

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031919\
 Data File : BF113158.D
 Acq On : 20 Mar 2019 7:20
 Operator : JU/SJ
 Sample : K1948-15
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-025-SW080-031319

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	5.345	549	554	557	rBV	3094481	3226100	92.69%	10.748%
2	6.369	723	728	731	rBV	3199369	3478122	99.93%	11.587%
3	6.492	745	749	753	rBV	3363530	3480707	100.00%	11.596%
4	6.557	758	760	773	rVB	45964	60033	1.72%	0.200%
5	6.722	784	788	791	rBV	1049651	863038	24.79%	2.875%
6	6.881	810	815	818	rBV	2871793	2579592	74.11%	8.594%
7	7.281	878	883	896	rBV	1705331	1869452	53.71%	6.228%
8	8.004	1002	1006	1022	rBV	1039521	994621	28.58%	3.314%
9	9.080	1184	1189	1192	rBV	3453818	3015259	86.63%	10.045%
10	9.475	1252	1256	1267	rBV	200606	225816	6.49%	0.752%
11	9.751	1300	1303	1315	rVB	1058857	1010347	29.03%	3.366%
12	10.539	1433	1437	1452	rBV	1758097	1691597	48.60%	5.636%
13	11.233	1551	1555	1562	rBV	937077	879045	25.25%	2.929%
14	11.768	1643	1646	1657	rBV2	293910	324920	9.33%	1.082%
15	12.439	1757	1760	1763	rBV	40957	46340	1.33%	0.154%
16	12.551	1776	1779	1788	rBV	90572	119734	3.44%	0.399%
17	12.668	1797	1799	1803	rVB	42954	34875	1.00%	0.116%
18	12.815	1819	1824	1827	rBV	2684639	2440605	70.12%	8.131%
19	13.298	1896	1906	1907	rBV4	33251	54601	1.57%	0.182%
