

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
 Data File : BF113235.D
 Acq On : 22 Mar 2019 15:28
 Operator : JU/SJ
 Sample : K2018-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-A

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	5.334	547	552	574	rBV	2824937	2929424	90.45%	9.013%
2	6.363	722	727	744	rBV	3003452	3090563	95.43%	9.509%
3	6.487	744	748	751	rBV	3360486	3062975	94.58%	9.424%
4	6.716	783	787	791	rBV	928969	870441	26.88%	2.678%
5	6.869	809	813	817	rBV	2547968	2267155	70.00%	6.975%
6	7.275	877	882	885	rBV	2001097	1885872	58.23%	5.802%
7	7.998	1000	1005	1019	rBV	1144169	1189914	36.74%	3.661%
8	9.075	1183	1188	1198	rBV	3360900	3238653	100.00%	9.964%
9	9.469	1251	1255	1263	rBV	229855	229825	7.10%	0.707%
10	9.745	1298	1302	1314	rVB	1370348	1348915	41.65%	4.150%
11	10.533	1432	1436	1449	rBV	2510273	2624124	81.03%	8.074%
12	11.227	1550	1554	1562	rBV	1586978	1487643	45.93%	4.577%
13	11.769	1642	1646	1656	rBV	598953	683909	21.12%	2.104%
14	12.439	1757	1760	1763	rBV	45141	48608	1.50%	0.150%
15	12.545	1775	1778	1790	rBV	166931	220921	6.82%	0.680%
16	12.663	1795	1798	1802	rVB	40582	42309	1.31%	0.130%
