

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
 Data File : BF110616.D
 Acq On : 9 Nov 2018 10:04
 Operator : JU/SJ
 Sample : J5813-03
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TS-C

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-BF110818.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	24	29	48	rVB	279861	393369	19.38%	1.774%
2	5.187	523	527	537	rBV	29802	44243	2.18%	0.200%
3	5.563	587	591	604	rBV	1620971	1729004	85.17%	7.797%
4	6.569	757	762	776	rBV	1711774	1935100	95.32%	8.727%
5	6.716	782	787	790	rBV	1987394	1857684	91.51%	8.378%
6	6.945	822	826	832	rBV	512847	461427	22.73%	2.081%
7	7.098	848	852	856	rBV	1603692	1377287	67.84%	6.211%
8	7.510	917	922	925	rBV	1188465	1148204	56.56%	5.178%
9	8.222	1039	1043	1054	rBV	613005	611587	30.13%	2.758%
10	9.298	1221	1226	1229	rBV	2271608	1886680	92.94%	8.509%
11	9.692	1289	1293	1299	rBV	241414	226531	11.16%	1.022%
12	9.986	1338	1343	1351	rVB	702398	643465	31.70%	2.902%
13	10.775	1473	1477	1489	rBV	829482	749208	36.91%	3.379%
14	11.475	1593	1596	1599	rBV	576750	539828	26.59%	2.435%
15	11.498	1599	1600	1605	rVB	44395	35164	1.73%	0.159%
16	11.998	1671	1685	1699	rBV	1109709	2030097	100.00%	9.155%
17	12.304	1734	1737	1742	rVB5	20811	30857	1.52%	0.139%
18	12.633	1789	1793	1797	rBV	41441	49496	2.44%	0.223%
19	12.698	1797	1804	1808	rVV	116800	188799	9.30%	0.851%
20	12.780	1811	1818	1838	rVV	877672	1649545	81.25%	7.439%
21	12.927	1841	1843	1849	rVB	77207	78194	3.85%	0.353%
22	13.063	1861	1866	1869	rVB	1209687	1143042	56.30%	5.155%
23	13.263	1897	1900	1904	rVB4	19916	26190	1.29%	0.118%
24	13.492	1936	1939	1941	rBV4	18446	24376	1.20%	0.110%
25	13.610	1956	1959	1966	rVB2	44490	67805	3.34%	0.306%
26	13.939	2011	2015	2020	rBV	127393	175821	8.66%	0.793%
27	14.127	2042	2047	2050	rBV	519226	495545	24.41%	2.235%
28	14.257	2065	2069	2072	rVB	122676	127916	6.30%	0.577%