20	13.733	1975	1980	1993	rBV2	98630	253424	7.28%	0.844%
21	13.862	1996	2002	2011	rVB	888895	917150	26.35%	3.056%
22	13.968	2017	2020	2024	rBV	93471	78417	2.25%	0.261%
23	14.039	2029	2032	2035	rBV	34408	37766	1.09%	0.126%
24	14.339	2080	2083	2085	rBV	45374	45924	1.32%	0.153%
25	14.368	2085	2088	2101	rVB3	123193	308116	8.85%	1.026%
26	14.580	2121	2124	2127	rVB	52627	45119	1.30%	0.150%
27	14.633	2130	2133	2137	rVB	56145	57314	1.65%	0.191%
28	14.768	2153	2156	2160	rVB	100232	94470	2.71%	0.315%
29	14.951	2183	2187	2190	rBV	115040	125644	3.61%	0.419%
30	14.998	2190	2195	2212	rVV3	225050	671643	19.30%	2.238%
31	15.268	2237	2241	2245	rBV	541367	657023	18.88%	2.189%
32	15.304	2245	2247	2252	rVB	54027	61123	1.76%	0.204%
33	15.492	2276	2279	2283	rVB5	32827	42229	1.21%	0.141%
34	15.709	2311	2316	2321	rVB	94135	136221	3.91%	0.454%

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ALS Vial : 35 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PST-025-SW080-031319

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	18.115	2719	2725	2733	rBV	33290	89802	2.58%	0.299%
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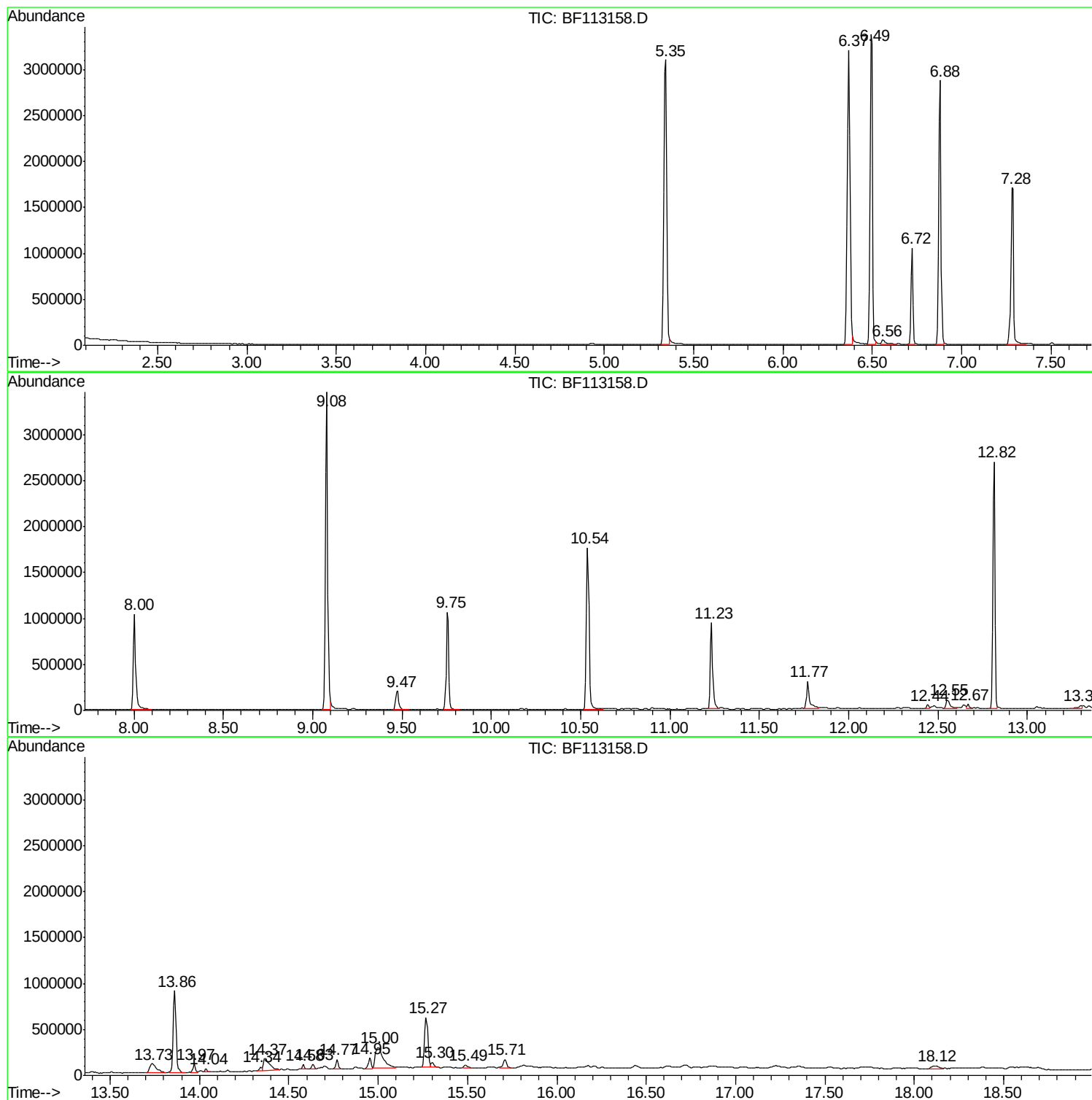
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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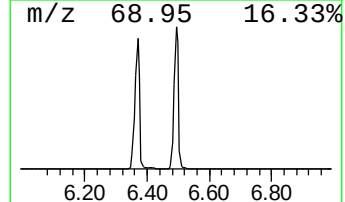
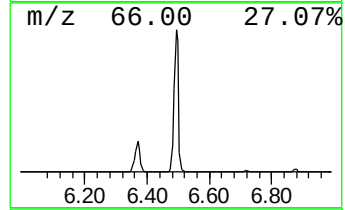
