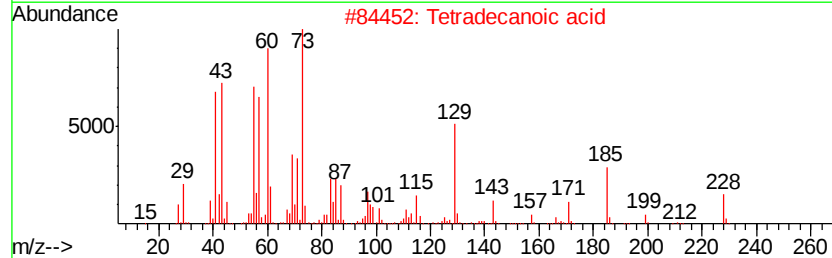
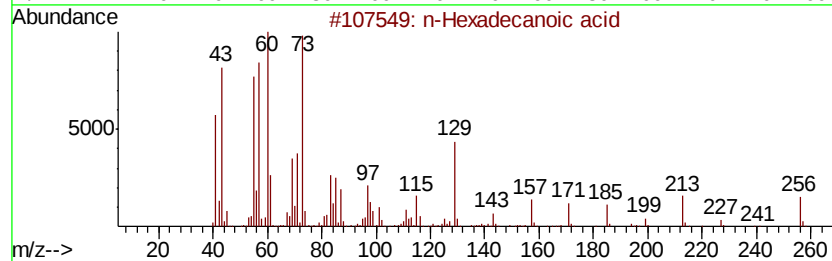
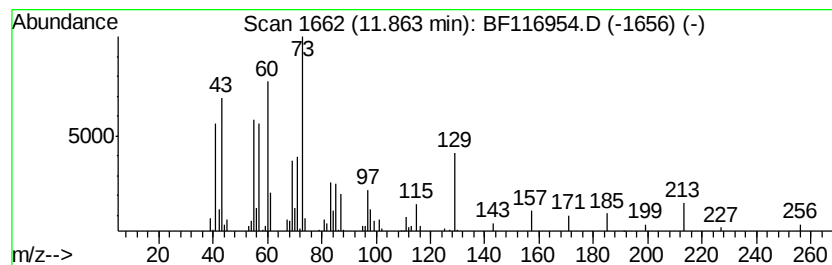
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	5.36 ng	197908	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	18
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	15



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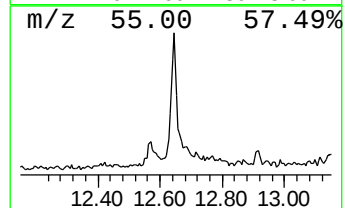
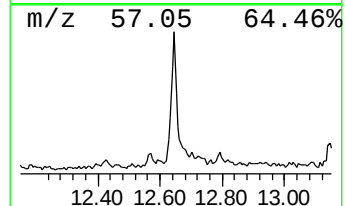
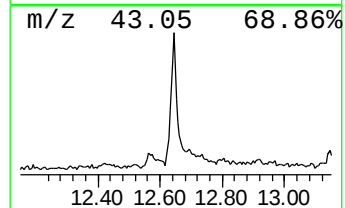
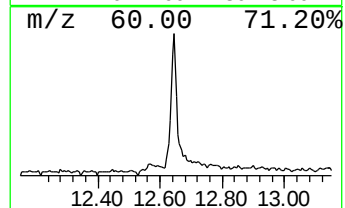
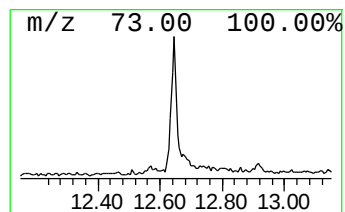
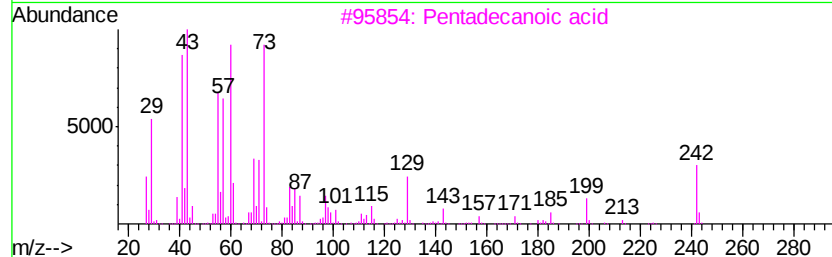
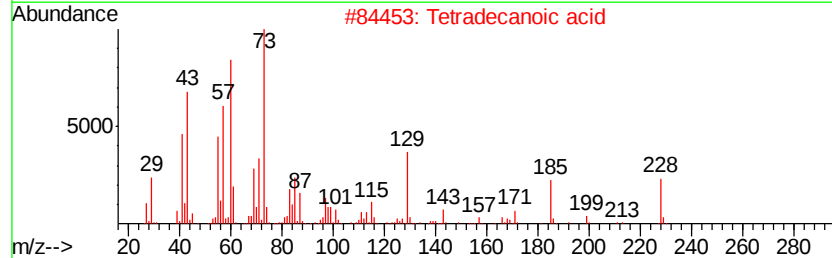
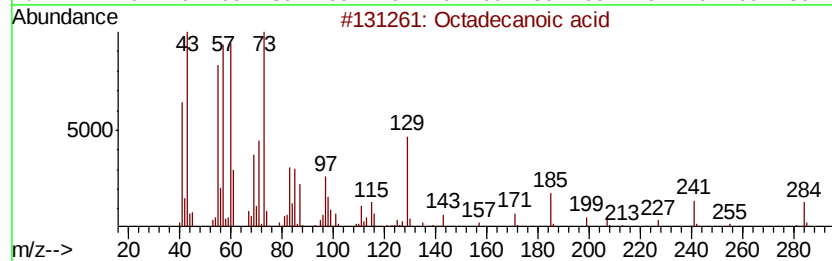
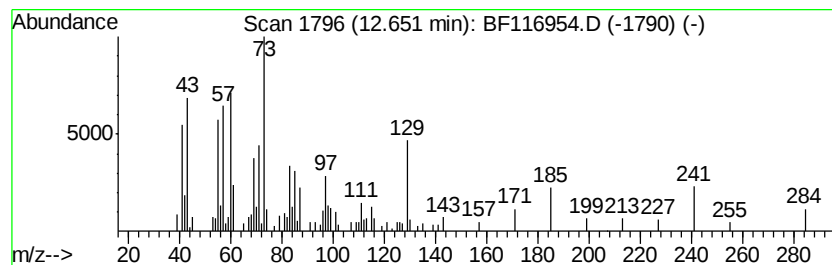
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.65	7.31 ng	269875	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	25
5	n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25



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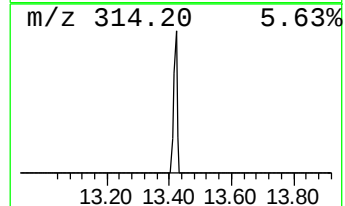
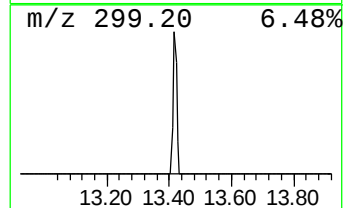
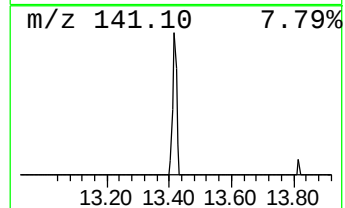
