

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062719\
 Data File : BF115239.D
 Acq On : 27 Jun 2019 16:34
 Operator : HP/JU
 Sample : K3534-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-050

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-BF062119.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	4.431	419	424	429	rVB	129708	153867	3.26%	0.327%
2	5.196	548	554	557	rBV	4383836	4311428	91.48%	9.159%
3	6.237	726	731	734	rBV	4164694	4595609	97.51%	9.762%
4	6.266	734	736	742	rVB	131334	113139	2.40%	0.240%
5	6.366	748	753	756	rBV	5074474	4712879	100.00%	10.011%
6	6.596	789	792	796	rBV	1539118	1221138	25.91%	2.594%
7	6.754	815	819	822	rBV	4514517	3684962	78.19%	7.828%
8	7.160	883	888	891	rBV	3062663	2880584	61.12%	6.119%
9	7.401	926	929	933	rVB	64711	54336	1.15%	0.115%
10	7.878	1006	1010	1013	rBV	1972634	1543119	32.74%	3.278%
11	8.954	1189	1193	1196	rBV	5350734	4659532	98.87%	9.898%
12	9.348	1257	1260	1265	rBV	989590	729598	15.48%	1.550%
13	9.625	1303	1307	1310	rBV	1866161	1741593	36.95%	3.700%
14	10.401	1435	1439	1443	rBV	3468302	3200893	67.92%	6.799%
15	11.095	1553	1557	1560	rBV	2234619	1865456	39.58%	3.963%
16	11.642	1647	1650	1666	rBV2	279623	391072	8.30%	0.831%
17	12.348	1765	1770	1779	rBV6	65427	151313	3.21%	0.321%
18	12.425	1779	1783	1796	rBV	576741	898086	19.06%	1.908%