17	12.810	1818	1823	1826	rBV	3433525	3235526	99.90%	9.955%
18	13.051	1860	1864	1874	rBV4	25147	45770	1.41%	0.141%
19	13.721	1974	1978	1994	rBV	298399	640382	19.77%	1.970%
20	13.857	1997	2001	2010	rVB	1274612	1213215	37.46%	3.733%
21	14.033	2027	2031	2034	rBV	74646	67410	2.08%	0.207%
22	14.333	2079	2082	2085	rBV	119749	115890	3.58%	0.357%
23	14.368	2085	2088	2096	rVB7	23653	45099	1.39%	0.139%
24	14.633	2129	2133	2138	rVB	147813	146496	4.52%	0.451%
25	14.945	2182	2186	2191	rBV	159241	184726	5.70%	0.568%
26	15.268	2236	2241	2244	rBV	783658	944914	29.18%	2.907%
27	15.298	2244	2246	2256	rVB	140830	180095	5.56%	0.554%
28	15.704	2310	2315	2322	rBV	116273	172324	5.32%	0.530%
29	15.798	2325	2331	2338	rBV8	42305	129293	3.99%	0.398%
30	16.168	2389	2394	2399	rBV	63101	108580	3.35%	0.334%
31	16.709	2483	2486	2491	rVB2	30514	51762	1.60%	0.159%

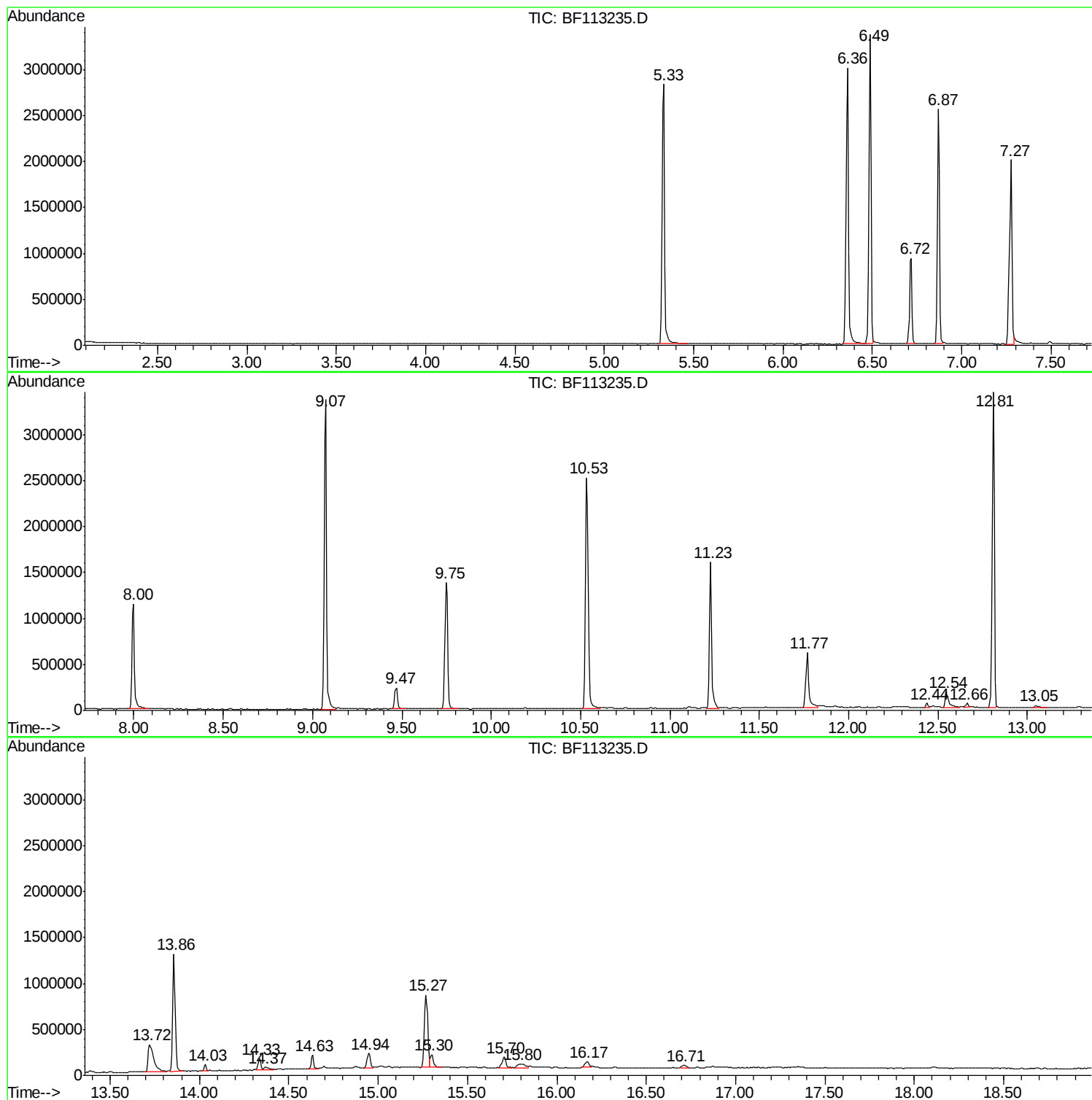
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ClientSampleId :
SP-1-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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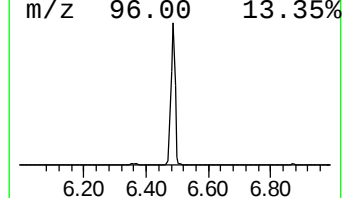
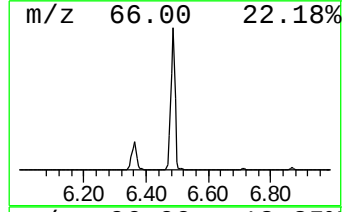
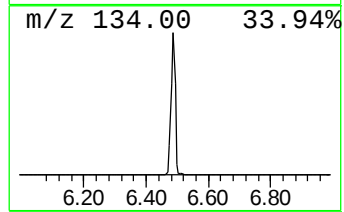