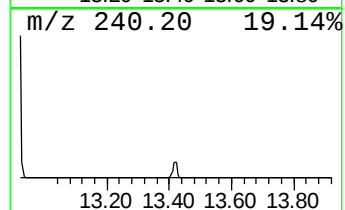
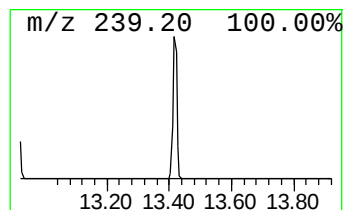
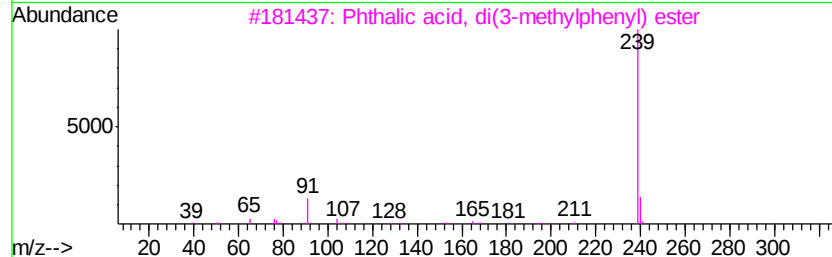
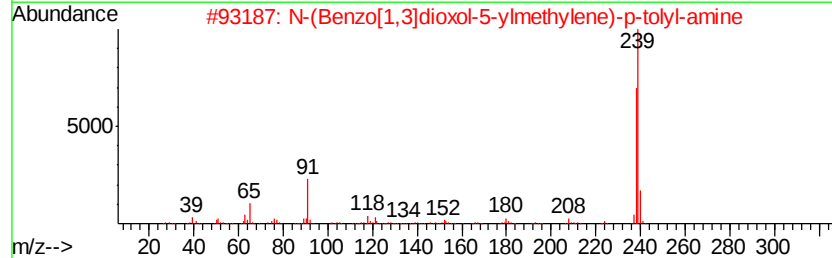
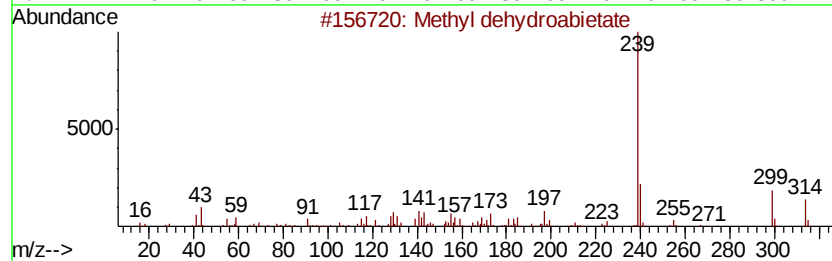
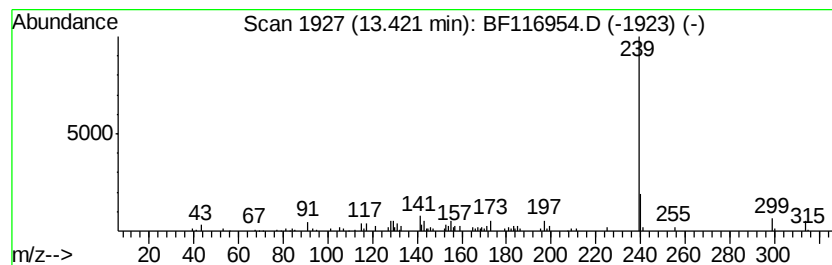
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Methyl dehydroabietate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	2.88 ng	104681	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl dehydroabietate	314	C21H30O2	001235-74-1	95
2		N-(Benzo[1,3]dioxol-5-ylmethyl)en...	239	C15H13NO2	007402-58-6	58
3		Phthalic acid, di(3-methylphenyl)...	346	C22H18O4	1000315-37-3	53
4		9,10-Anthracenedione, 1-amino-4-...	239	C14H9NO3	000116-85-8	53
5		Imidazolo[2,1-b]thiazole, 5-(3-i...	239	C13H9N3S	327097-37-0	50



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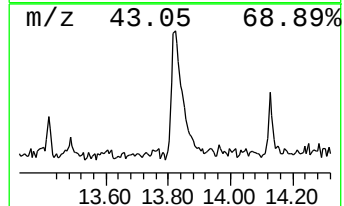
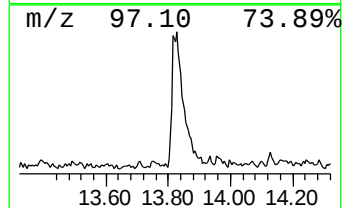
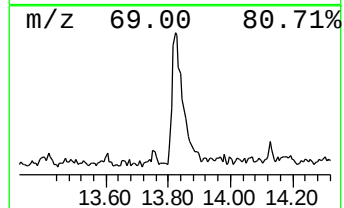
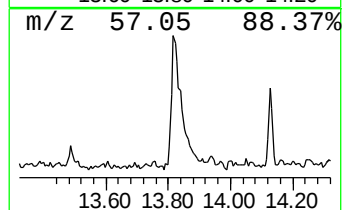
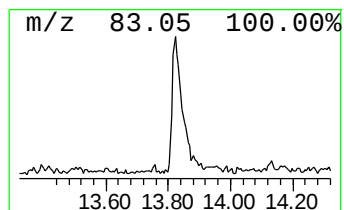
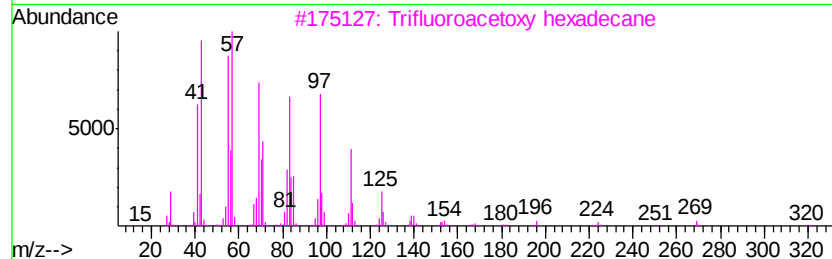
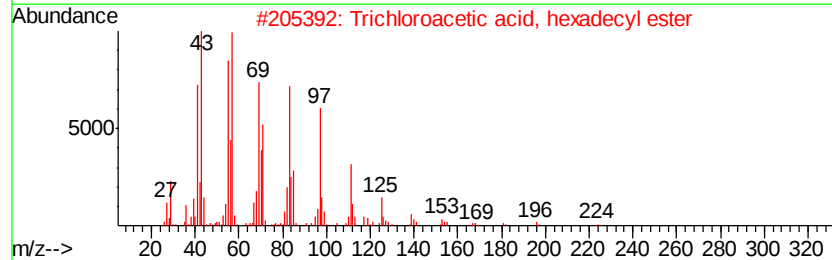