19	12.577	1806	1809	1817	rVB	64469	104502	2.22%	0.222%
20	12.677	1822	1826	1829	rBV	5157695	4587522	97.34%	9.745%
21	13.142	1902	1905	1911	rBV5	40672	94442	2.00%	0.201%
22	13.601	1980	1983	1985	rBV	101715	90866	1.93%	0.193%
23	13.654	1985	1992	1998	rVV3	155397	512485	10.87%	1.089%
24	13.713	1998	2002	2005	rVB	1976379	1772779	37.62%	3.766%
25	13.919	2034	2037	2041	rBV	93909	83501	1.77%	0.177%
26	14.219	2084	2088	2093	rBV2	207891	222391	4.72%	0.472%
27	14.513	2135	2138	2142	rBV	213448	209321	4.44%	0.445%
28	14.577	2146	2149	2153	rVB	213501	187285	3.97%	0.398%
29	14.813	2185	2189	2193	rBV	396781	407118	8.64%	0.865%
30	15.071	2229	2233	2237	rVB	1312435	1389509	29.48%	2.952%
31	15.142	2242	2245	2250	rVB	183337	212475	4.51%	0.451%
32	15.524	2306	2310	2314	rBV	219251	292897	6.21%	0.622%

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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-BF062119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

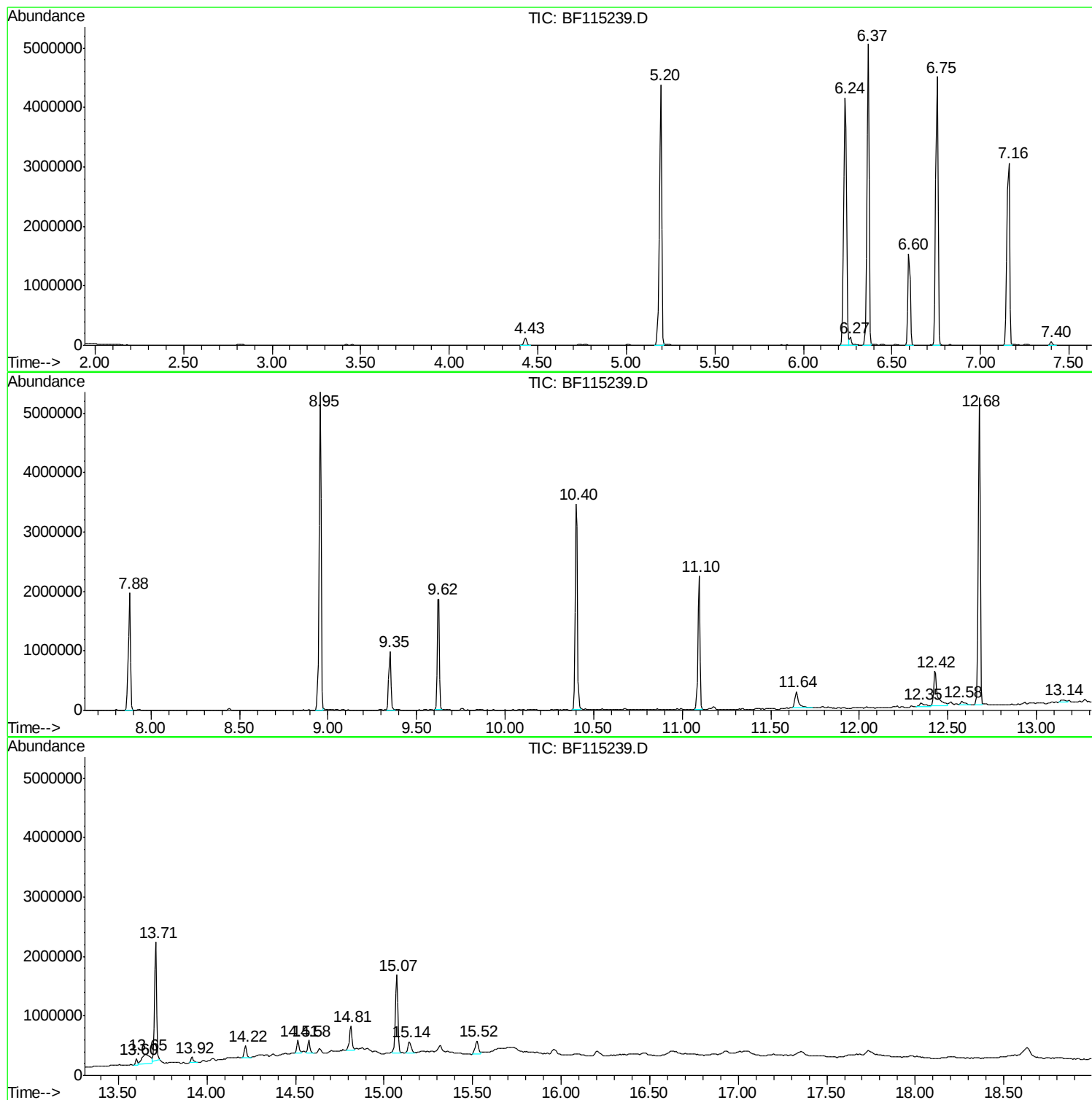
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF062119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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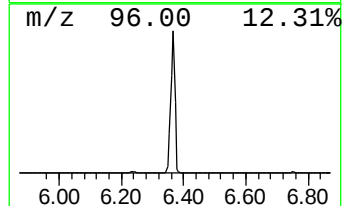
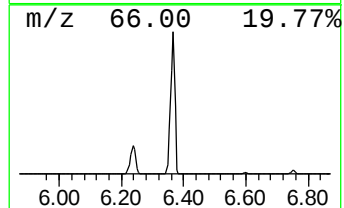
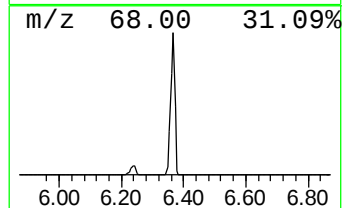
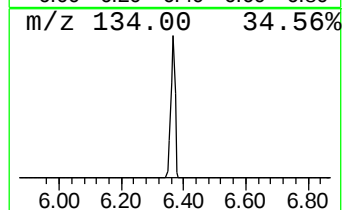