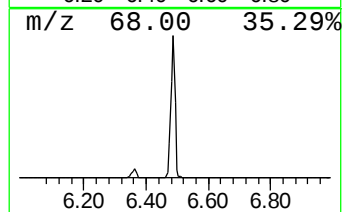
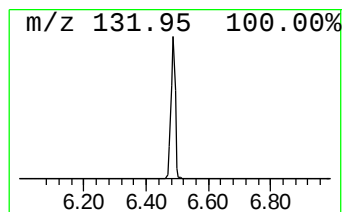
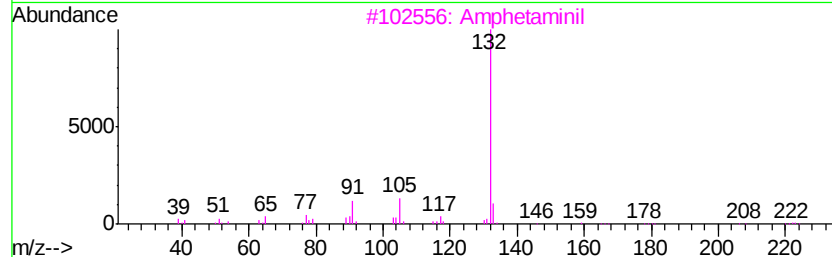
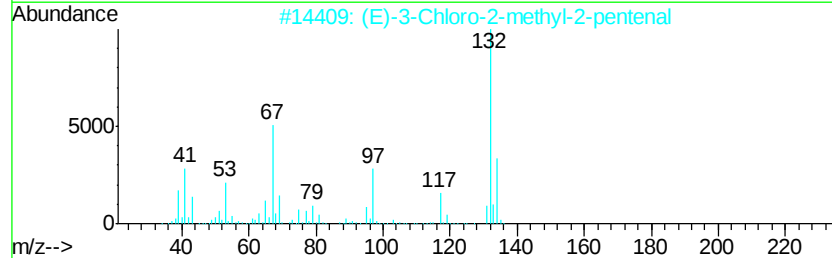
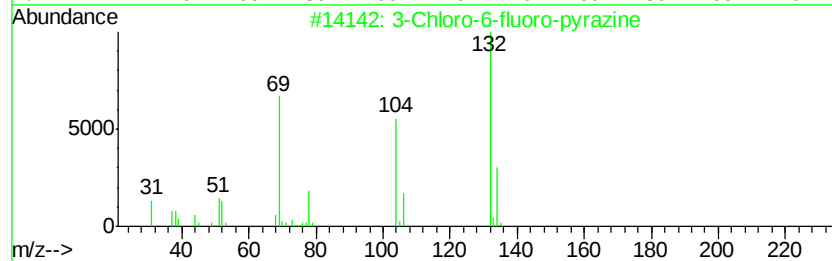
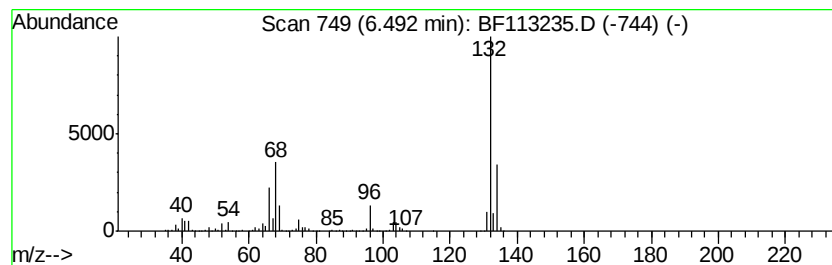
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	70.38 ng	3062980	1,4-Dichlorobenzene-d4	6.72

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	12
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Xenon	132	Xe	007440-63-3	9



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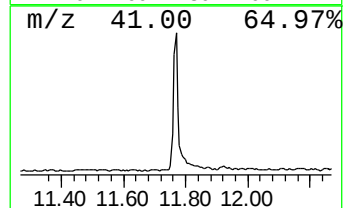
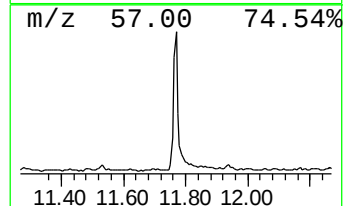
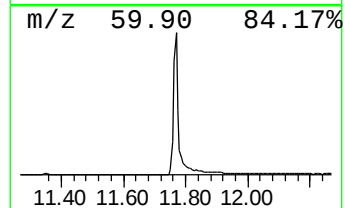
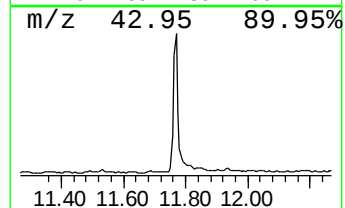
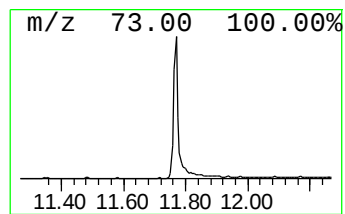
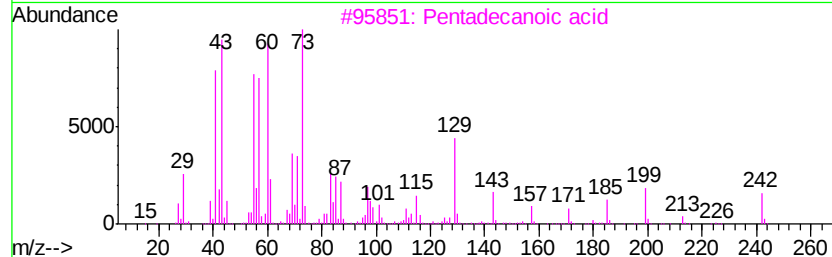
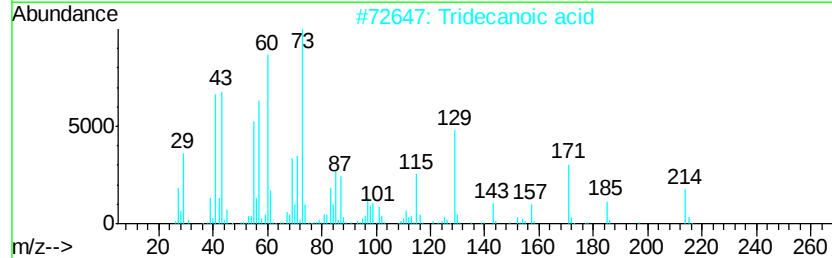
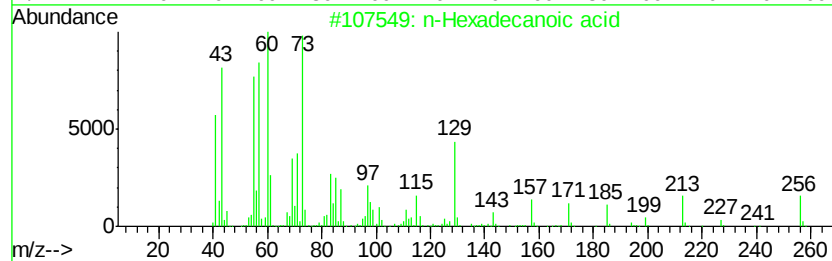
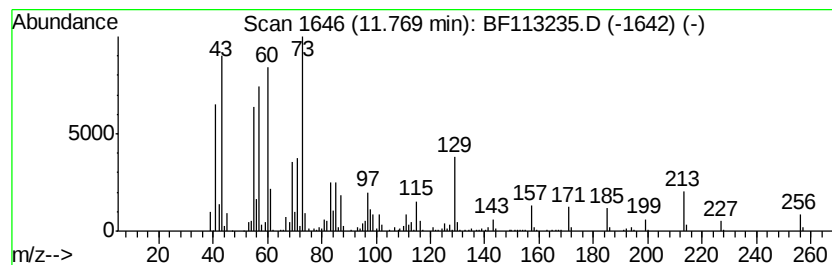
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	9.19 ng	683909	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5		n-Decanoic acid	172	C10H20O2	000334-48-5	55



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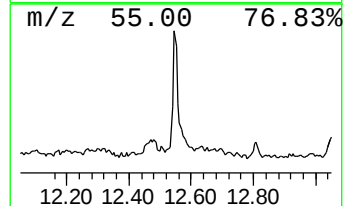