29	14.557	2116	2120	2123	rBV	301137	292169	14.39%	1.318%
30	14.874	2169	2174	2179	rBV	398498	490444	24.16%	2.212%
31	15.027	2198	2200	2205	rBV4	41373	47122	2.32%	0.213%
32	15.227	2230	2234	2239	rVB	392506	458115	22.57%	2.066%
33	15.621	2297	2301	2304	rBV	261480	370670	18.26%	1.672%
34	15.651	2304	2306	2311	rVB	296881	327168	16.12%	1.475%

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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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35	16.074	2373	2378	2385	rVB	208752	307489	15.15%	1.387%
36	16.604	2463	2468	2477	rVB	87121	154317	7.60%	0.696%

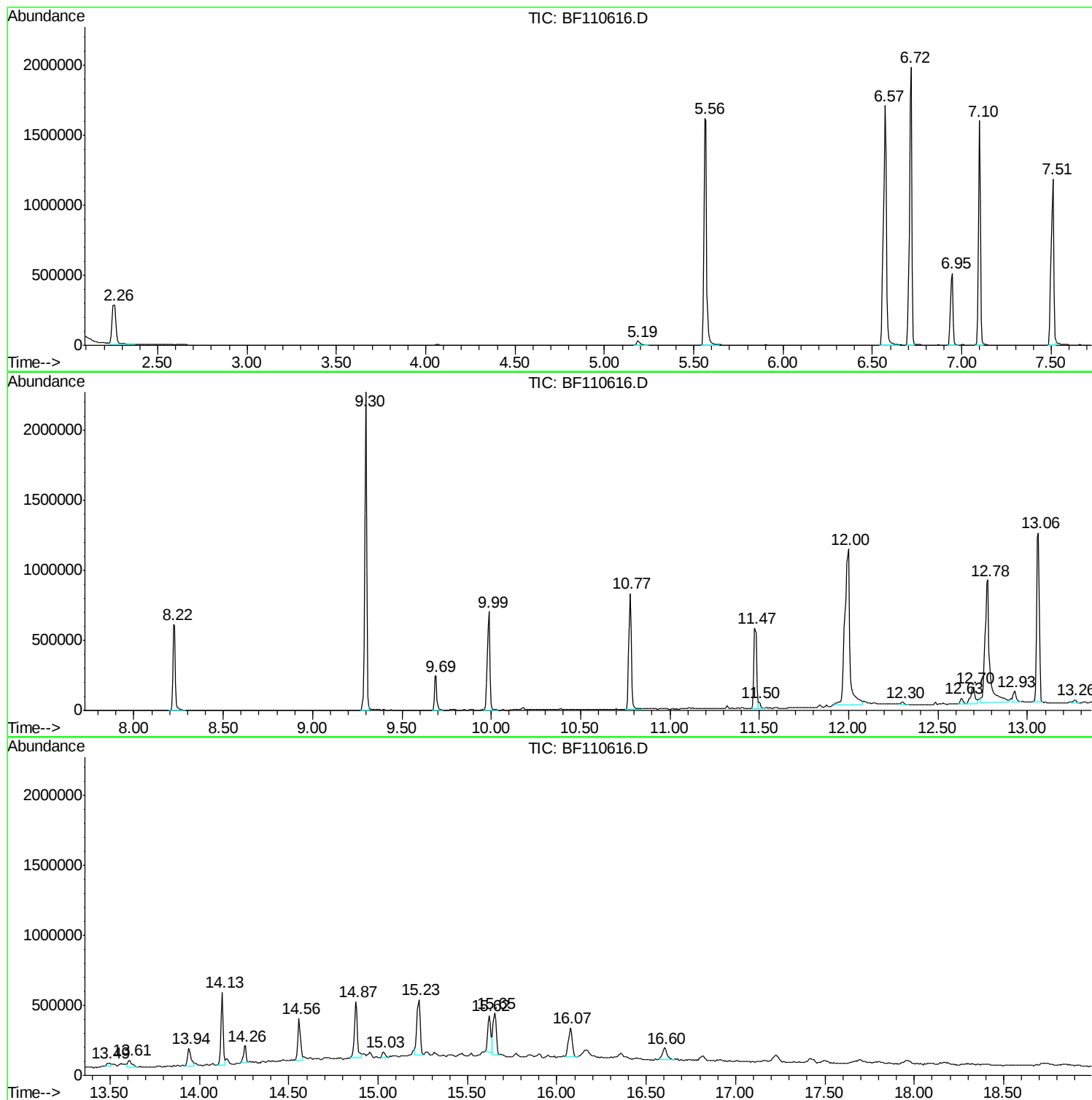
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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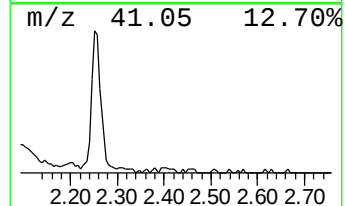
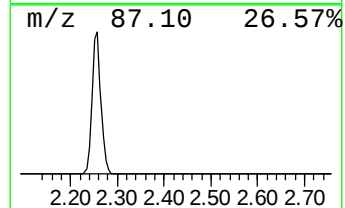
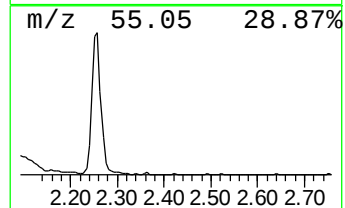
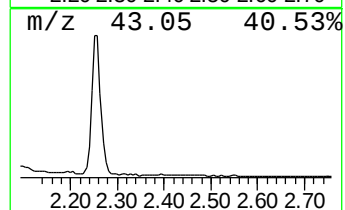