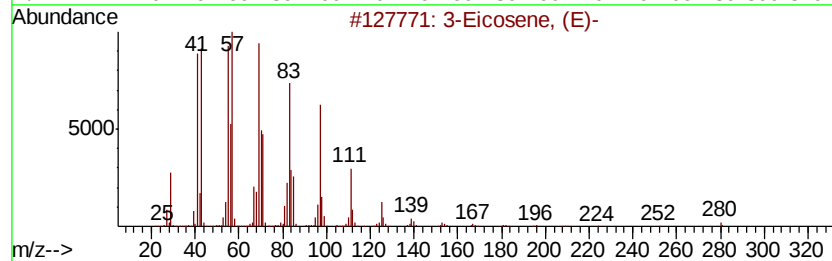
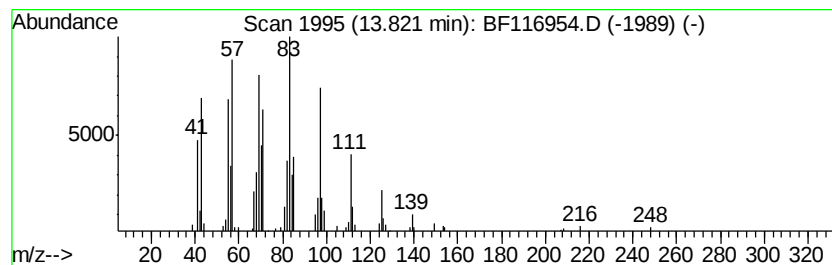
Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.82	8.11 ng	294486	Chrysene-d12	13.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116954.D
Acq On : 11 Sep 2019 18:54
Operator : HP/JU
Sample : K4786-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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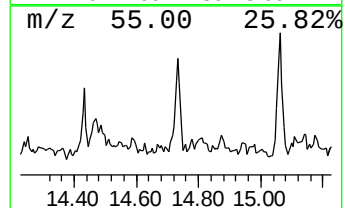
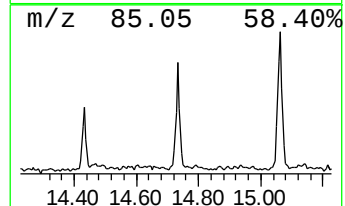
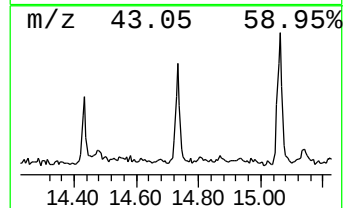
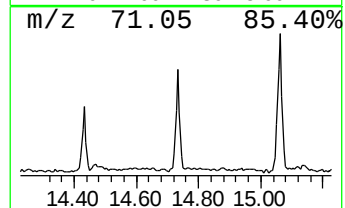
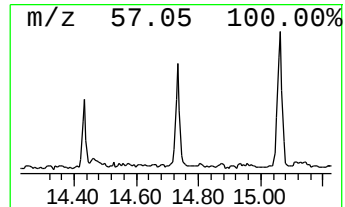
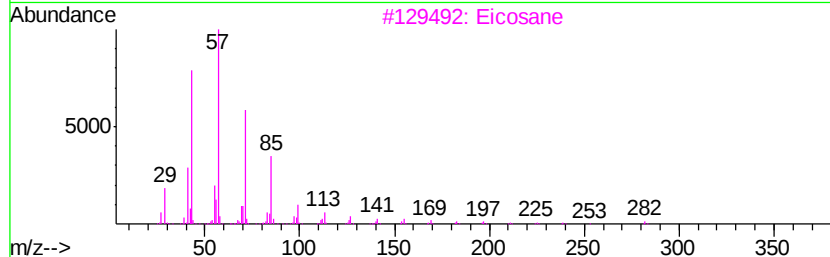
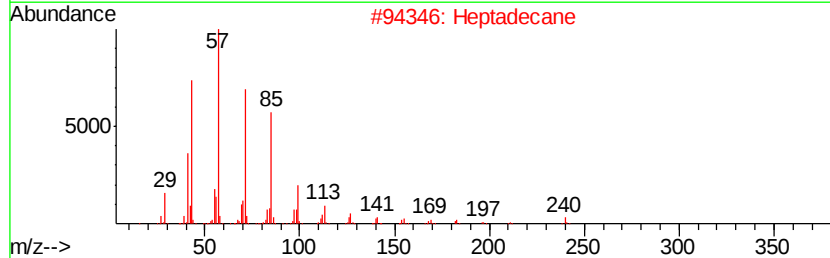
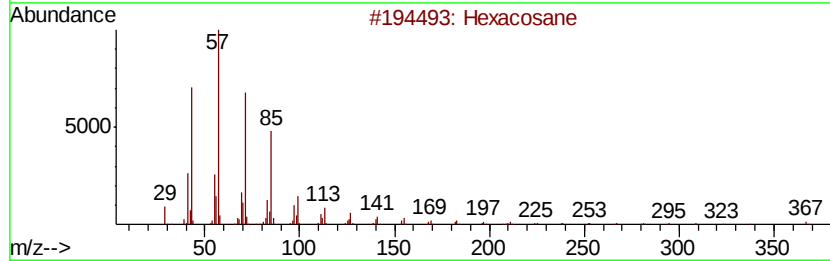
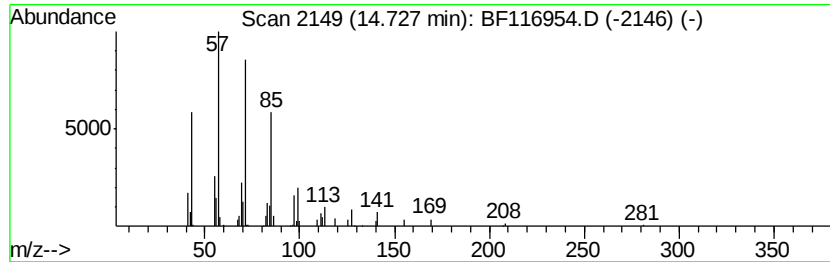
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.33 ng	90508	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	87
2		Heptadecane	240	C17H36	000629-78-7	86
3		Eicosane	282	C20H42	000112-95-8	80
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5		Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