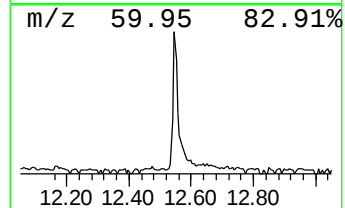
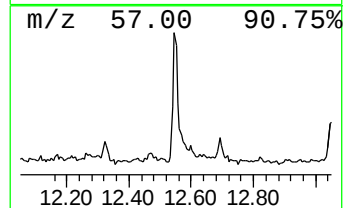
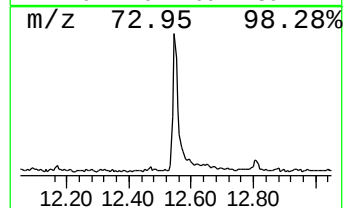
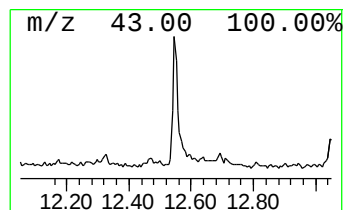
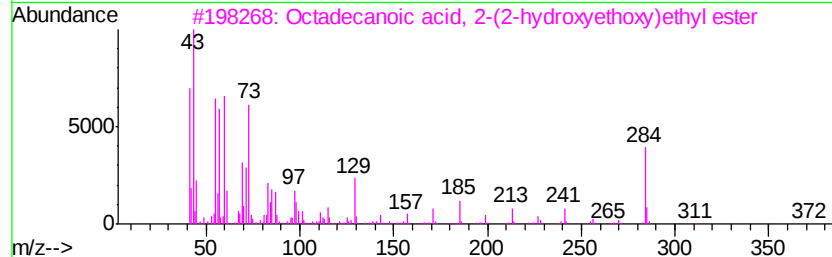
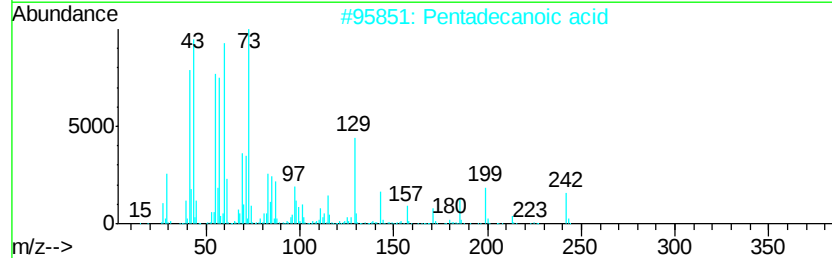
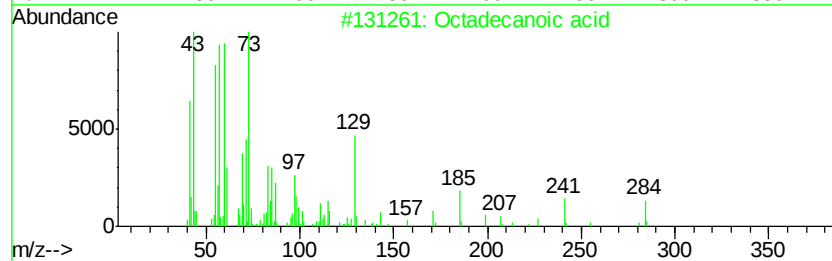
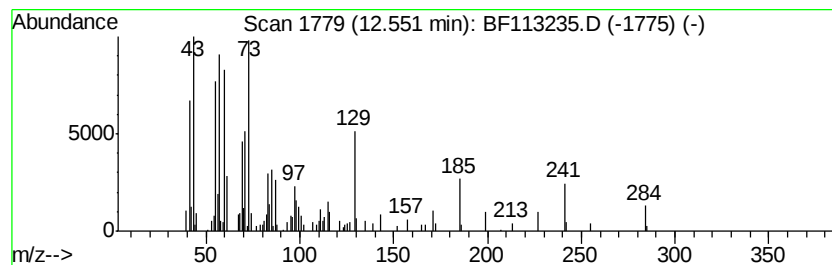
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Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	3.64 ng	220921	Chrysene-d12	13.86

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		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



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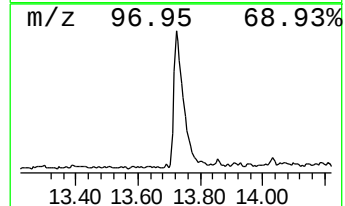
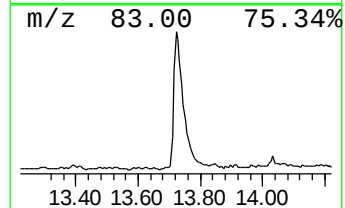
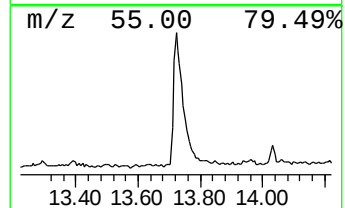
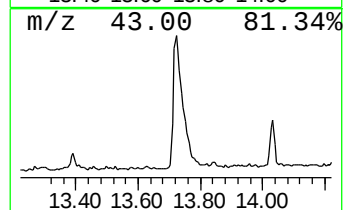
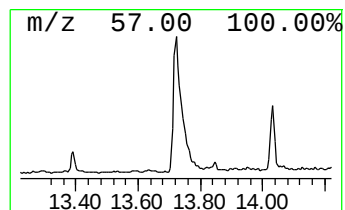
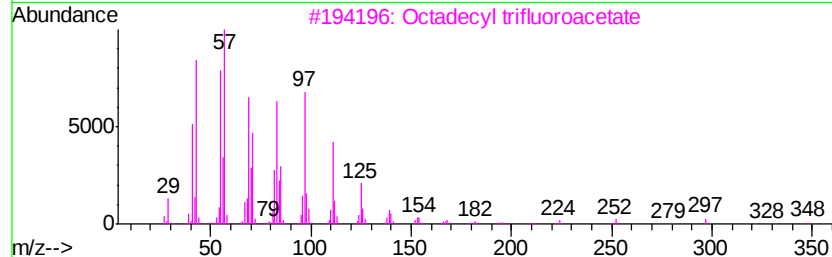
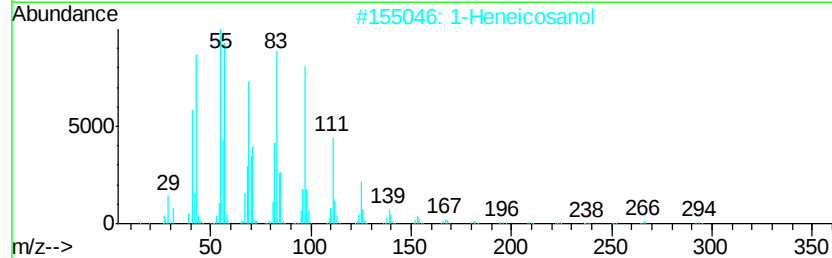
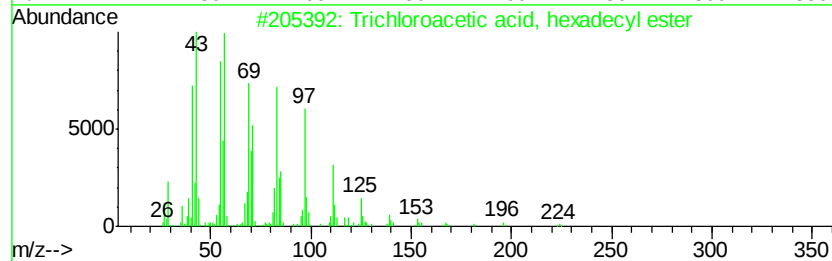
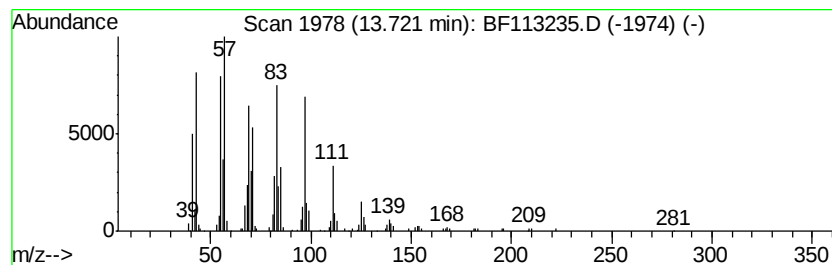
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 Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	10.56 ng	640382	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5		Octacosanol	410	C28H58O	000557-61-9	91