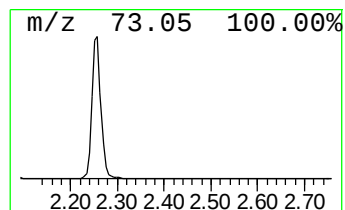
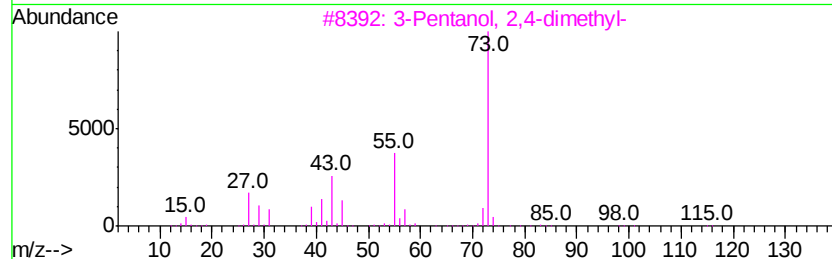
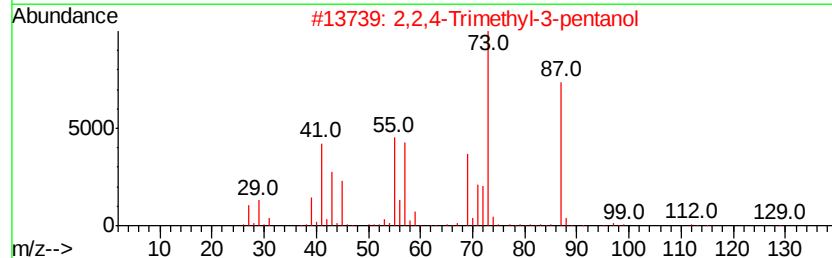
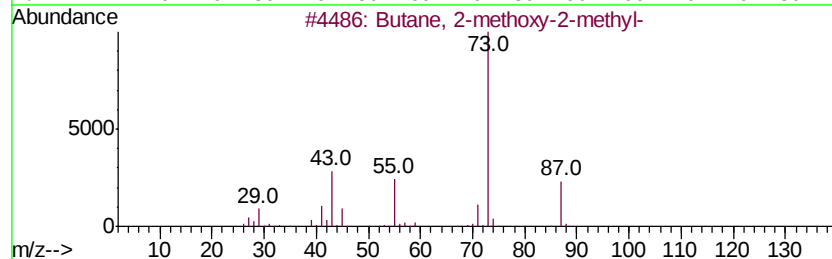
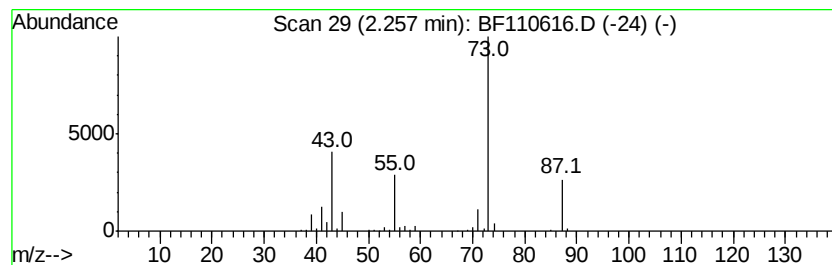
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	17.05 ng	393369	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16



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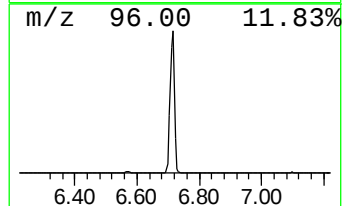
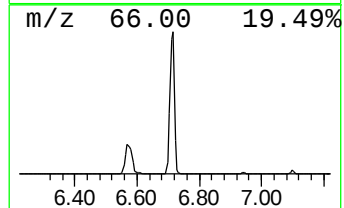
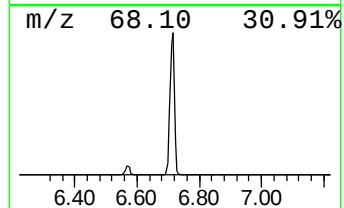
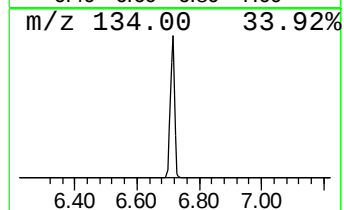
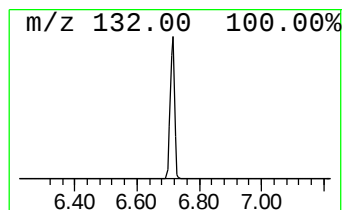
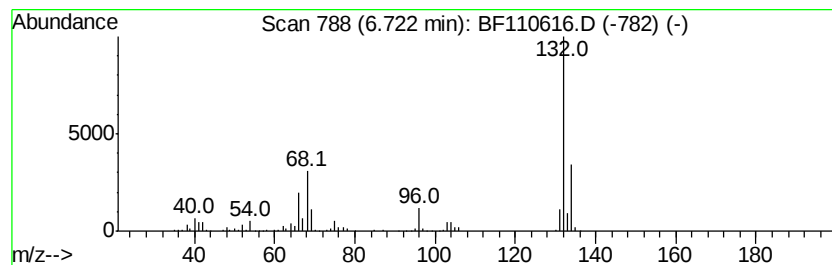
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	80.52 ng	1857680	1,4-Dichlorobenzene-d4	6.95

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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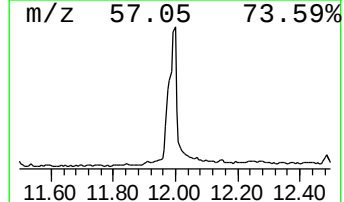