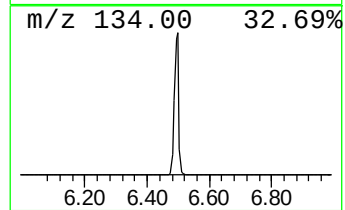
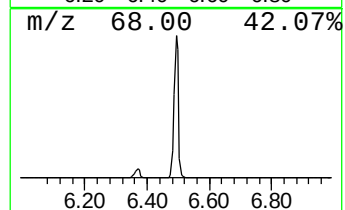
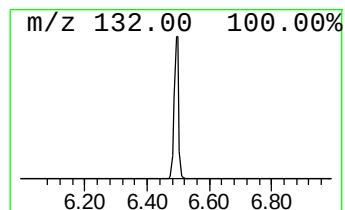
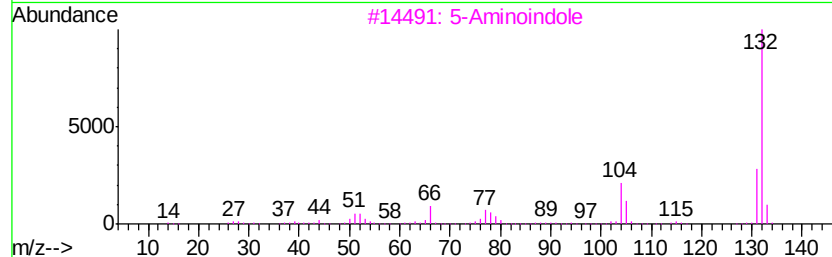
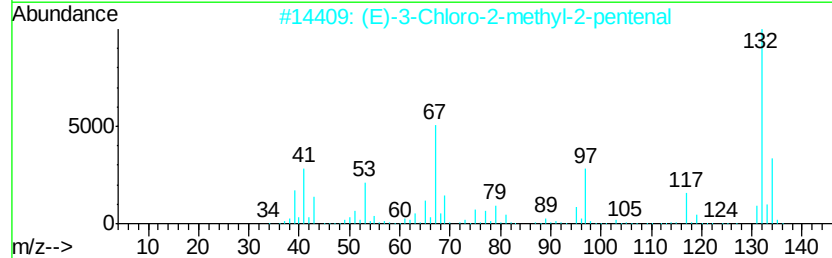
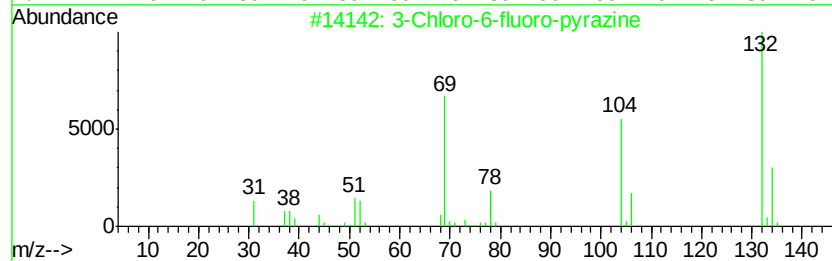
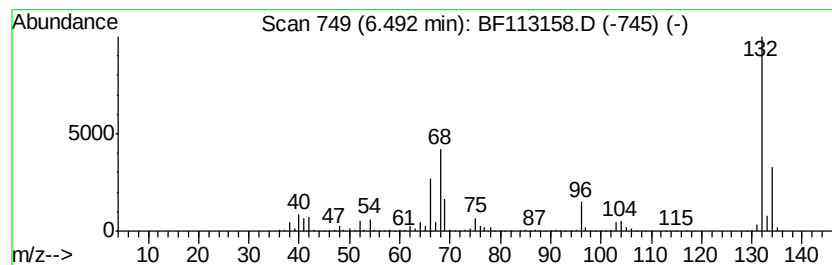
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	80.66 ng	3480710	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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Amphetaminil	250	C17H18N2	017590-01-1	10
5		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10



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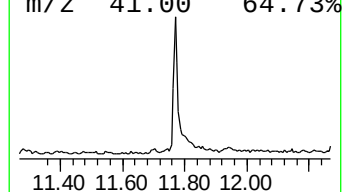
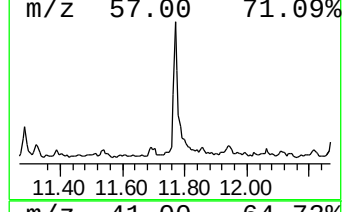
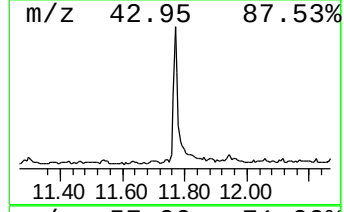
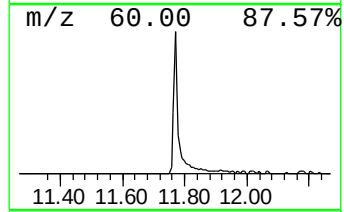
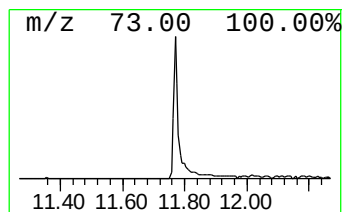
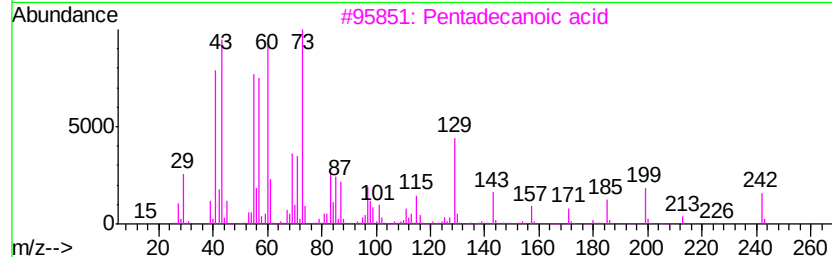
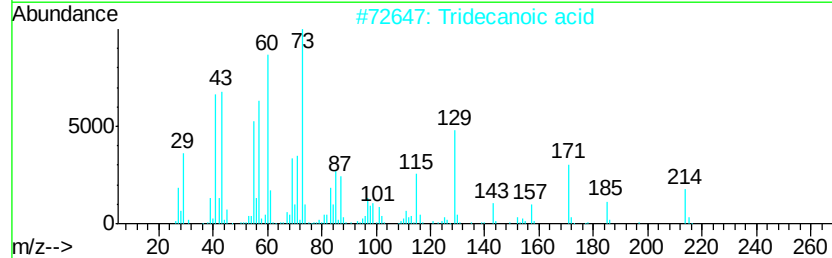
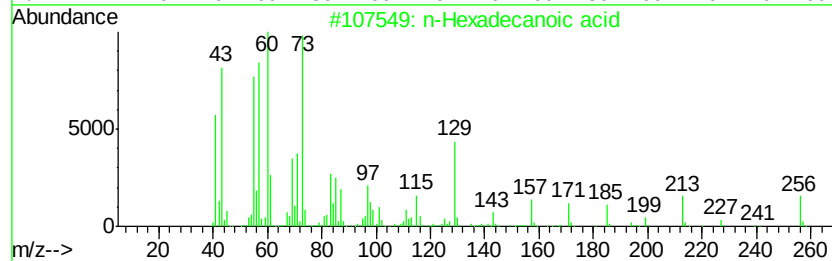
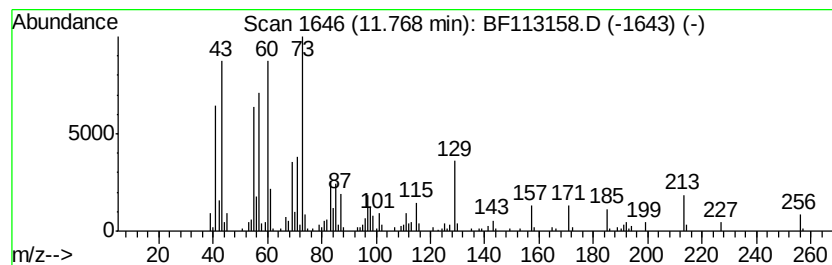
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.77	7.39 ng	324920	Phenanthrene-d10		11.23	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	83
5	Heptanoic acid		130	C7H14O2	000111-14-8	47



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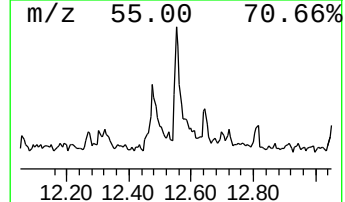
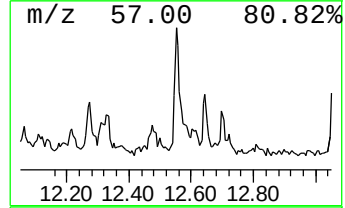