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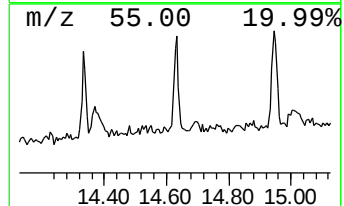
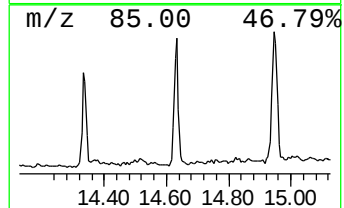
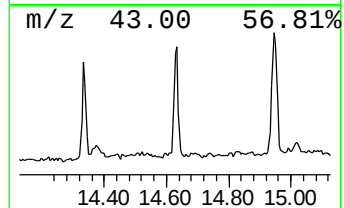
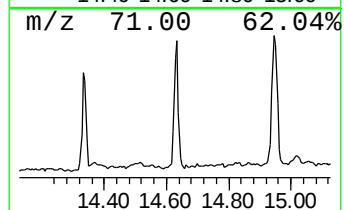
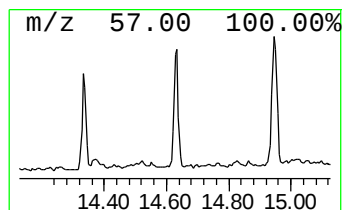
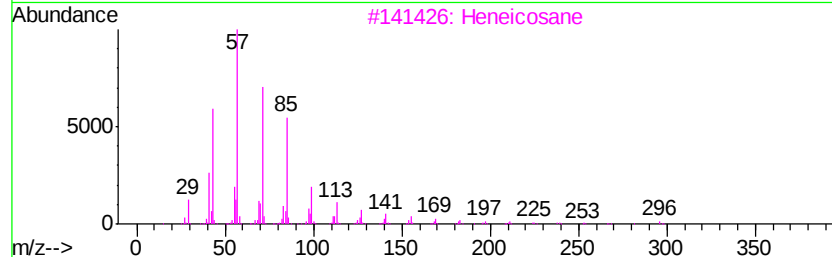
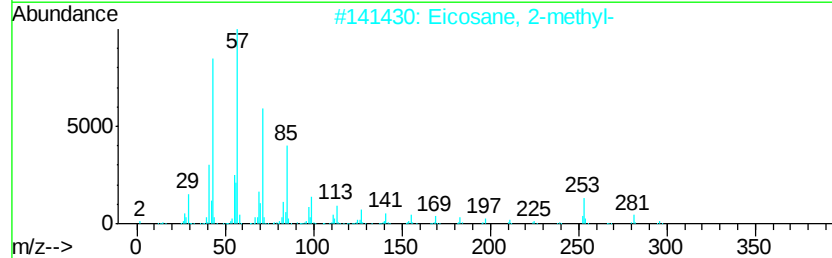
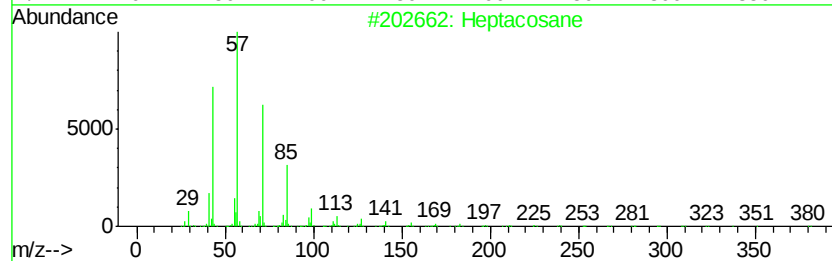
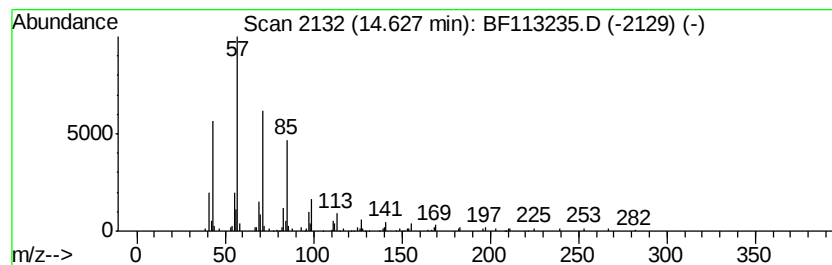
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	3.10 ng	146496	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Octacosane	394	C28H58	000630-02-4	90



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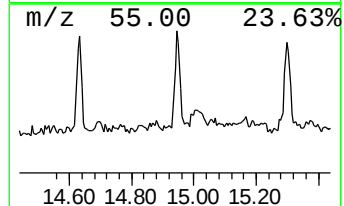
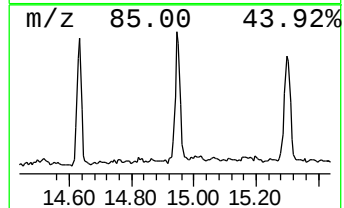
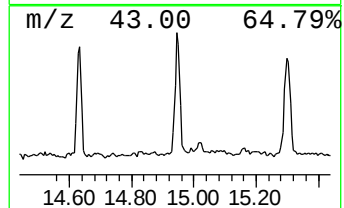
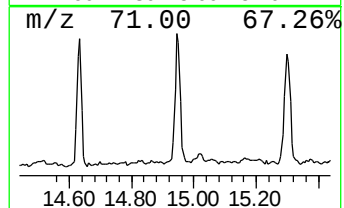
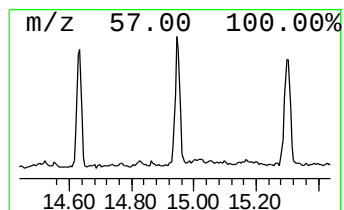
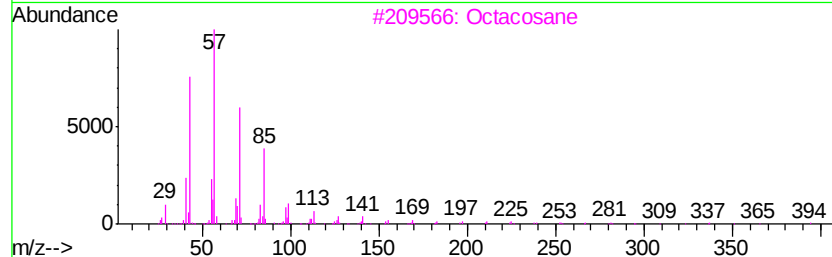
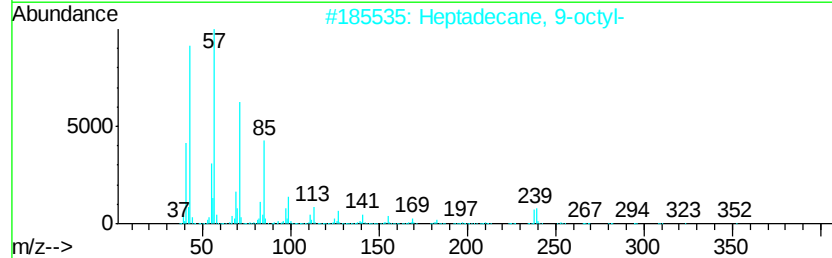
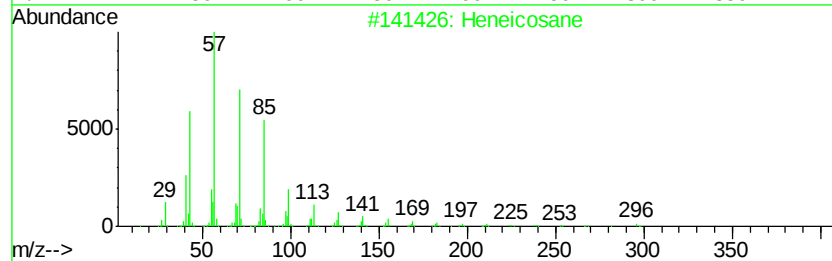
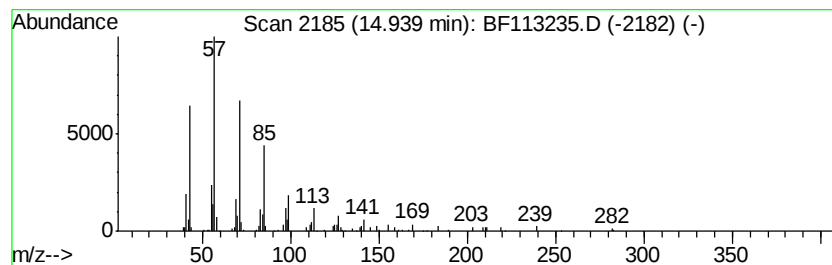