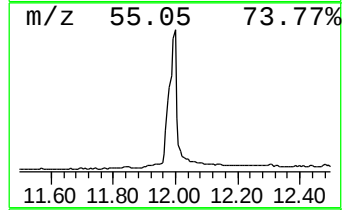
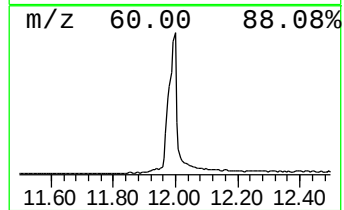
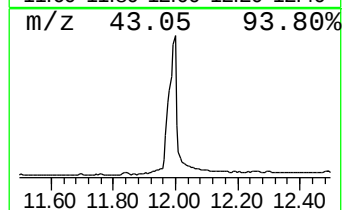
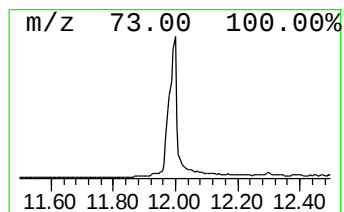
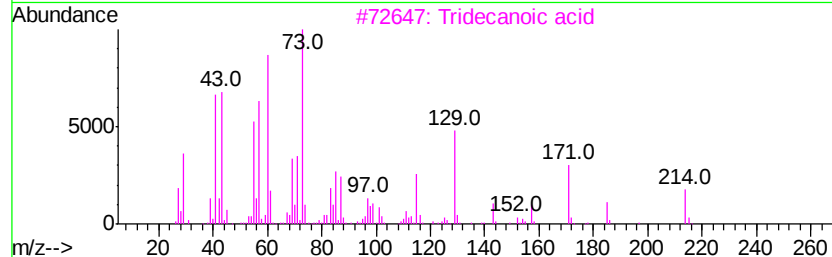
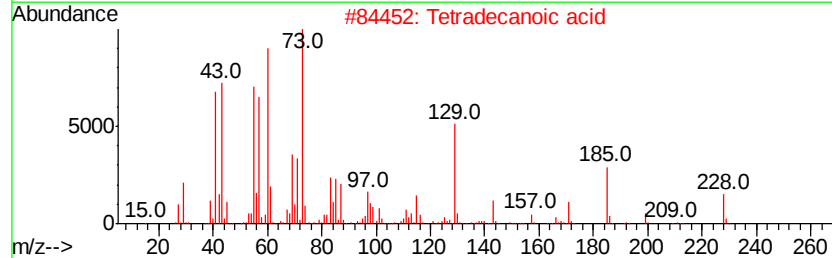
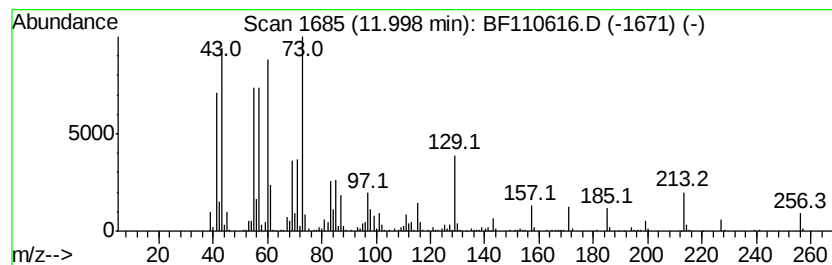
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	75.21 ng	2030100	Phenanthrene-d10	11.47

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	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	92
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



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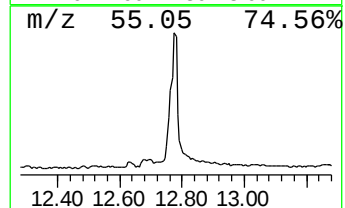
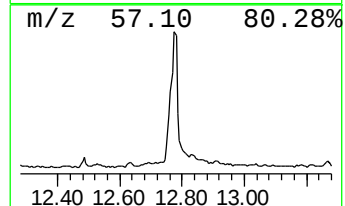
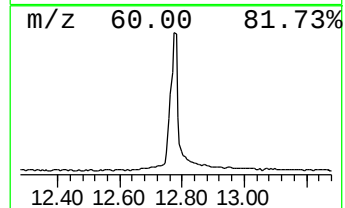
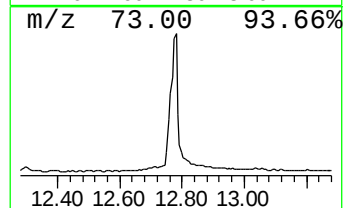
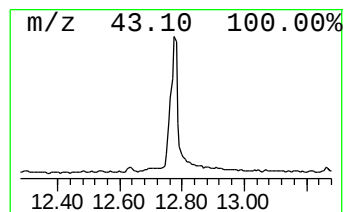
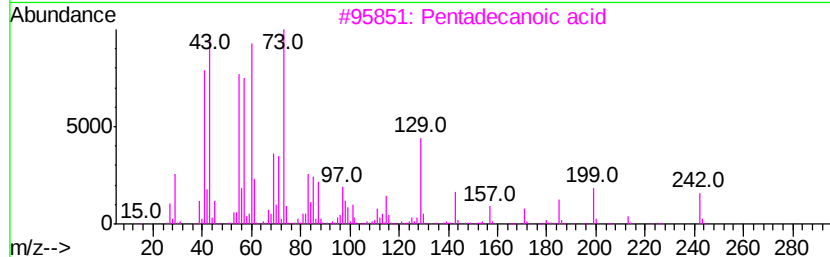
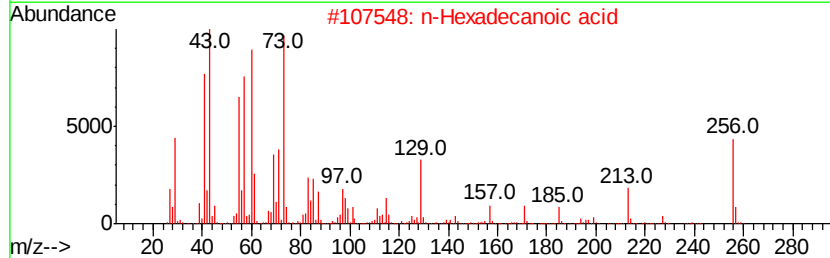
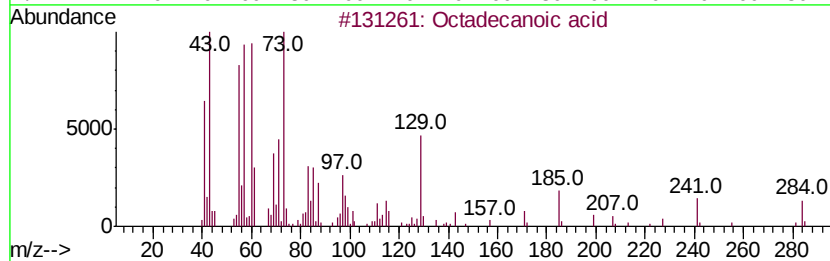