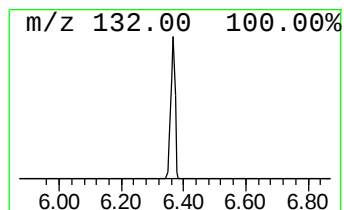
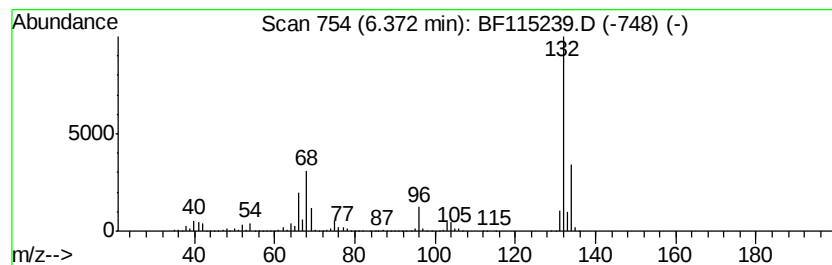
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	77.19 ng	4712880	1,4-Dichlorobenzene-d4	6.60

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		2H-Cyclopentaf[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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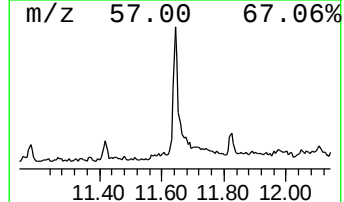
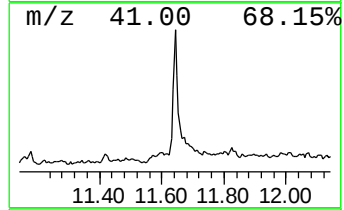
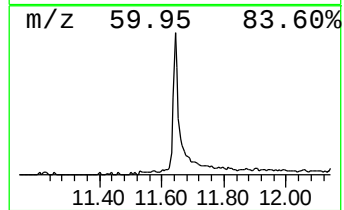
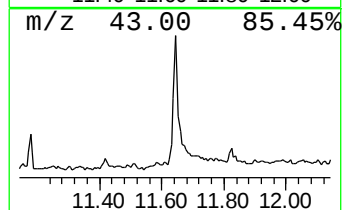
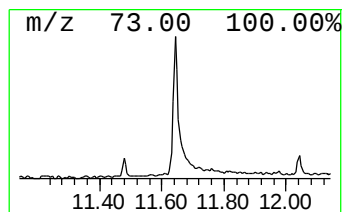
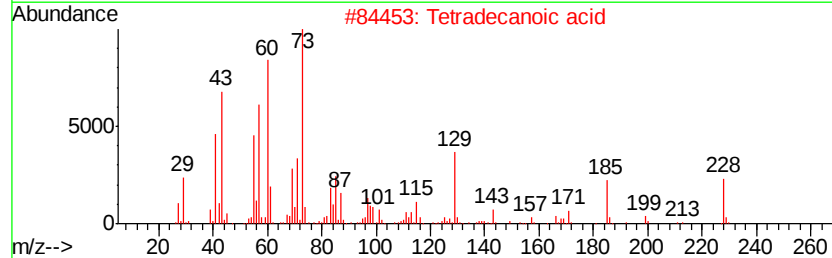
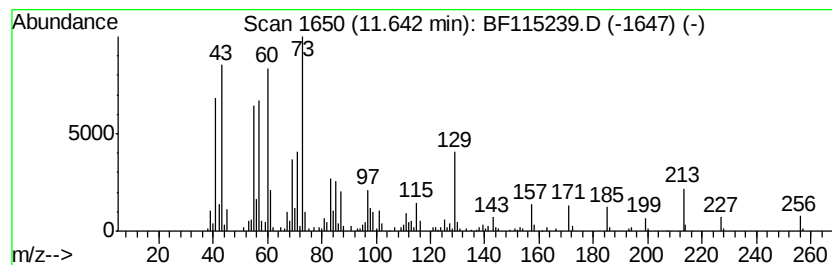
Instrument :
BNA_F
ClientSampleId :
FK-PS-01-050

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF062119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.64	4.19 ng	391072	Phenanthrene-d10		11.10	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4		Tridecanoic acid	214	C13H26O2	000638-53-9	91
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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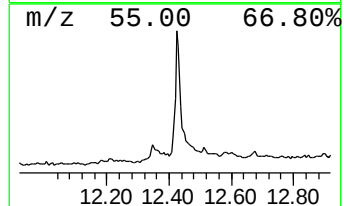
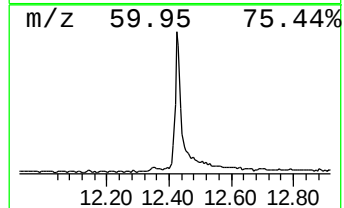
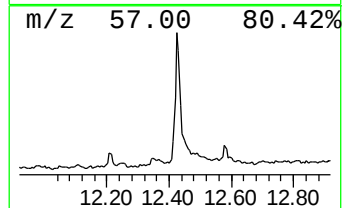
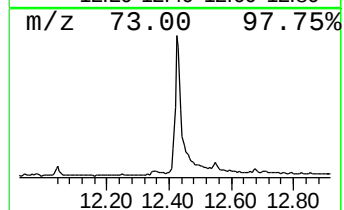
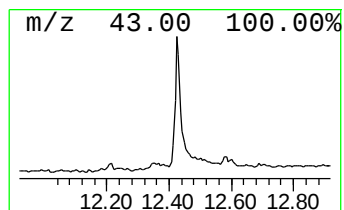
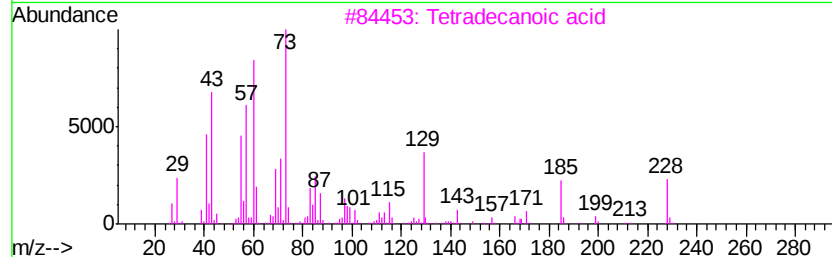