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	3.91 ng	184726	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
3	Octacosane		394	C28H58	000630-02-4	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\BF032219\
Data File : BF113235.D
Acq On : 22 Mar 2019 15:28
Operator : JU/SJ
Sample : K2018-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-A

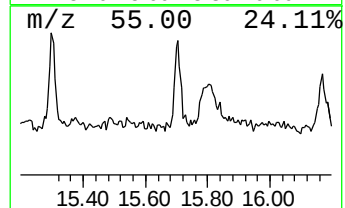
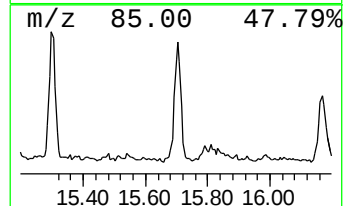
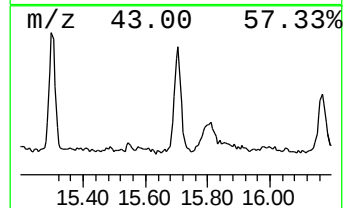
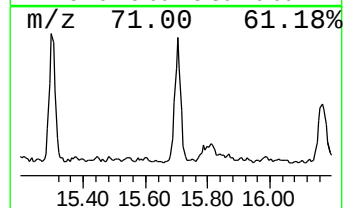
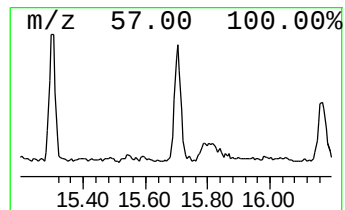
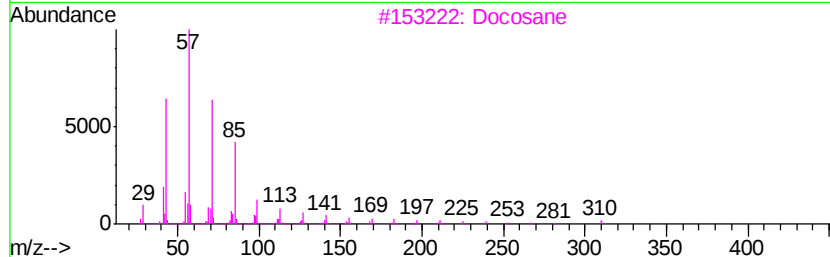
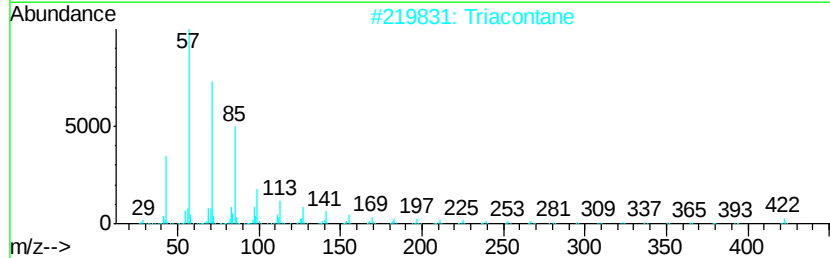
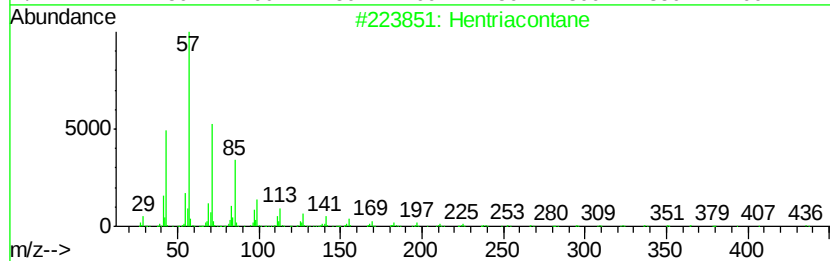
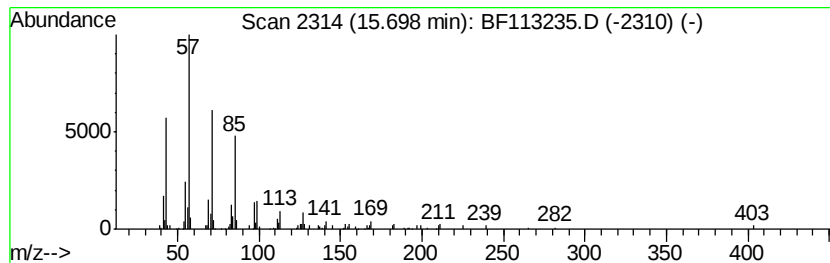
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	3.65 ng	172324	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	90
2	triacontane		422	C30H62	000638-68-6	87
3	Docosane		310	C22H46	000629-97-0	87
4	Octacosane		394	C28H58	000630-02-4	87
5	Tetracosane		338	C24H50	000646-31-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
Data File : BF113235.D
Acq On : 22 Mar 2019 15:28
Operator : JU/SJ
Sample : K2018-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-A