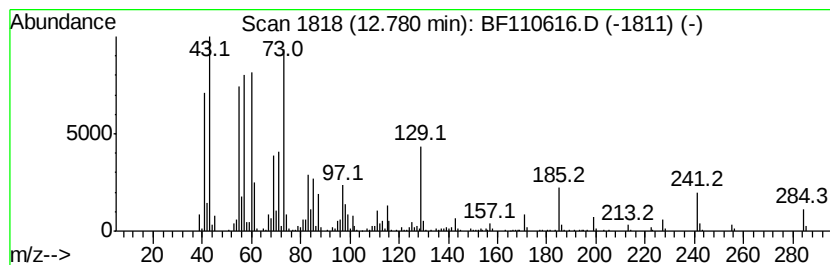
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	61.11 ng	1649550	Phenanthrene-d10	11.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Tridecanoic acid	214	C13H26O2	000638-53-9	76



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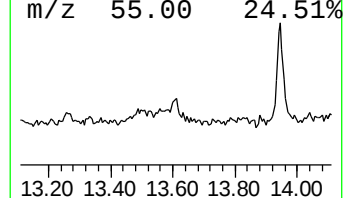
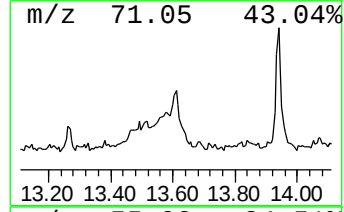
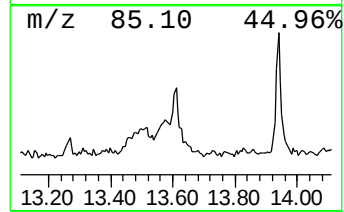
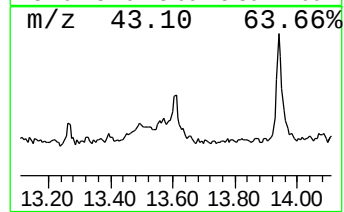
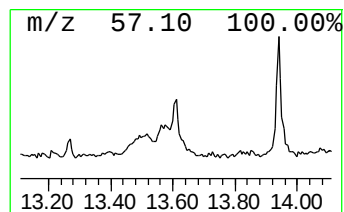
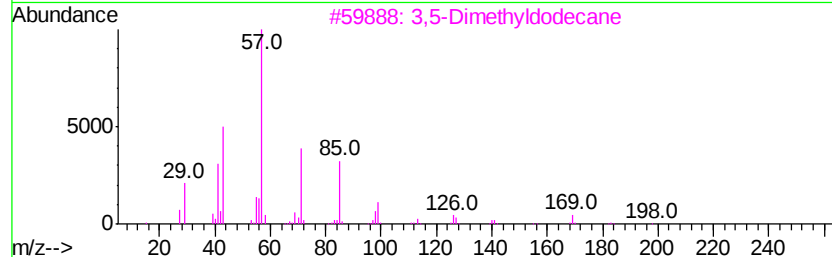
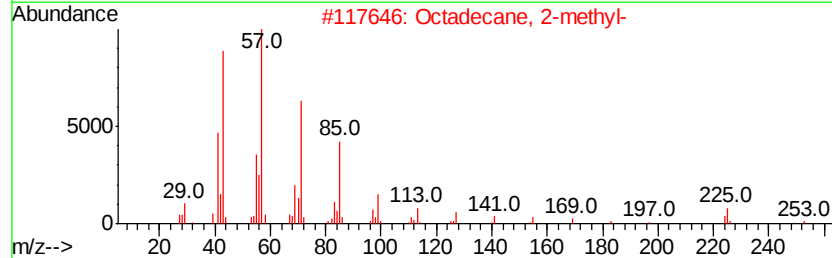
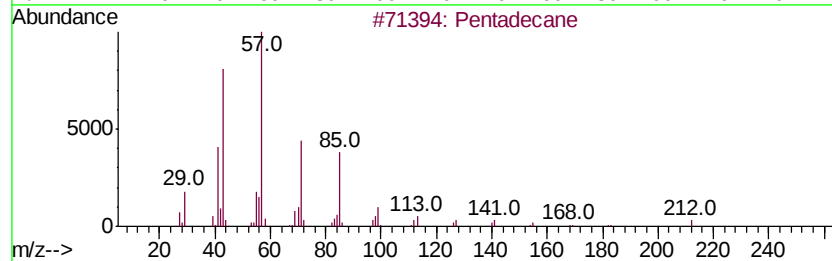
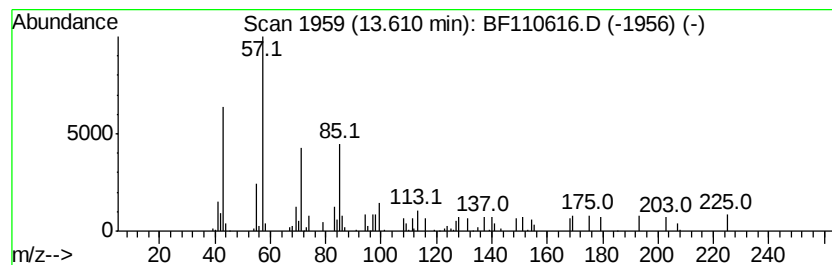
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	2.74 ng	67805	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	64
2		Octadecane, 2-methyl-	268	C19H40	001560-88-9	64
3		3,5-Dimethyldodecane	198	C14H30	107770-99-0	59
4		Hentriacontane	437	C31H64	000630-04-6	52