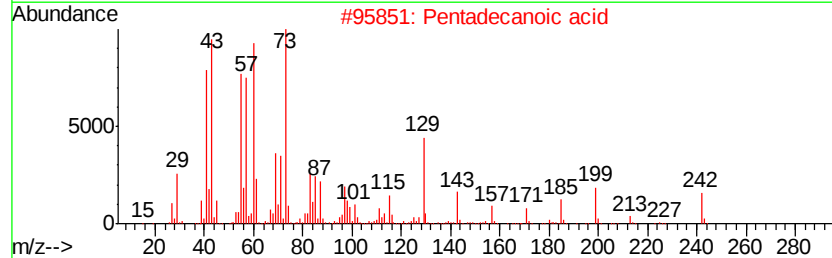
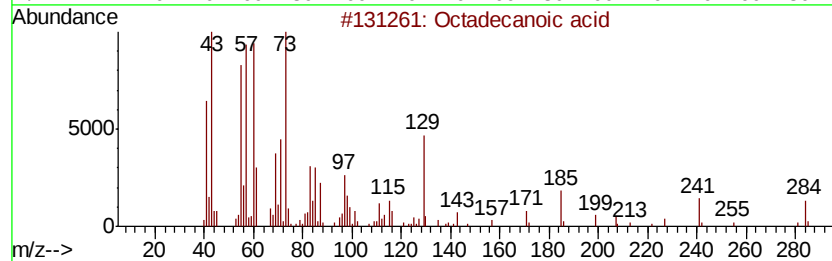
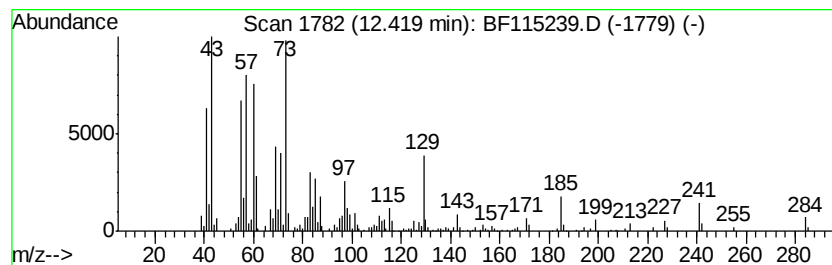
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.42	10.13 ng	898086	Chrysene-d12		13.71	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62



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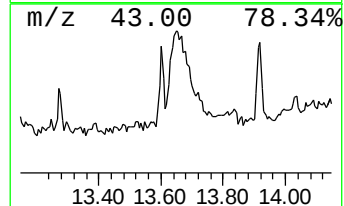
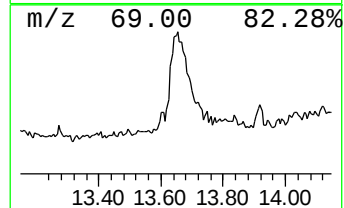
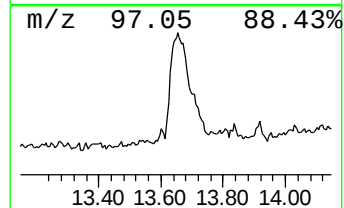
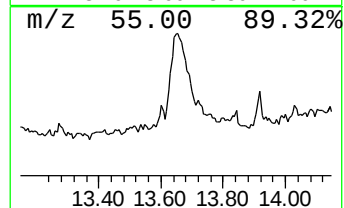
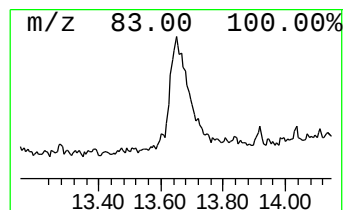
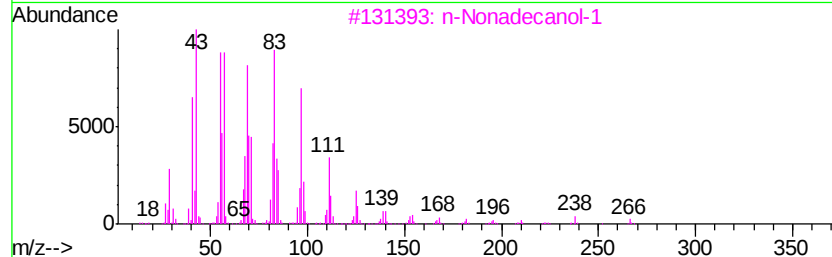
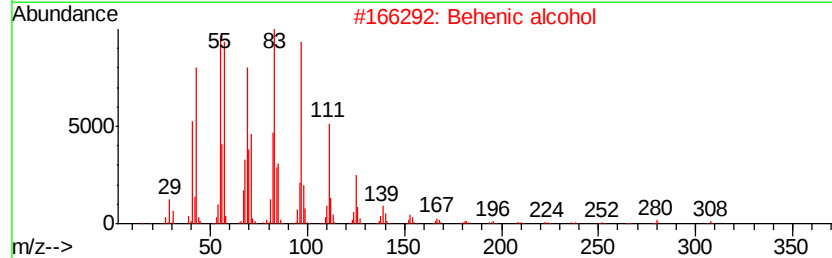
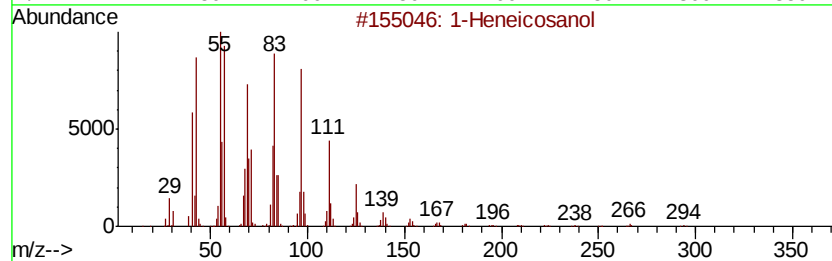
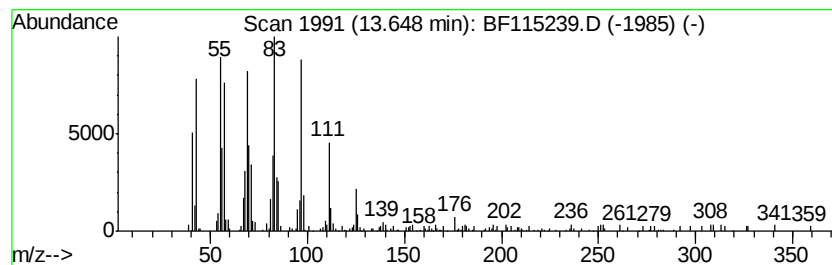
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	5.78 ng	512485	Chrysene-d12	13.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	93
2	Behenic alcohol		326	C22H46O	000661-19-8	93
3	n-Nonadecanol-1		284	C19H40O	001454-84-8	93
4	3-Eicosene, (E)-		280	C20H40	074685-33-9	92
5	3-Octadecene, (E)-		252	C18H36	007206-19-1	86



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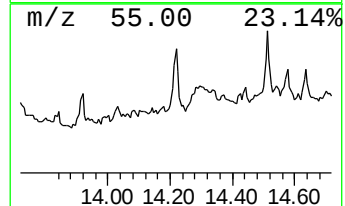
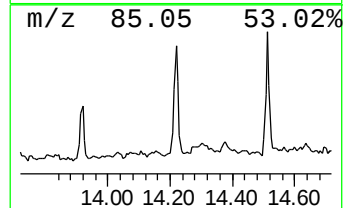
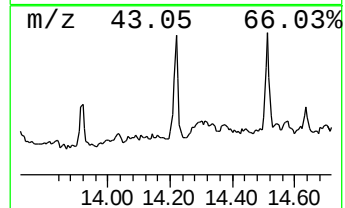
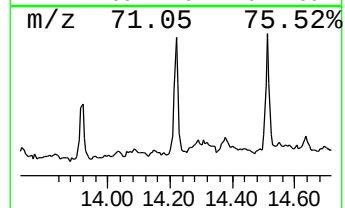
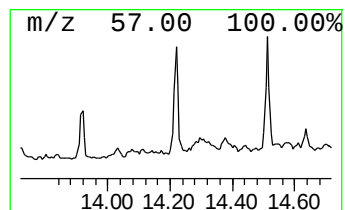
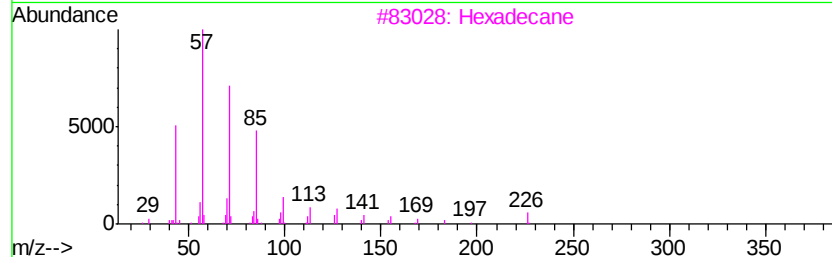