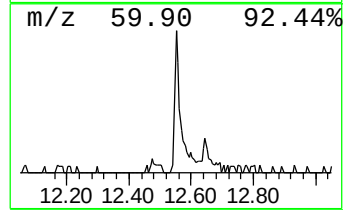
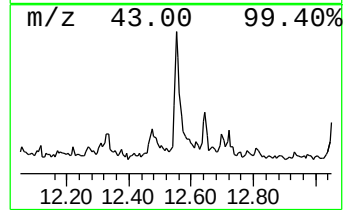
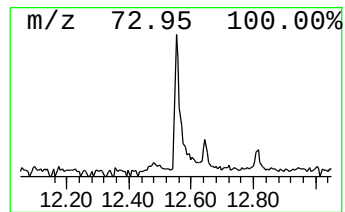
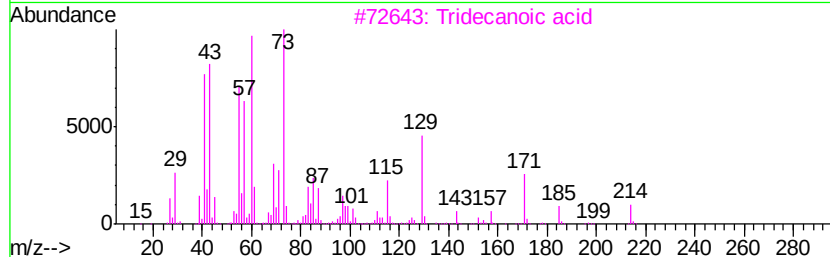
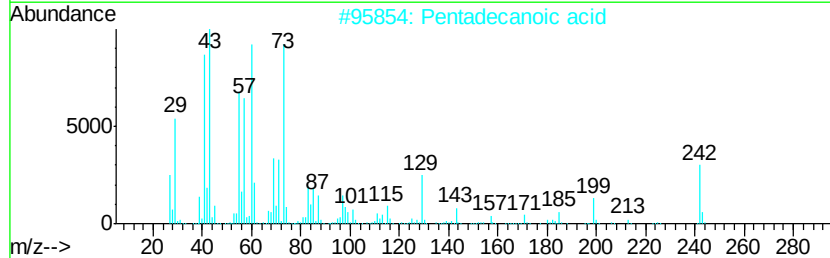
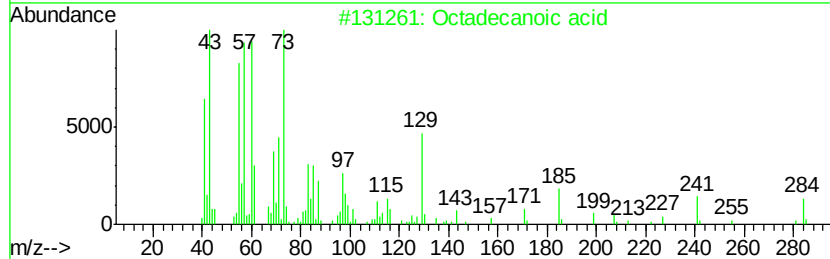
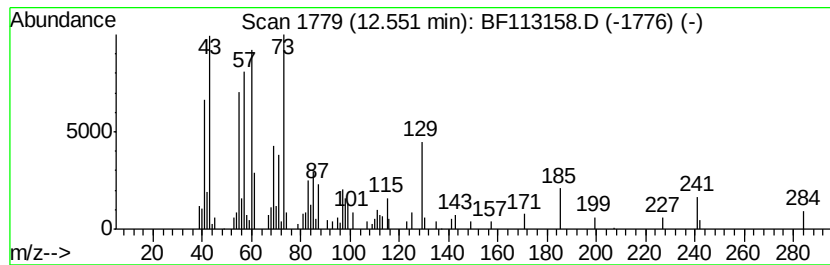
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.55	2.61 ng	119734	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	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



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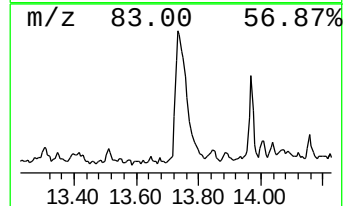
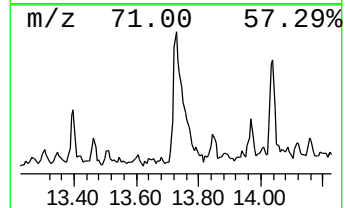
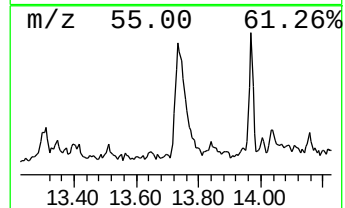
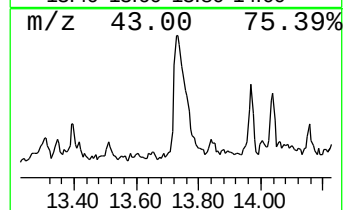
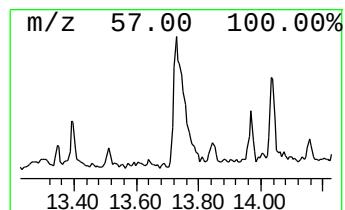
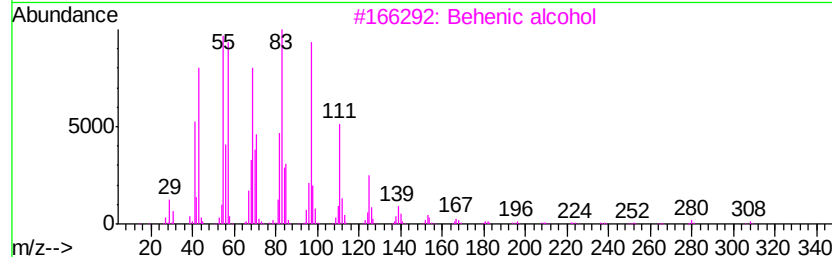
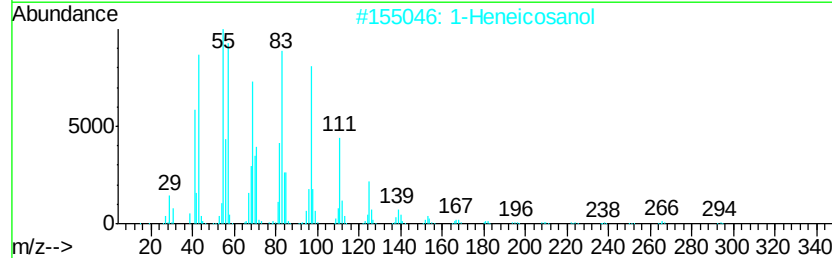
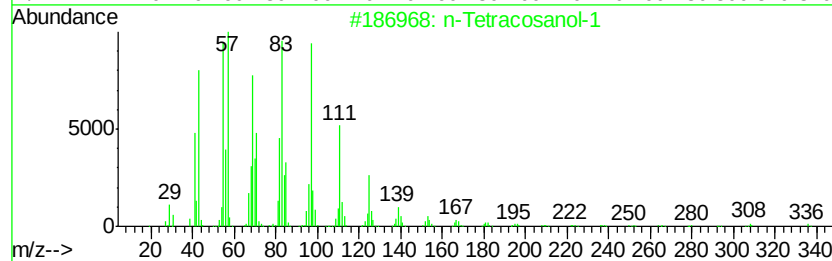
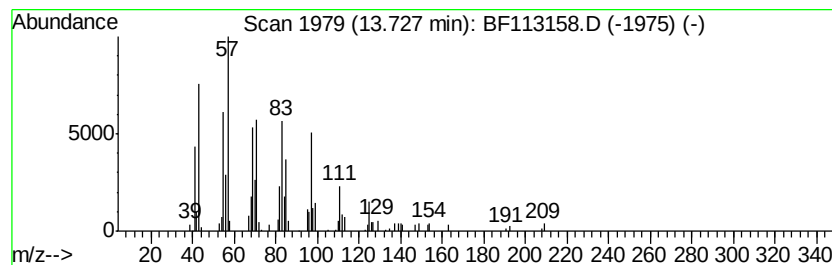
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.73	5.53 ng	253424	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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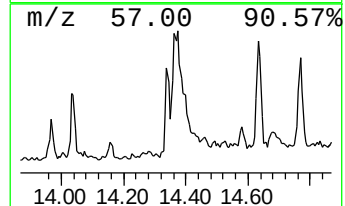
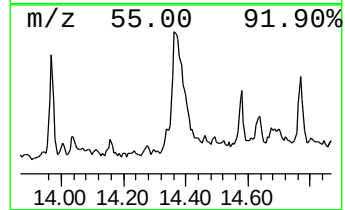
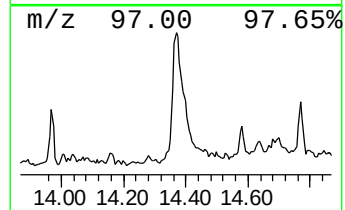
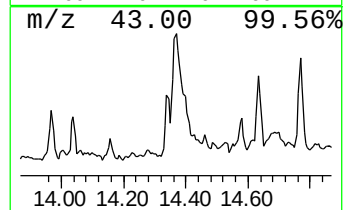
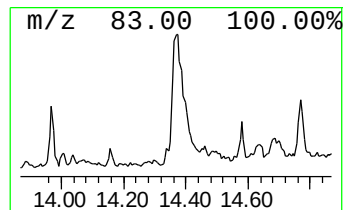
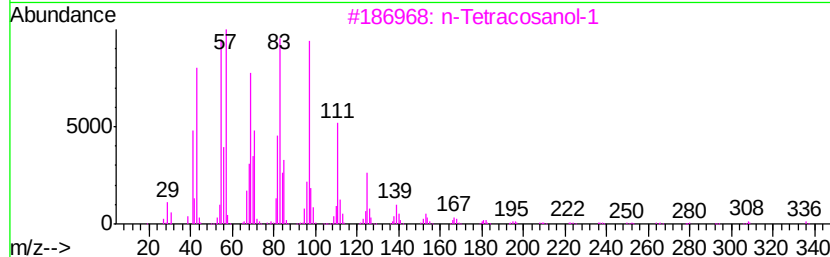
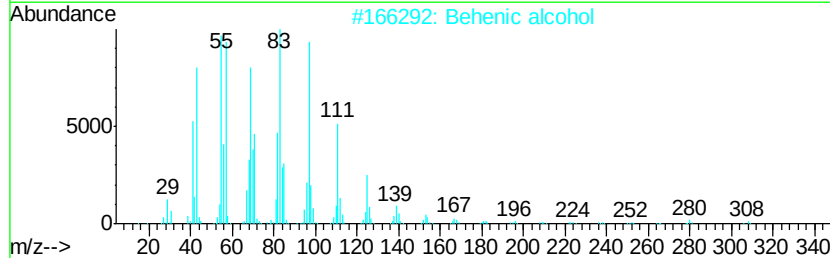