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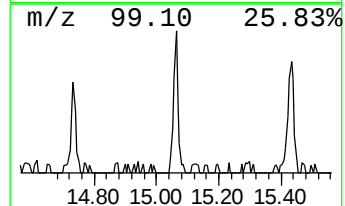
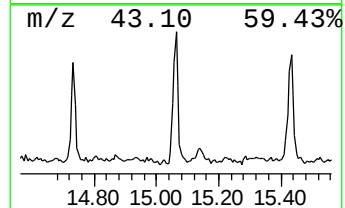
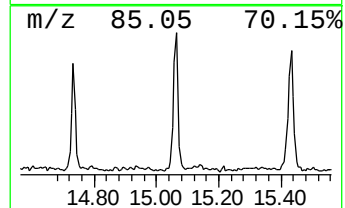
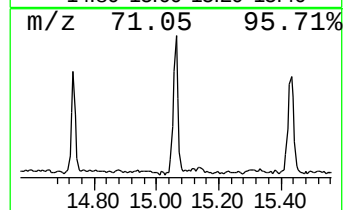
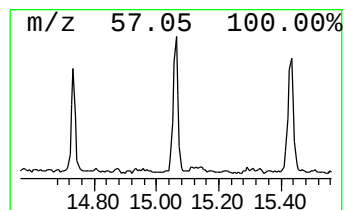
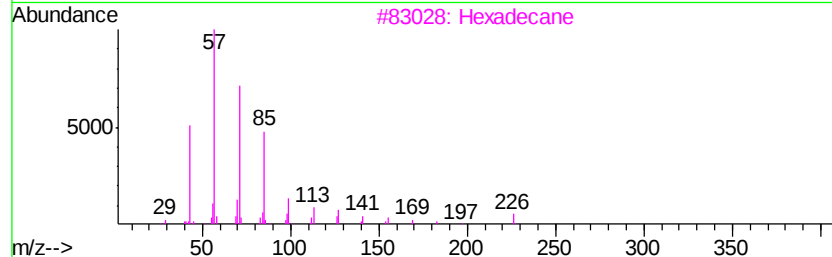
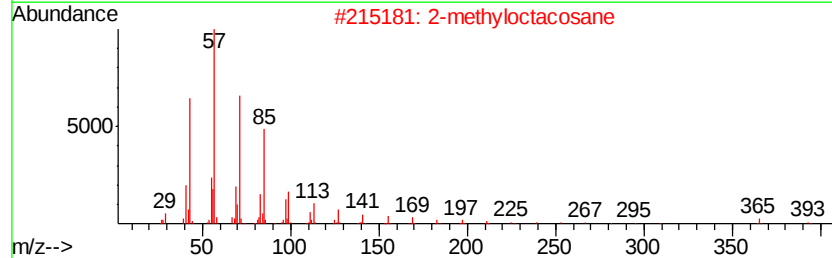
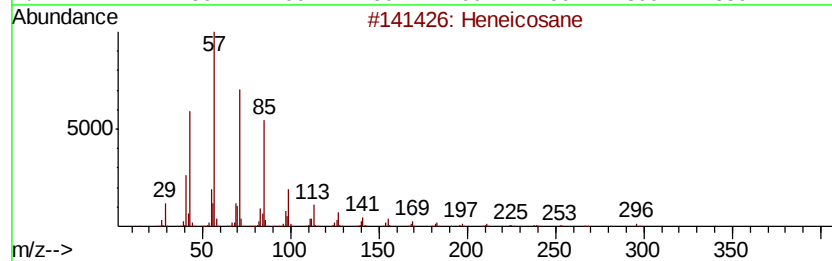
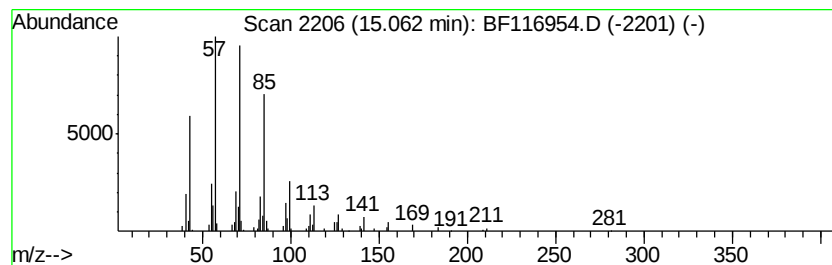
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	3.89 ng	151324	Perylene-d12	15.42

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	87
3	Hexadecane		226	C16H34	000544-76-3	87
4	triacontane		422	C30H62	000638-68-6	86
5	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116954.D
Acq On : 11 Sep 2019 18:54
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Sample : K4786-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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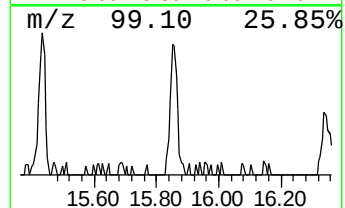
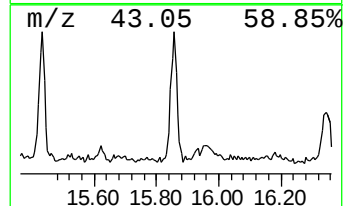
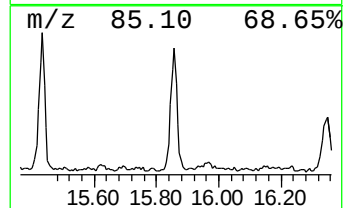
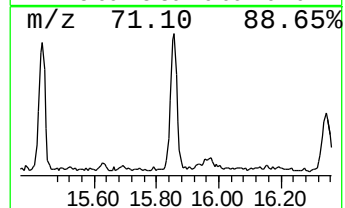
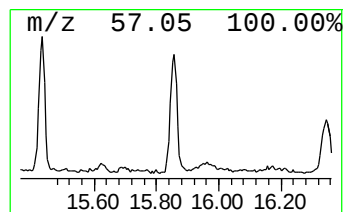
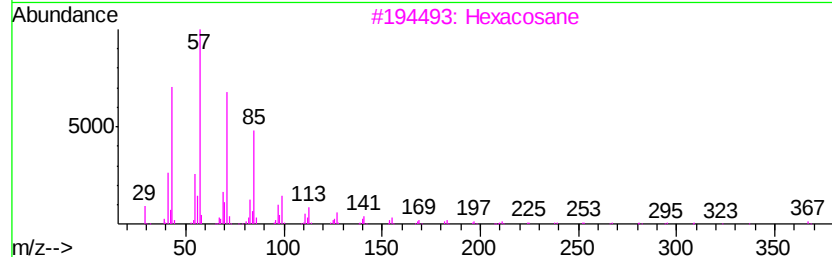