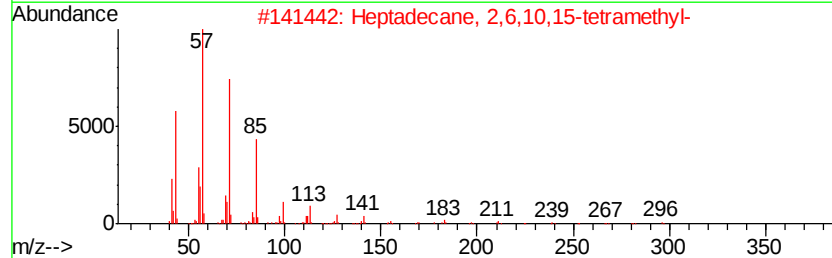
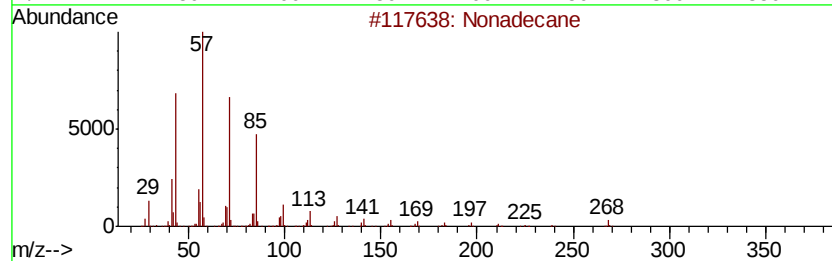
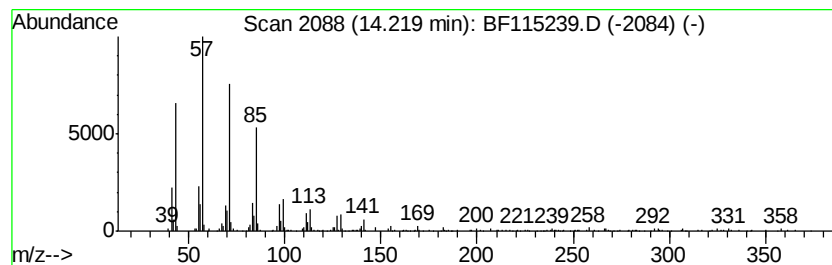
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	2.51 ng	222391	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	93
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3		Hexadecane	226	C16H34	000544-76-3	91
4		Hexatriacontane	507	C36H74	000630-06-8	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



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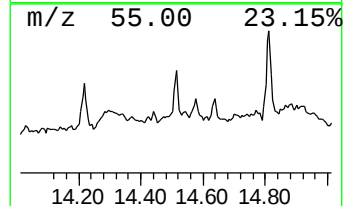
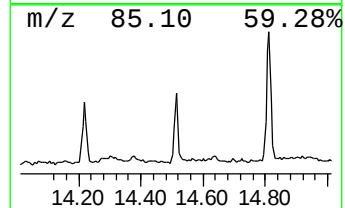
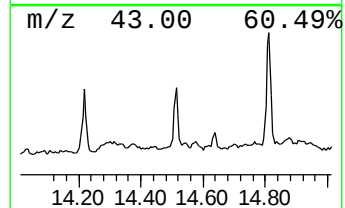
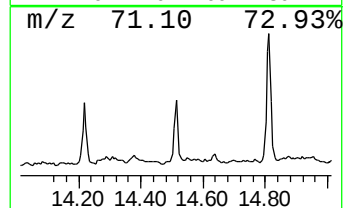
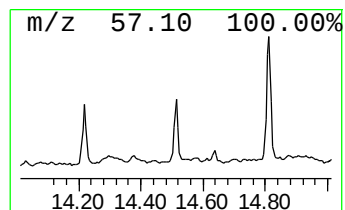
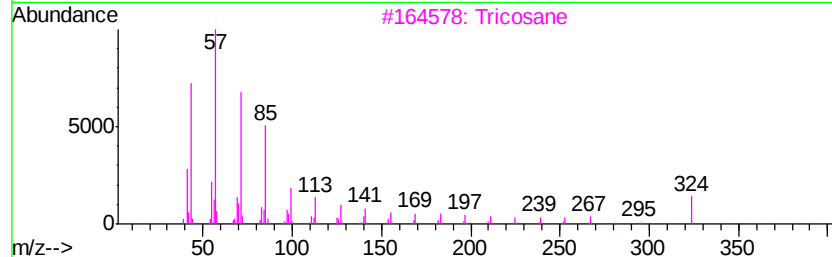
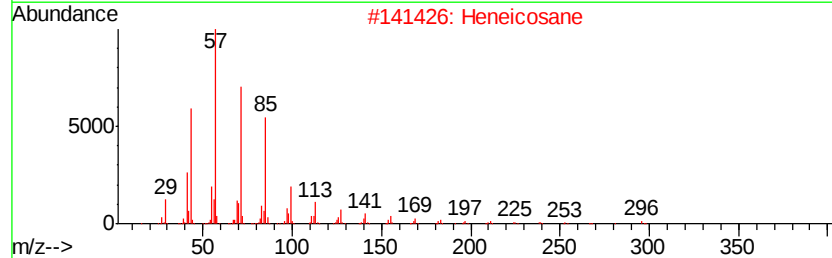
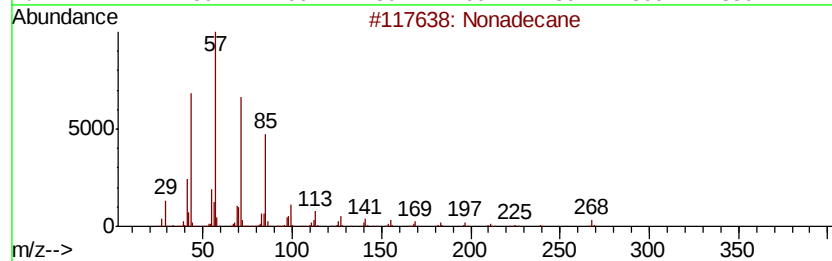
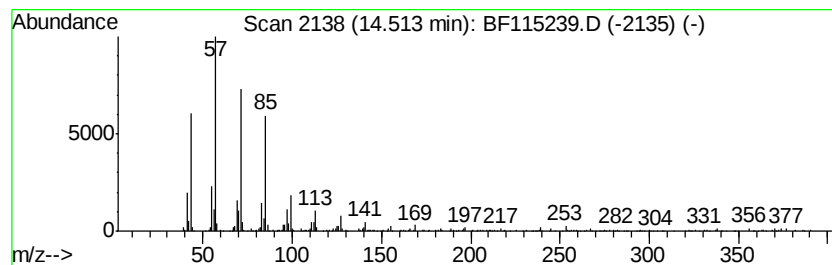
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	3.01 ng	209321	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	93
2		Heneicosane	296	C21H44	000629-94-7	87
3		Tricosane	324	C23H48	000638-67-5	87
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
5		Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062719\
Data File : BF115239.D
Acq On : 27 Jun 2019 16:34
Operator : HP/JU