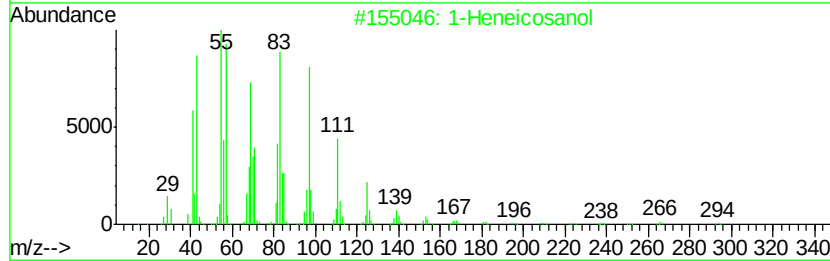
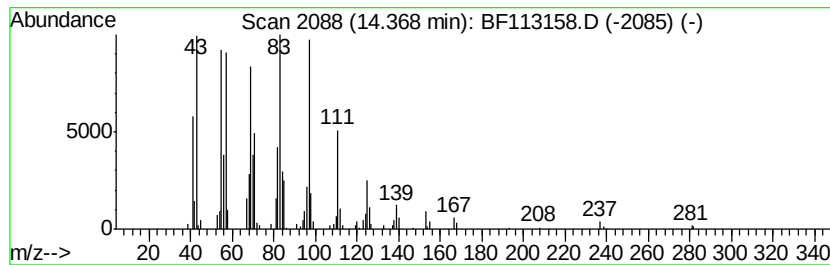
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Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.37	6.72 ng	308116	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	93



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Misc :
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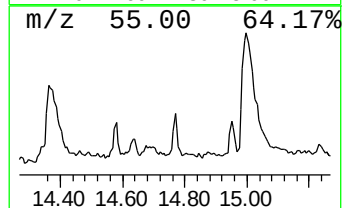
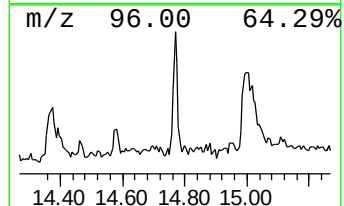
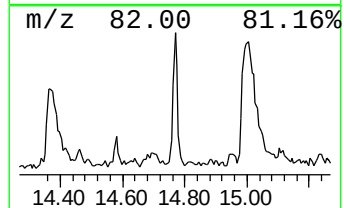
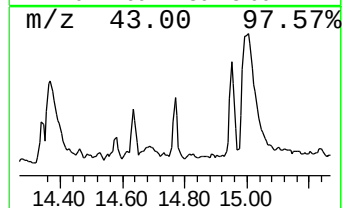
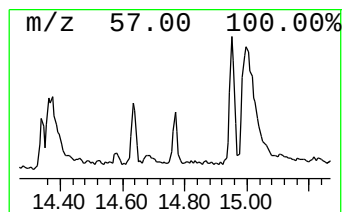
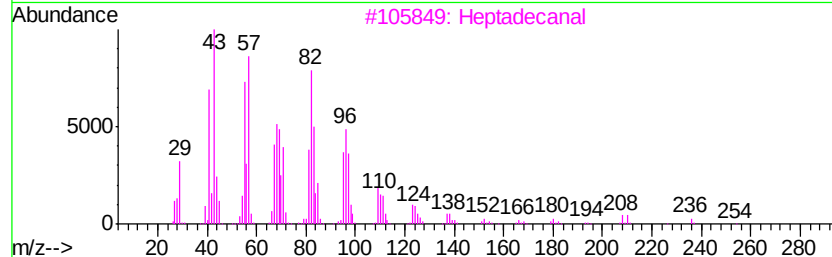
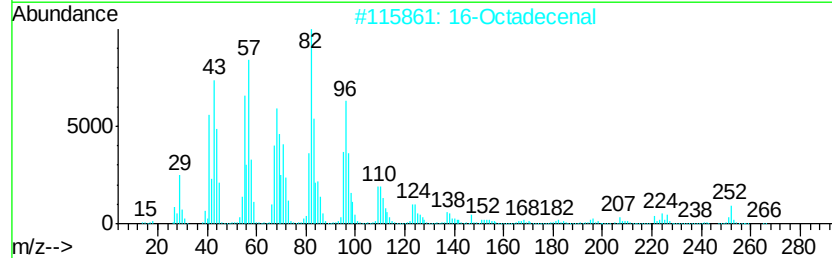
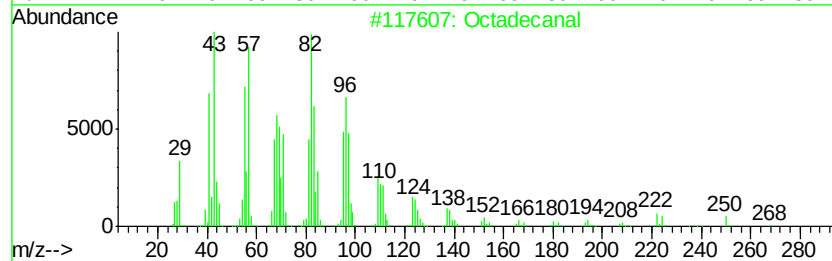
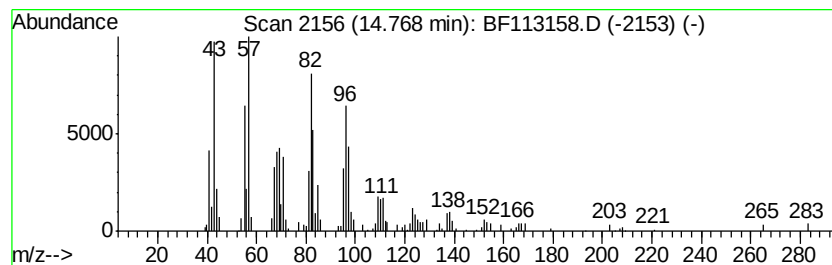
Instrument :
BNA_F
ClientSampleId :
PST-025-SW080-031319

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

Peak Number 7 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.77	2.88 ng	94470	Perylene-d12		15.27
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	16-Octadecenal	266	C18H34O	056554-87-1	90
3	Heptadecanal	254	C17H34O	1000376-70-0	87
4	Pentadecanal-	226	C15H30O	002765-11-9	86
5	Hexadecanal	240	C16H32O	000629-80-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031919\
Data File : BF113158.D
Acq On : 20 Mar 2019 7:20
Operator : JU/SJ
Sample : K1948-15