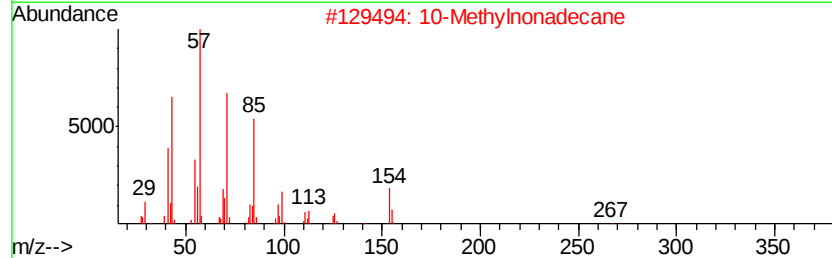
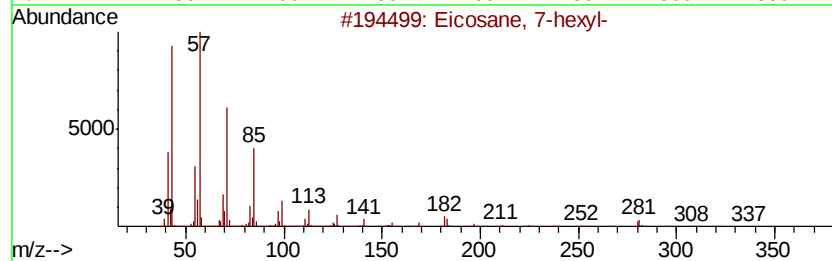
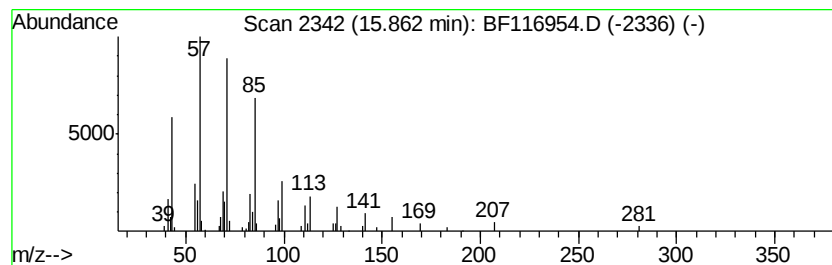
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	4.02 ng	156643	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
2		10-Methylnonadecane	282	C20H42	056862-62-5	90
3		Hexacosane	366	C26H54	000630-01-3	87
4		Octacosane	394	C28H58	000630-02-4	86
5		Hexadecane	226	C16H34	000544-76-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116954.D
Acq On : 11 Sep 2019 18:54
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Misc :
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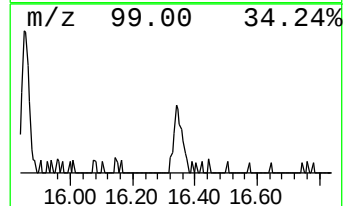
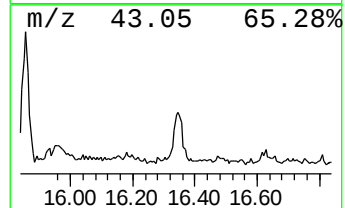
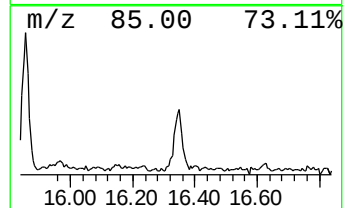
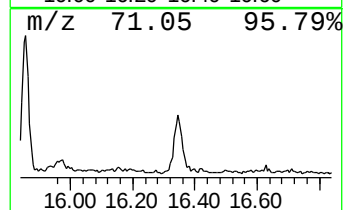
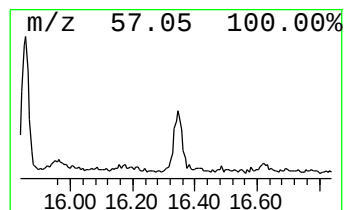
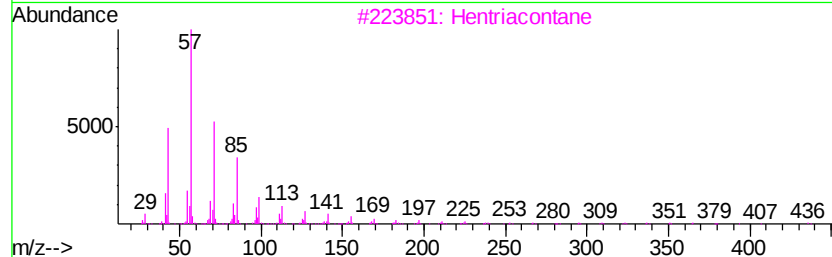
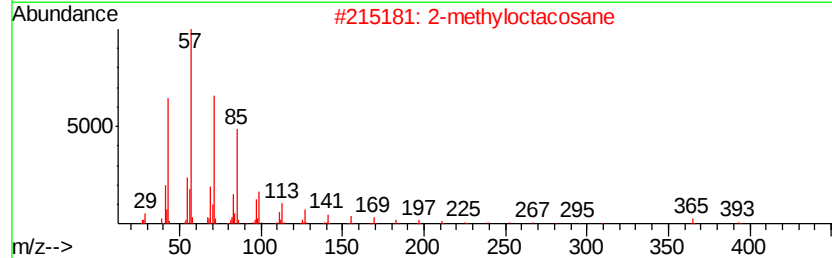
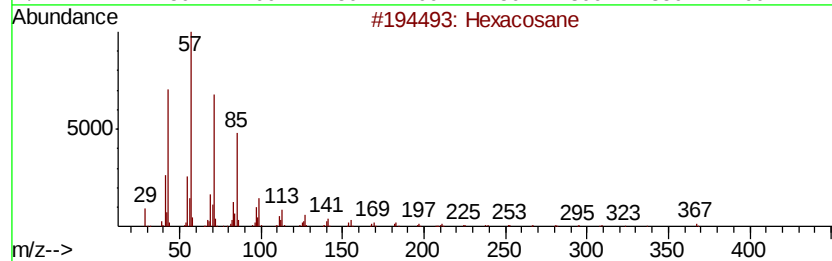
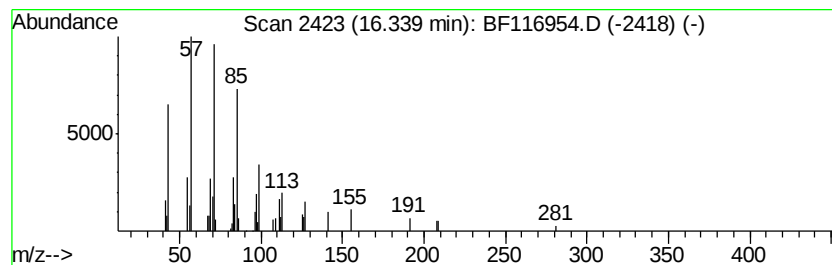
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.34	2.01 ng	78234	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	87