Sample : K3534-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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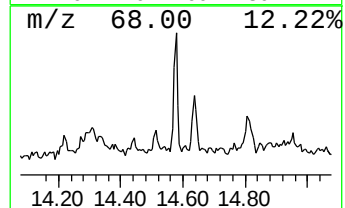
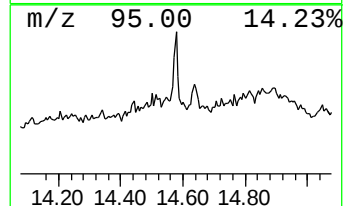
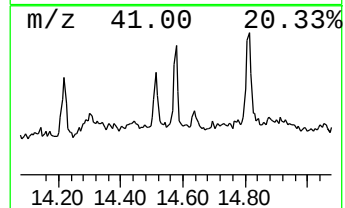
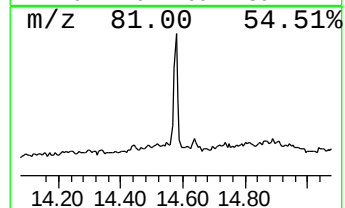
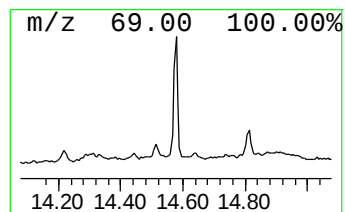
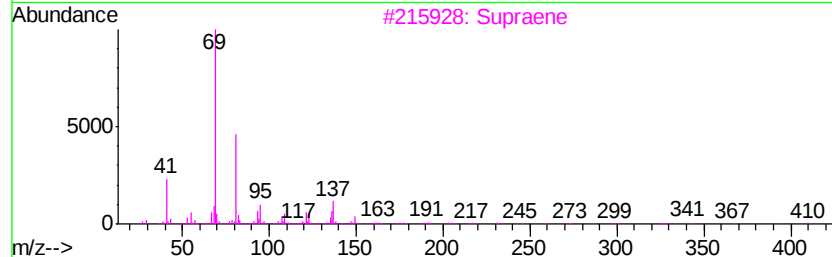
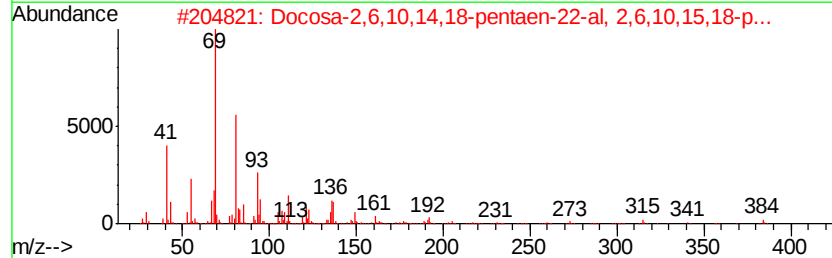
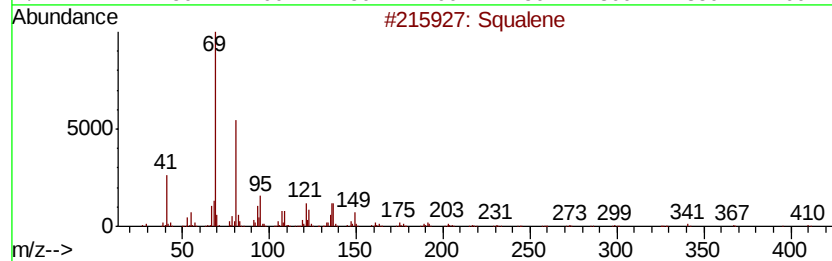
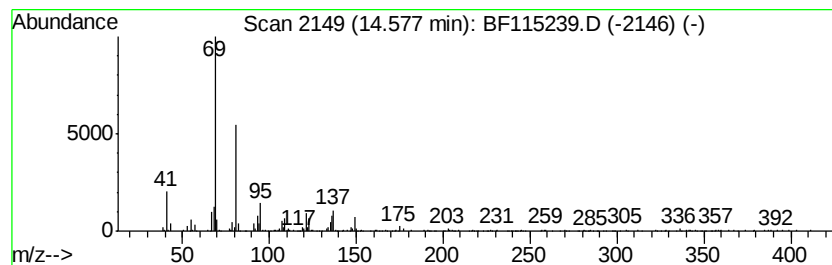
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	2.70 ng	187285	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
3		Supraene	410	C30H50	007683-64-9	83
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062719\
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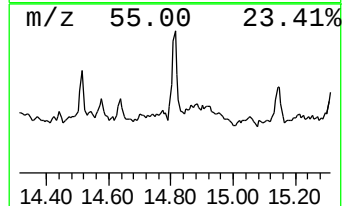
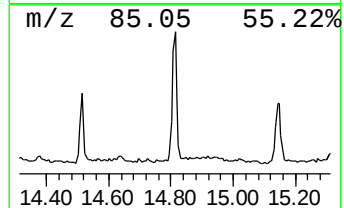
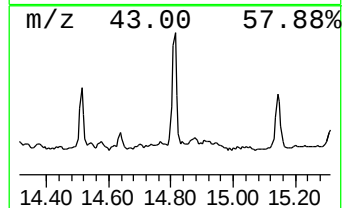
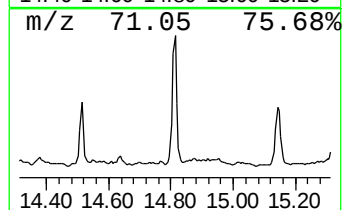
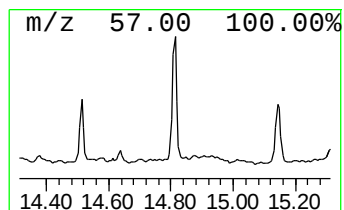
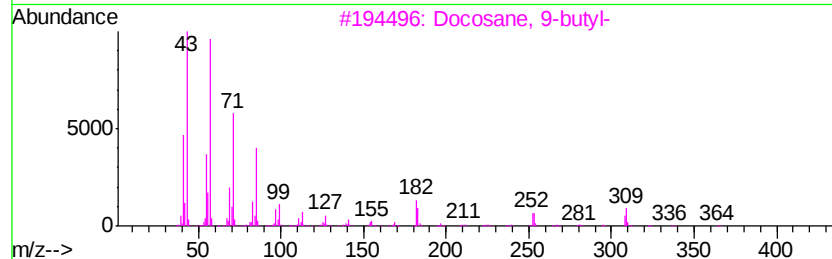
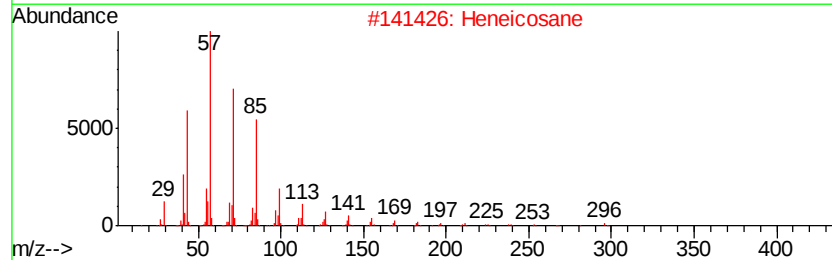
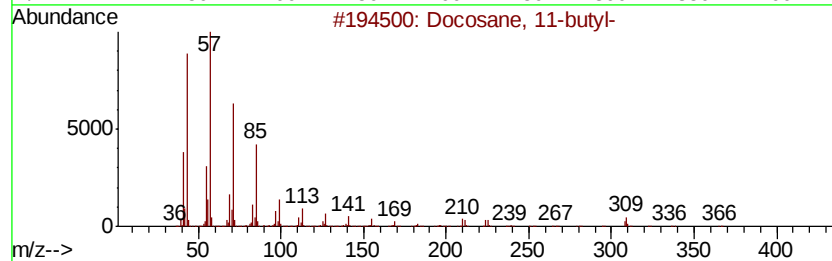
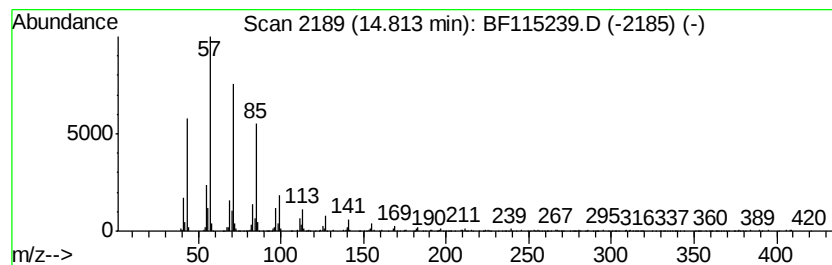
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Docosane, 11-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	5.86 ng	407118	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 11-butyl-	366	C26H54	013475-76-8	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Docosane, 9-butyl-	366	C26H54	055282-14-9	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062719\