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-025-SW080-031319

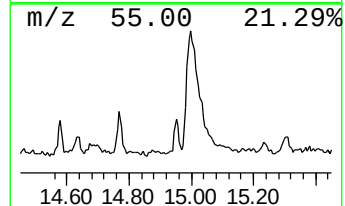
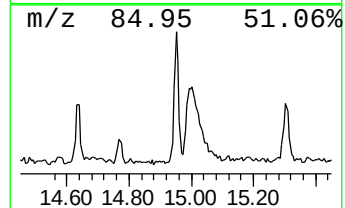
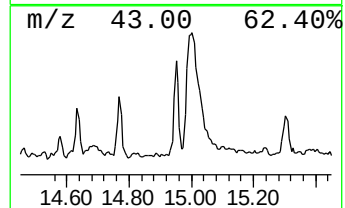
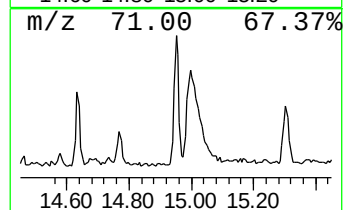
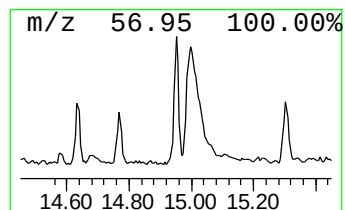
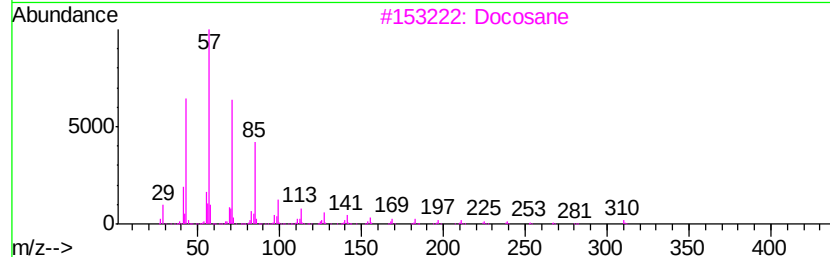
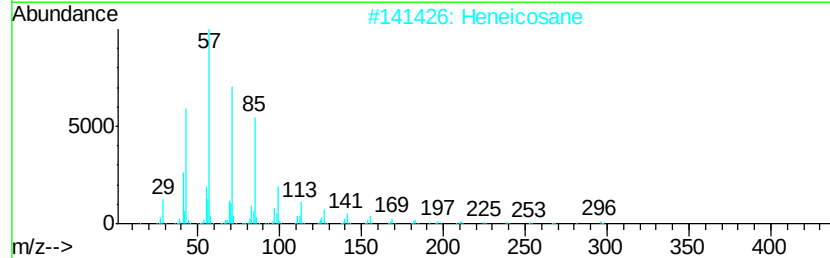
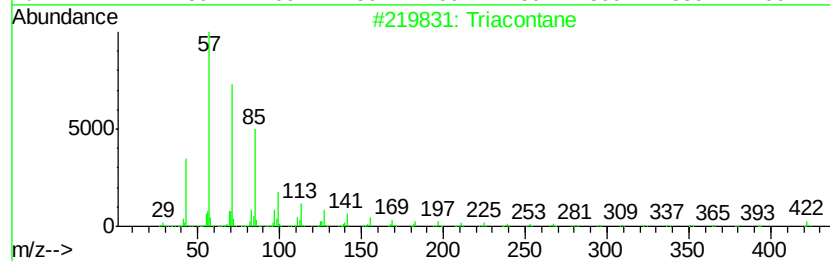
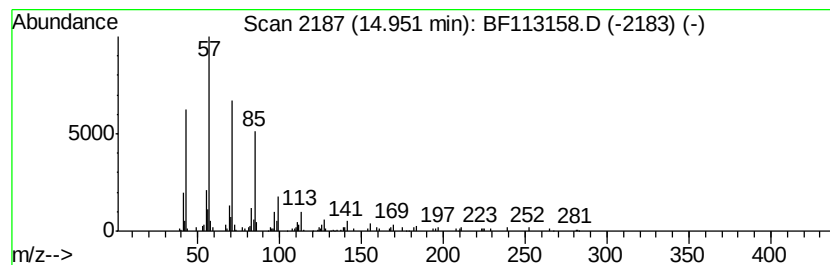
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.82 ng	125644	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Docosane	310	C22H46	000629-97-0	87
4		Octadecane	254	C18H38	000593-45-3	86
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031919\
Data File : BF113158.D
Acq On : 20 Mar 2019 7:20
Operator : JU/SJ
Sample : K1948-15
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-025-SW080-031319

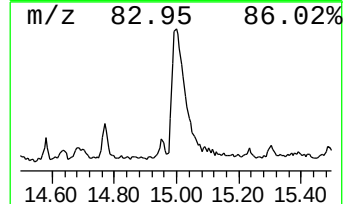
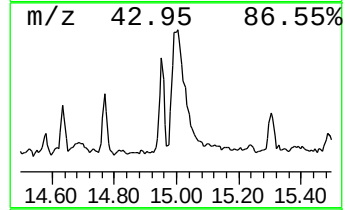
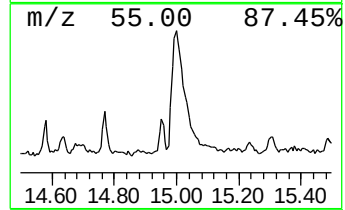
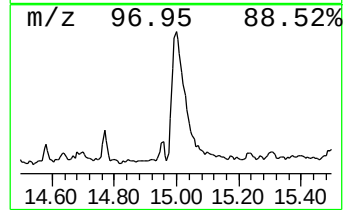
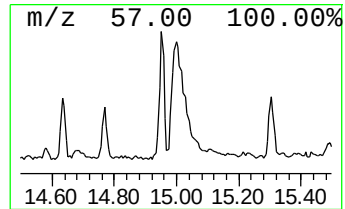
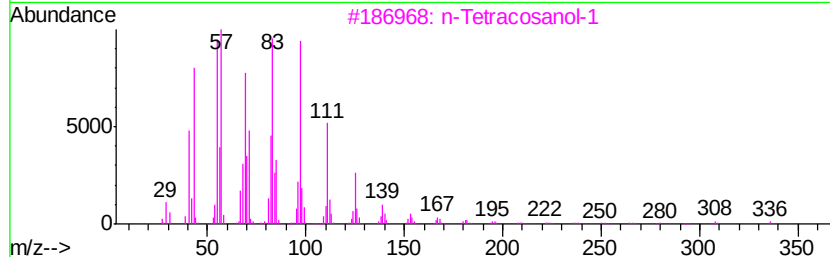
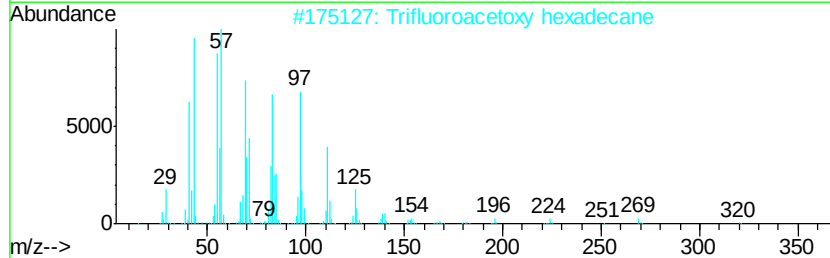
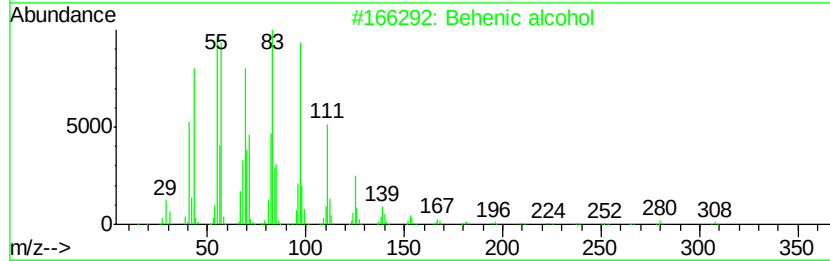
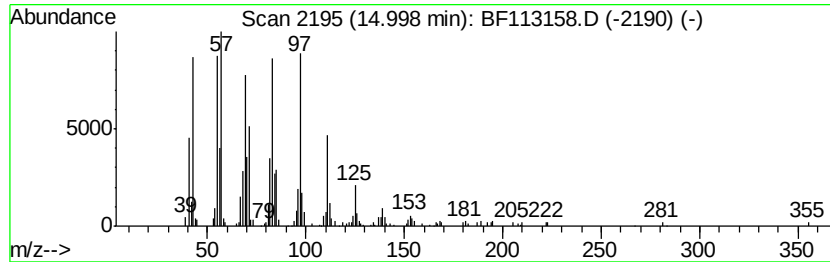
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	20.45 ng	671643	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4		1-Heneicosanol	312	C21H44O	015594-90-8	95