5		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	52



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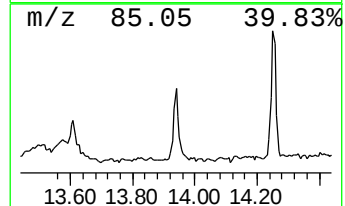
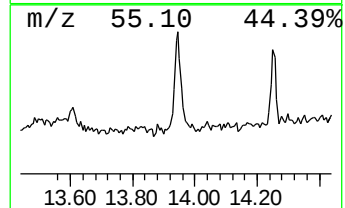
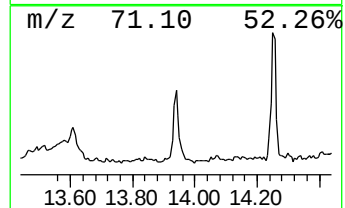
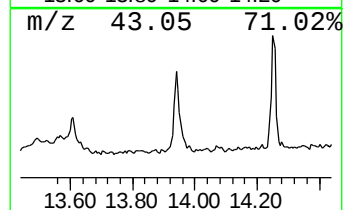
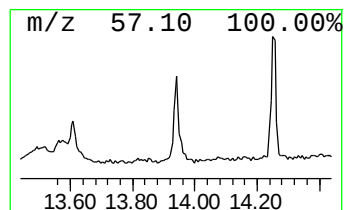
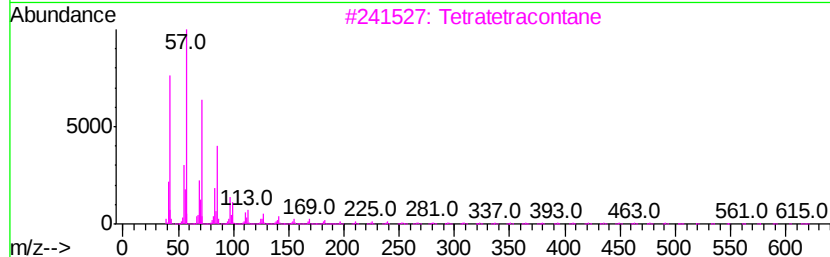
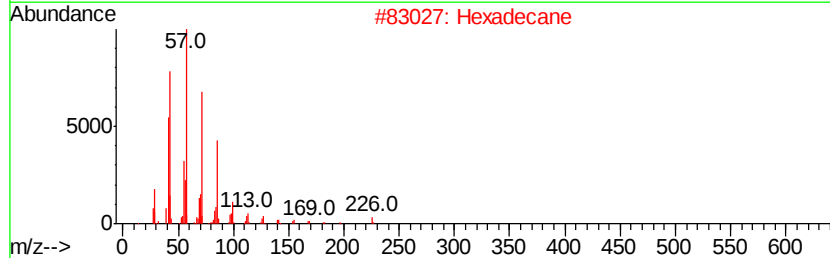
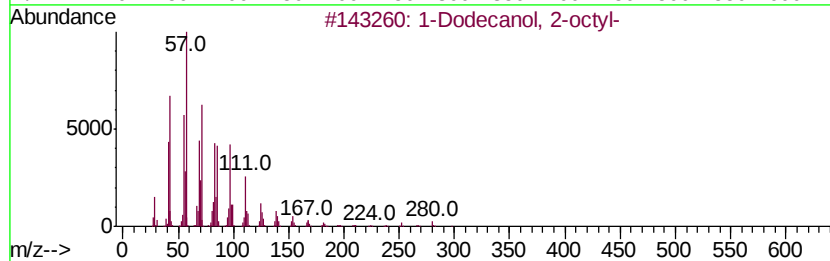
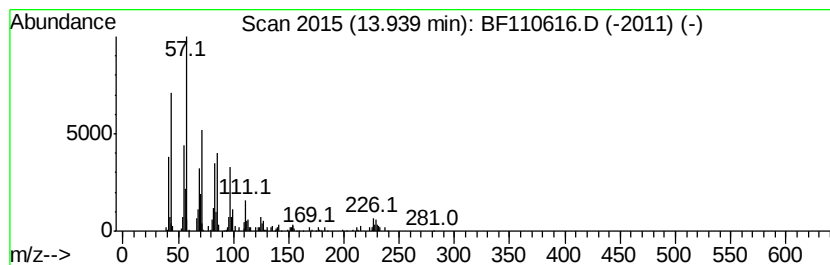
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	7.10 ng	175821	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2		Hexadecane	226	C16H34	000544-76-3	89
3		Tetratetracontane	619	C44H90	007098-22-8	80
4		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	72
5		Oxalic acid, isobutyl tridecyl e...	328	C19H36O4	1000309-37-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110616.D
Acq On : 9 Nov 2018 10:04
Operator : JU/SJ