Data File : BF115239.D
Acq On : 27 Jun 2019 16:34
Operator : HP/JU
Sample : K3534-01
Misc :
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Instrument :
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ClientSampleId :
FK-PS-01-050

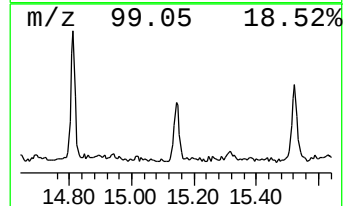
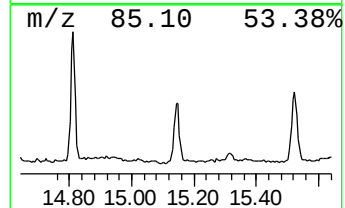
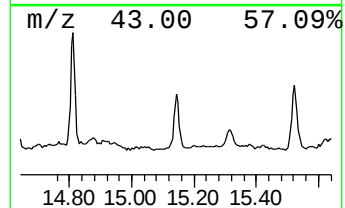
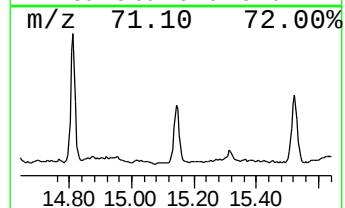
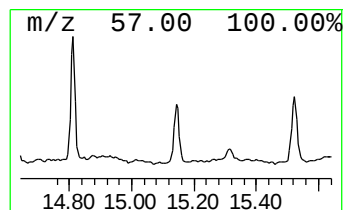
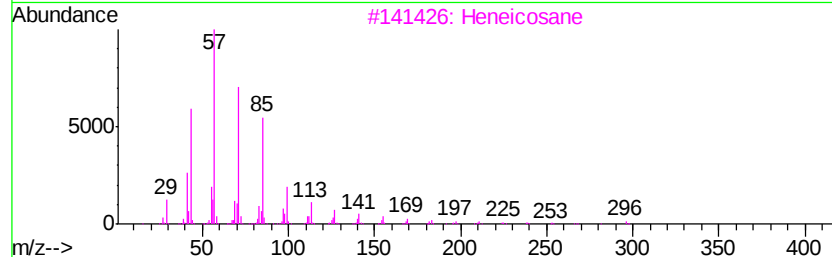
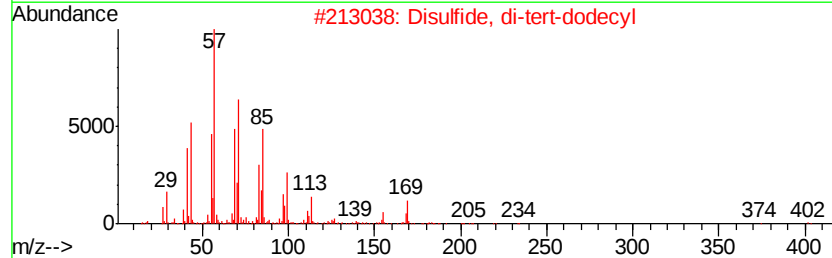
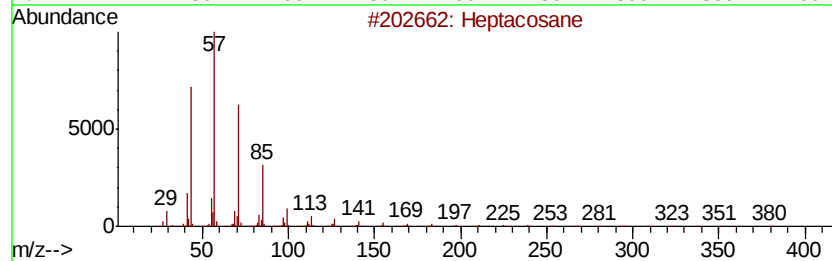
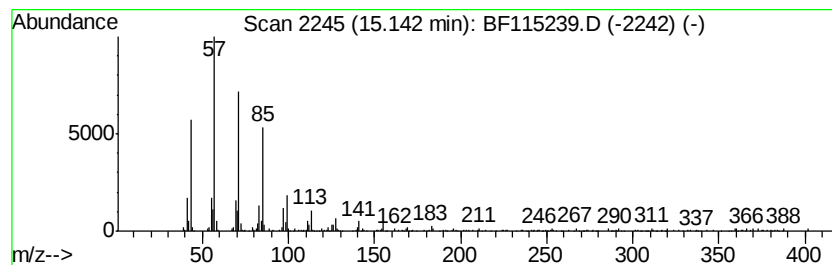
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	3.06 ng	212475	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	95
2		Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Dodecane, 2-methyl-	184	C13H28	001560-97-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062719\
Data File : BF115239.D
Acq On : 27 Jun 2019 16:34
Operator : HP/JU
Sample : K3534-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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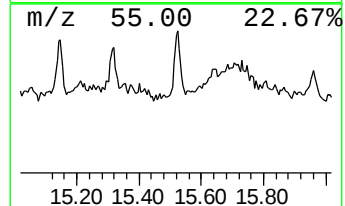
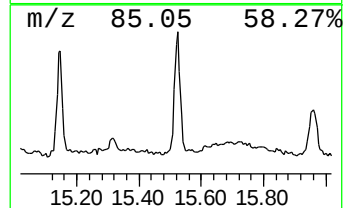