5		1-Heptacosanol	396	C27H56O	002004-39-9	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031919\
Data File : BF113158.D
Acq On : 20 Mar 2019 7:20
Operator : JU/SJ
Sample : K1948-15
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-025-SW080-031319

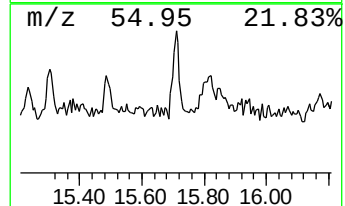
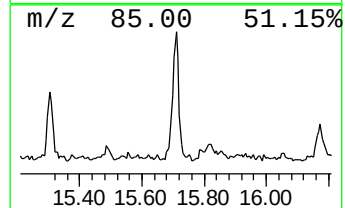
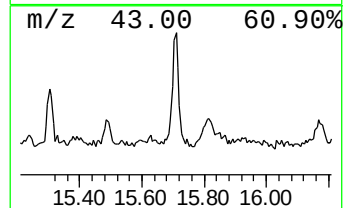
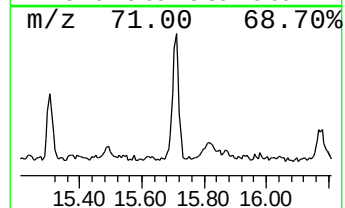
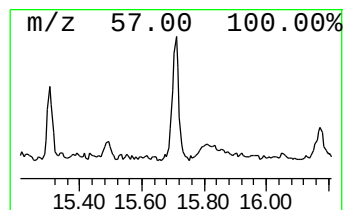
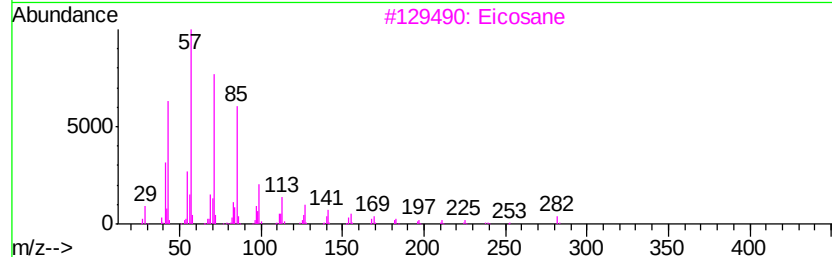
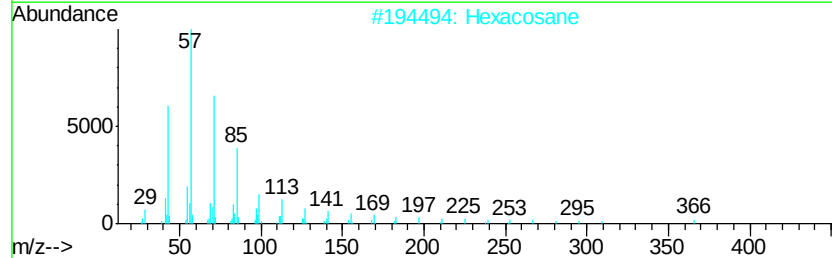
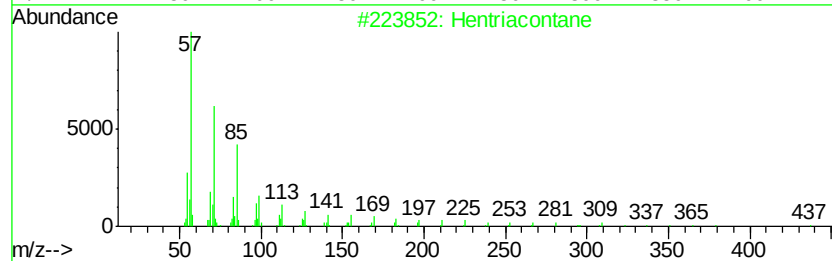
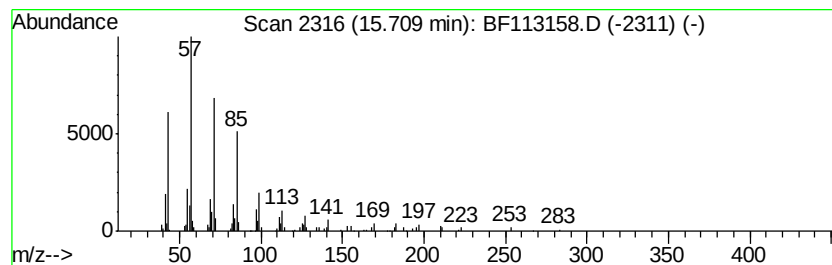
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	4.15 ng	136221	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Eicosane	282	C20H42	000112-95-8	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031919\
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Acq On : 20 Mar 2019 7:20
Operator : JU/SJ
Sample : K1948-15
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PST-025-SW080-031319

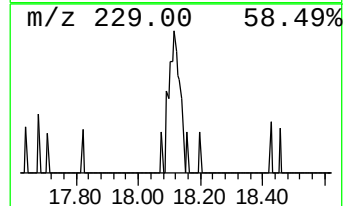
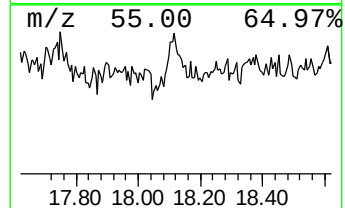
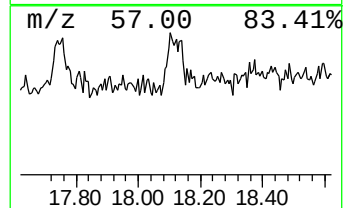
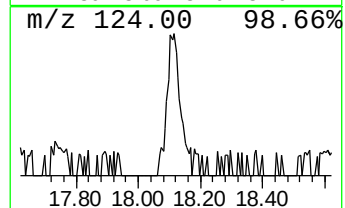
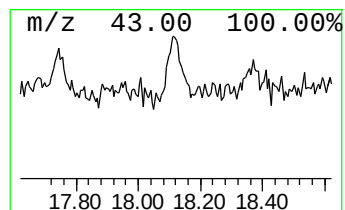
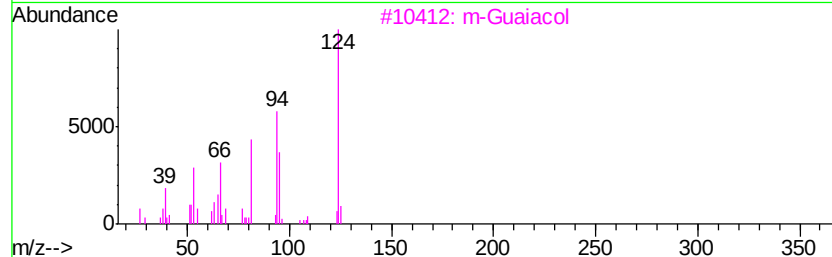
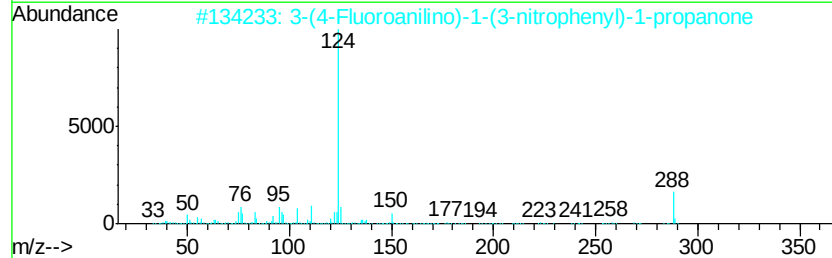