2		2-methyloctacosane	408	C29H60	1000376-72-8	87
3		Hentriacontane	437	C31H64	000630-04-6	86
4		Heptacosane	380	C27H56	000593-49-7	86
5		Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116954.D
Acq On : 11 Sep 2019 18:54
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Sample : K4786-03
Misc :
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Instrument :
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ClientSampleId :
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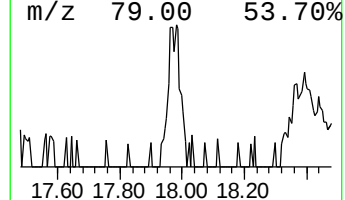
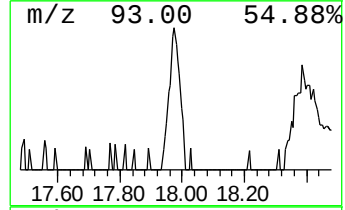
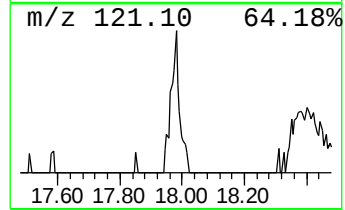
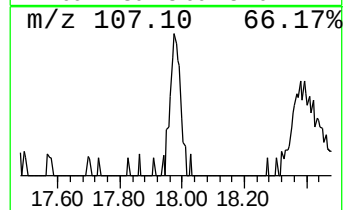
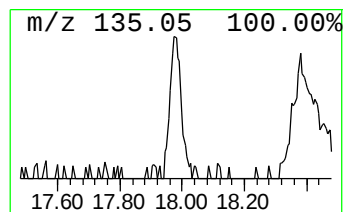
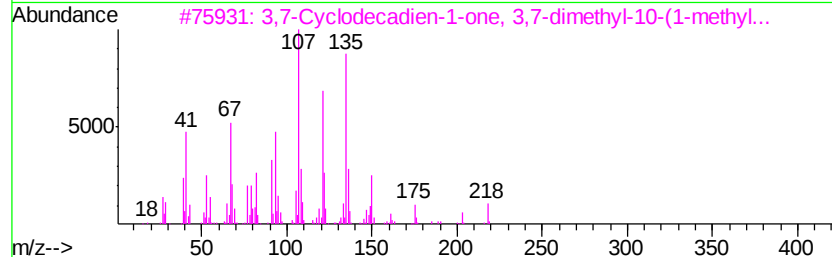
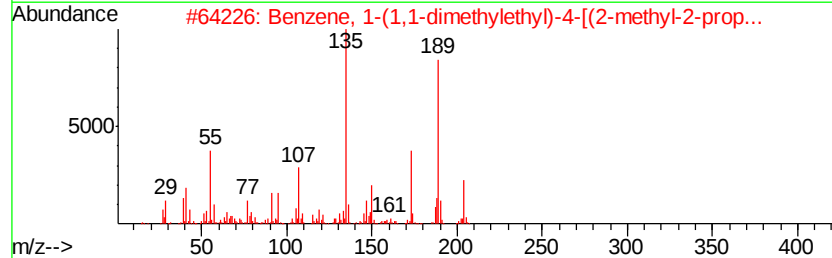
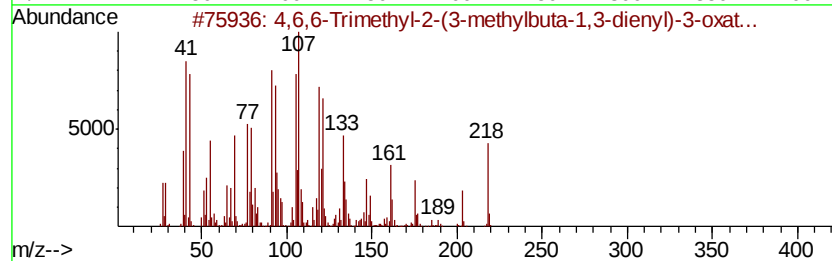
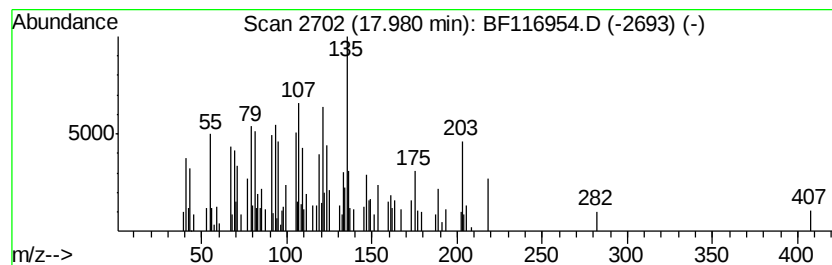
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 4,6,6-Trimethyl-2-(3-methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	4.01 ng	155937	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,6,6-Trimethyl-2-(3-methylbuta-...	218	C15H22O	1000190-22-2	51