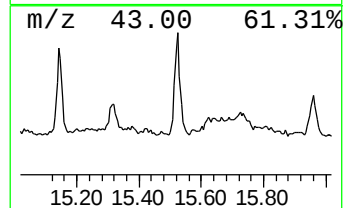
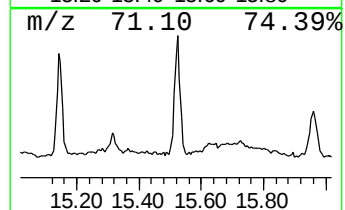
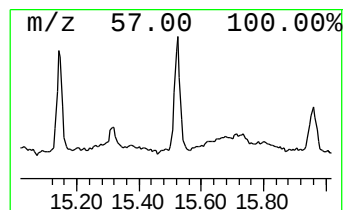
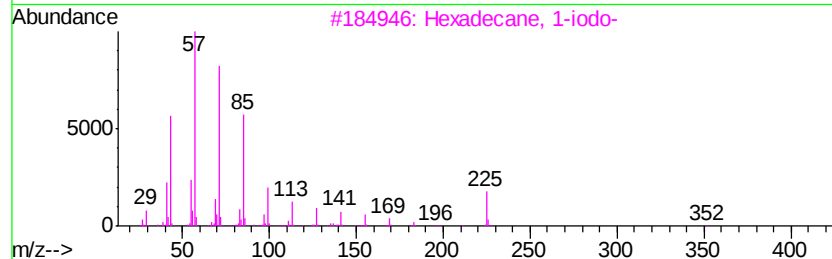
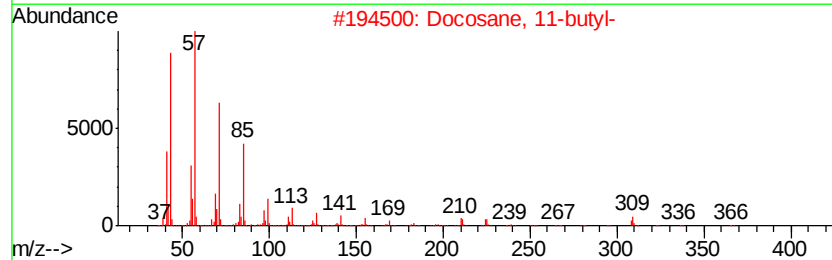
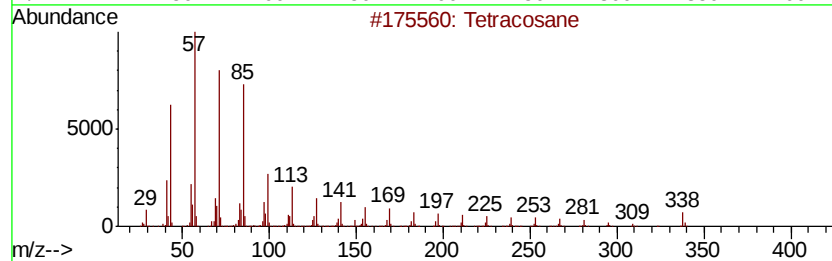
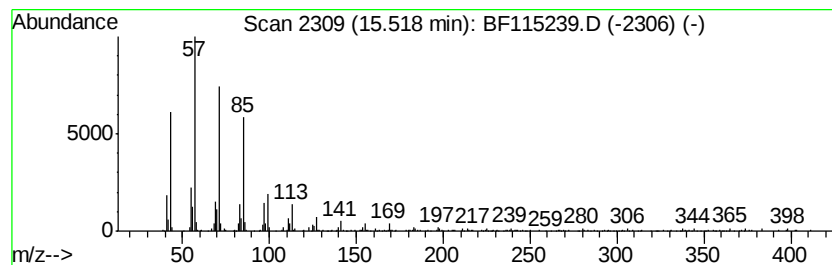
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.52	4.22 ng	292897	Perylene-d12	15.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	95
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	94
3		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
4		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062719\
Data File : BF115239.D
Acq On : 27 Jun 2019 16:34
Operator : HP/JU
Sample : K3534-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-050

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.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	11.64	4.2	ng	391072	4	11.10	1865460	20.0
Octadecanoic acid	12.42	10.1	ng	898086	5	13.71	1772780	20.0
1-Heneicosanol	13.65	5.8	ng	512485	5	13.71	1772780	20.0
Nonadecane	14.22	2.5	ng	222391	5	13.71	1772780	20.0
Heneicosane	14.51	3.0	ng	209321	6	15.07	1389510	20.0
Squalene	14.58	2.7	ng	187285	6	15.07	1389510	20.0
Docosane, 11-butyl-	14.81	5.9	ng	407118	6	15.07	1389510	20.0
Heptacosane	15.14	3.1	ng	212475	6	15.07	1389510	20.0
Tetracosane	15.52	4.2	ng	292897	6	15.07	1389510	20.0