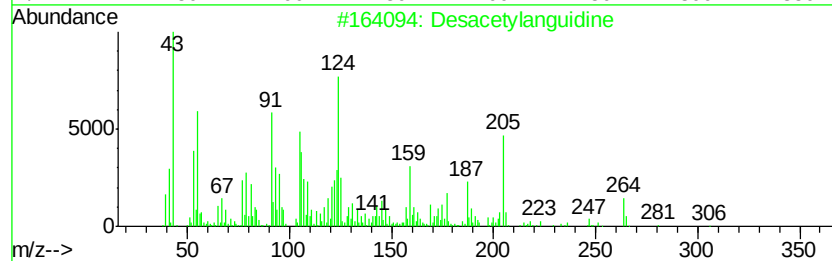
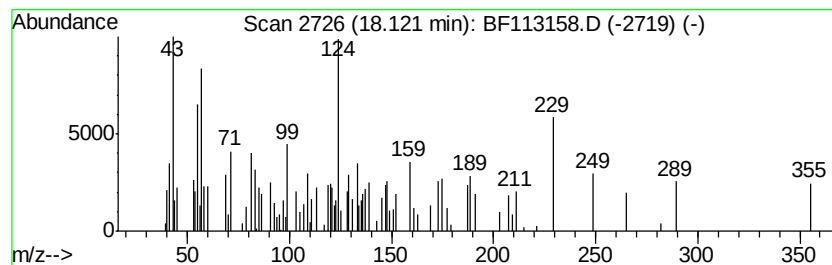
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown18.12 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.12	2.73 ng	89802	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Desacetylanguidine	324	C17H24O6	002623-22-5	27
2		3-(4-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	350039-84-8	22
3		m-Guaiacol	124	C7H8O2	000150-19-6	18
4		4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	001004-36-0	18
5		4,5-Dimethyl-2-pyrimidone	124	C6H8N2O	034939-17-8	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031919\
 Data File : BF113158.D
 Acq On : 20 Mar 2019 7:20
 Operator : JU/SJ
 Sample : K1948-15
 Misc :
 ALS Vial : 35 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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n-Hexadecanoic acid	11.77	7.4	ng	324920	4	11.23	879045	20.0
Octadecanoic acid	12.55	2.6	ng	119734	5	13.86	917150	20.0
n-Tetracosanol-1	13.73	5.5	ng	253424	5	13.86	917150	20.0
1-Heneicosanol	14.37	6.7	ng	308116	5	13.86	917150	20.0
Octadecanal	14.77	2.9	ng	94470	6	15.27	657023	20.0
Triacontane	14.95	3.8	ng	125644	6	15.27	657023	20.0
Behenic alcohol	15.00	20.4	ng	671643	6	15.27	657023	20.0
Hentriacontane	15.71	4.2	ng	136221	6	15.27	657023	20.0
unknown18.12	18.12	2.7	ng	89802	6	15.27	657023	20.0