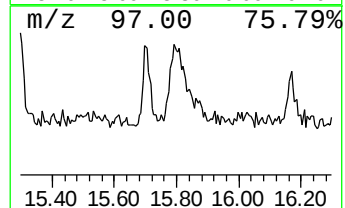
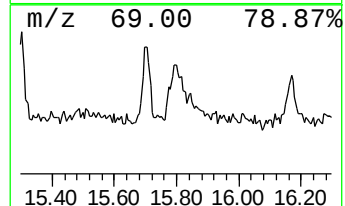
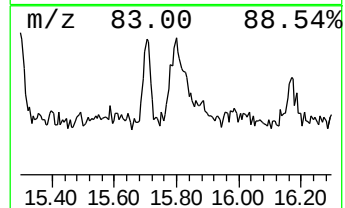
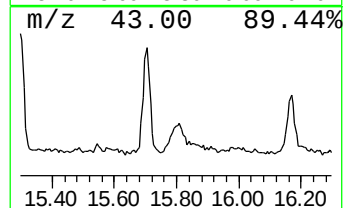
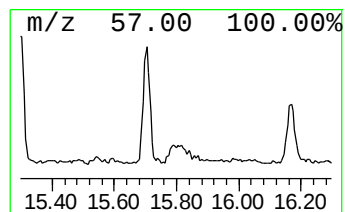
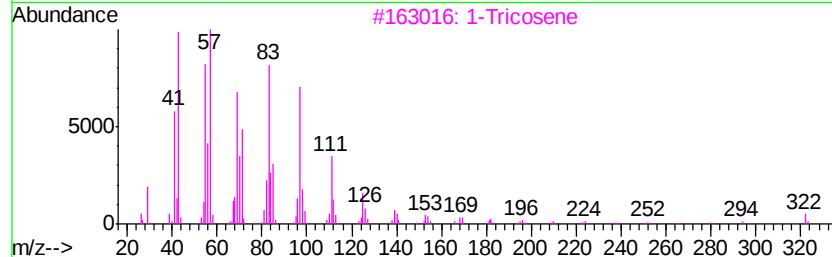
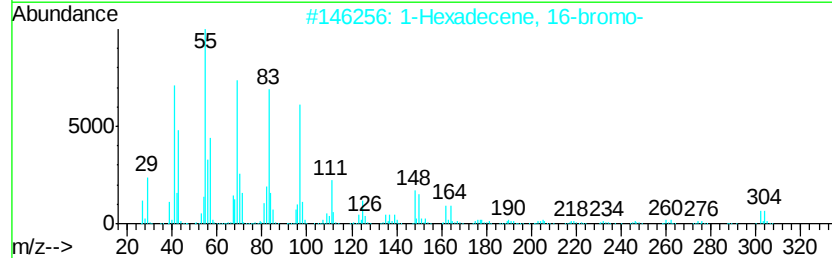
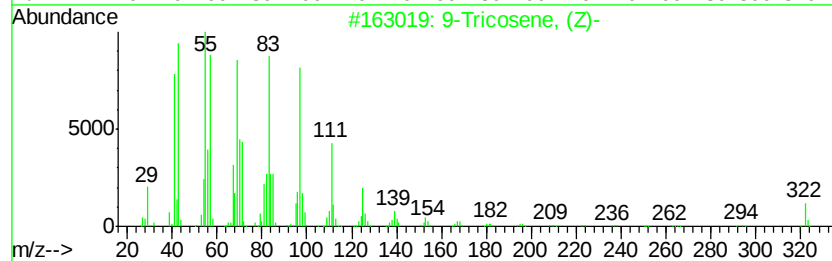
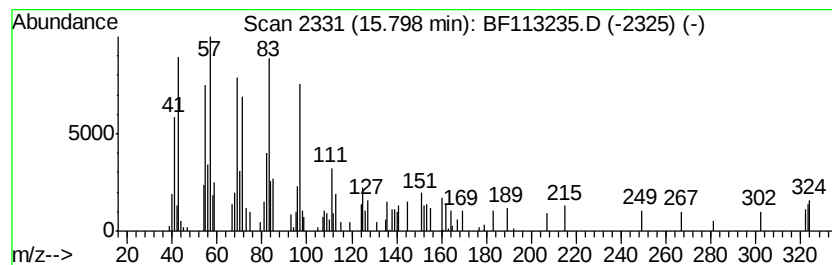
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Tricosene, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	2.74 ng	129293	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
2		1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	76
3		1-Tricosene	322	C23H46	018835-32-0	70
4		Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	58
5		Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	56



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
Data File : BF113235.D
Acq On : 22 Mar 2019 15:28
Operator : JU/SJ
Sample : K2018-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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BNA_F
ClientSampleId :
SP-1-A

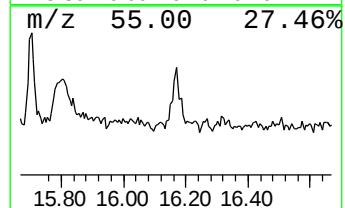
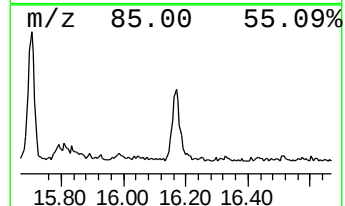