2		Benzene, 1-(1,1-dimethylethyl)-4...	204	C14H20O	054932-87-5	35
3		3,7-Cyclodecadien-1-one, 3,7-dim...	218	C15H22O	006902-91-6	30
4		2-Heptenoic acid, 4-cyclopropyl-...	194	C12H18O2	074793-23-0	27
5		2,6,10,10-Tetramethylbicyclo[7.2...	204	C15H24	136296-37-2	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116954.D
Acq On : 11 Sep 2019 18:54
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ALS Vial : 5 Sample Multiplier: 1

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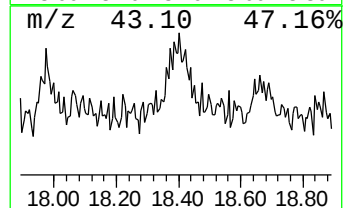
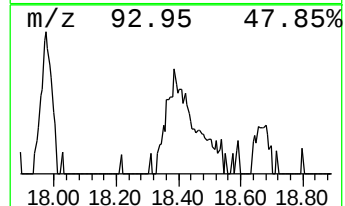
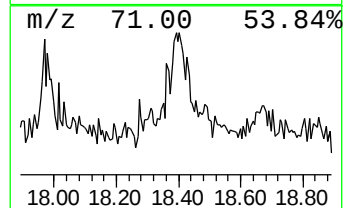
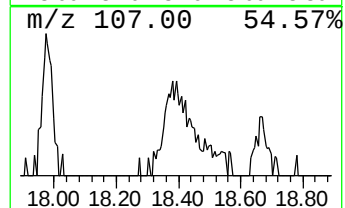
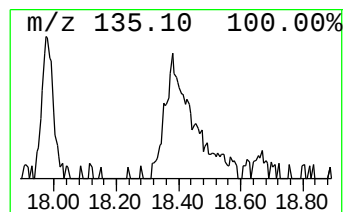
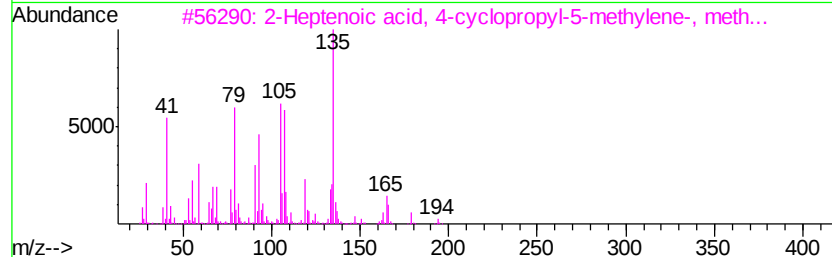
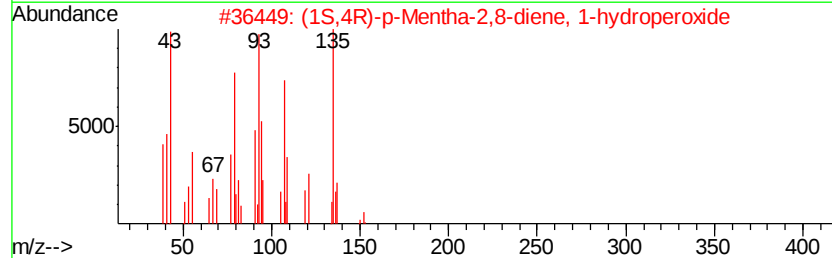
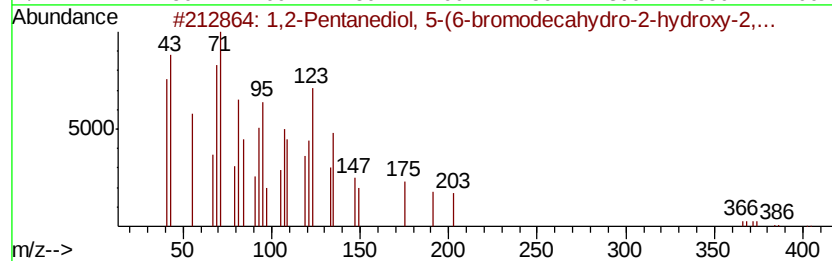
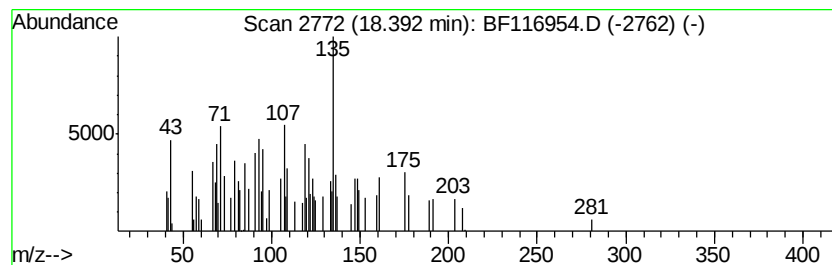
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown18.39 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.06 ng	79997	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Pentanediol, 5-(6-bromodecah...	402	C20H35BrO3	115346-29-7	43