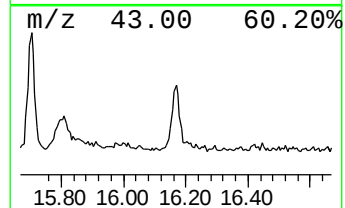
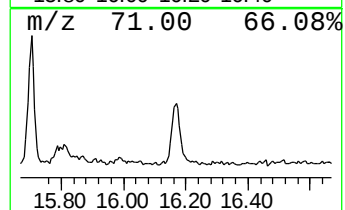
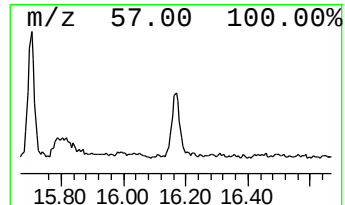
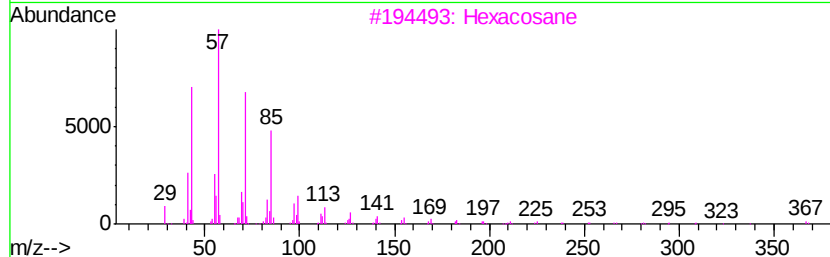
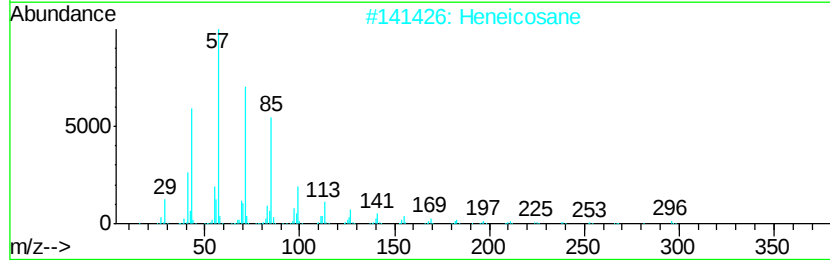
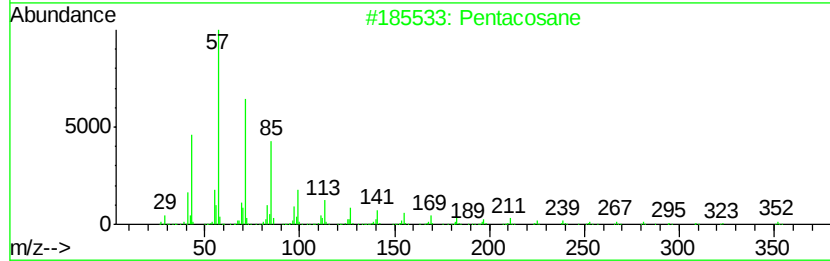
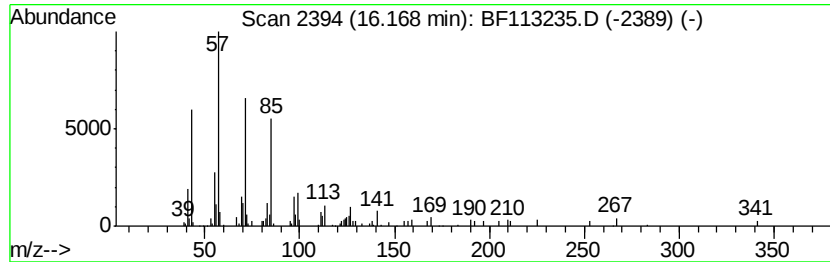
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.30 ng	108580	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexacosane	366	C26H54	000630-01-3	90
4		Heptacosane	380	C27H56	000593-49-7	90
5		Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
 Data File : BF113235.D
 Acq On : 22 Mar 2019 15:28
 Operator : JU/SJ
 Sample : K2018-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.49	6.49	70.4	ng	3062980	1	6.72	870441	20.0
n-Hexadecanoic acid	11.77	9.2	ng	683909	4	11.23	1487640	20.0
Octadecanoic acid	12.55	3.6	ng	220921	5	13.86	1213220	20.0
Trichloroacetic a...	13.72	10.6	ng	640382	5	13.86	1213220	20.0
Heptacosane	14.63	3.1	ng	146496	6	15.27	944914	20.0
Heneicosane	14.94	3.9	ng	184726	6	15.27	944914	20.0
Hentriacontane	15.70	3.6	ng	172324	6	15.27	944914	20.0
9-Tricosene, (Z)-	15.80	2.7	ng	129293	6	15.27	944914	20.0
Pentacosane	16.17	2.3	ng	108580	6	15.27	944914	20.0