2		(1S,4R)-p-Mentha-2,8-diene, 1-hy...	168	C10H16O2	1000292-73-9	35
3		2-Heptenoic acid, 4-cyclopropyl-...	194	C12H18O2	074793-23-0	35
4		Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	27
5		Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091119\
Data File : BF116954.D
Acq On : 11 Sep 2019 18:54
Operator : HP/JU
Sample : K4786-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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
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n-Hexadecanoic acid	11.86	5.4	ng	197908	4	11.33	737929	20.0
Octadecanoic acid	12.65	7.3	ng	269875	4	11.33	737929	20.0
Methyl dehydroabi...	13.42	2.9	ng	104681	5	13.97	726527	20.0
3-Eicosene, (E)-	13.82	8.1	ng	294486	5	13.97	726527	20.0
Hexacosane	14.73	2.3	ng	90508	6	15.42	778376	20.0
Heneicosane	15.06	3.9	ng	151324	6	15.42	778376	20.0
Eicosane, 7-hexyl-	15.86	4.0	ng	156643	6	15.42	778376	20.0
2-methyloctacosane	16.34	2.0	ng	78234	6	15.42	778376	20.0
4,6,6-Trimethyl-2...	17.98	4.0	ng	155937	6	15.42	778376	20.0
unknown18.39	18.39	2.1	ng	79997	6	15.42	778376	20.0