Sample : J5813-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

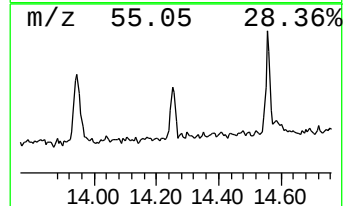
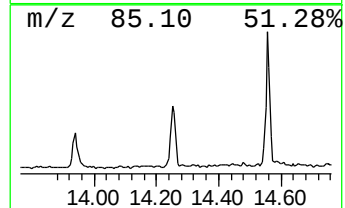
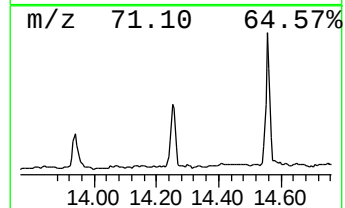
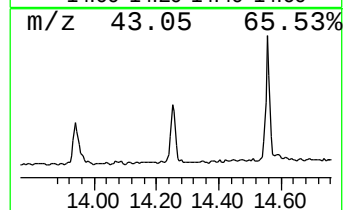
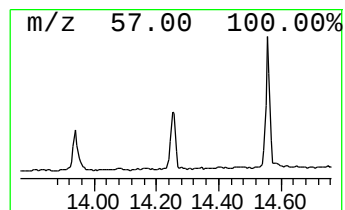
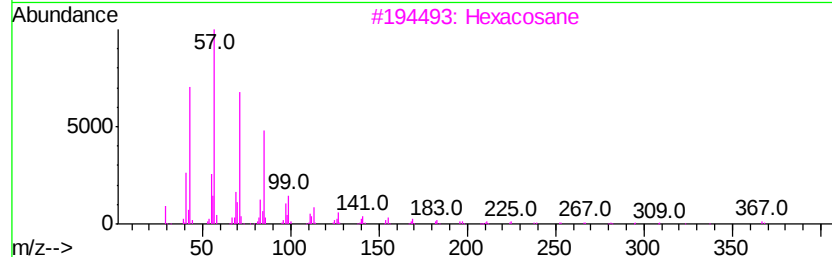
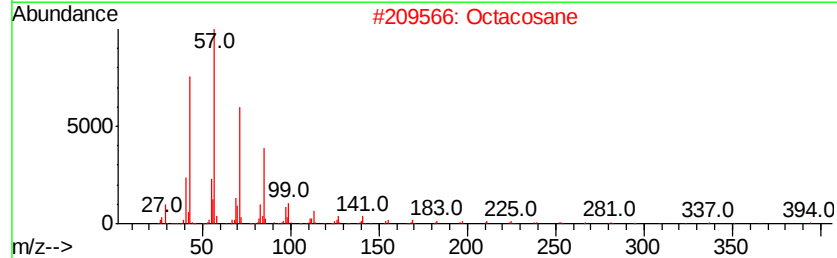
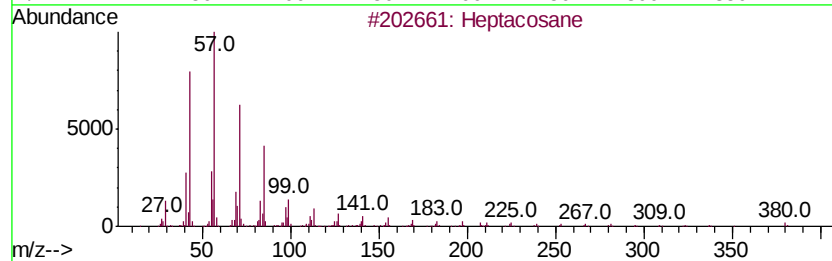
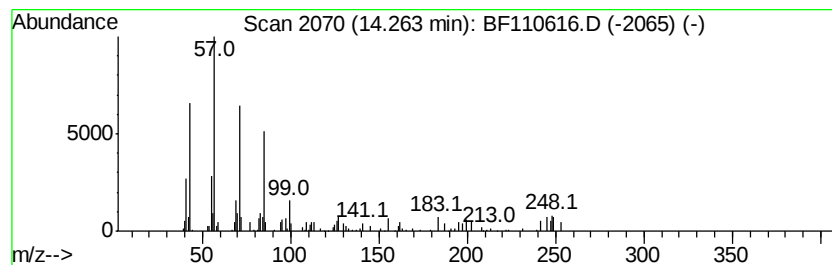
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	5.16 ng	127916	Chrysene-d12	14.13
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	90
2	Octacosane	394 C28H58	000630-02-4	90
3	Hexacosane	366 C26H54	000630-01-3	90
4	Tetracosane	338 C24H50	000646-31-1	90
5	Heneicosane	296 C21H44	000629-94-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
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Sample : J5813-03
Misc :
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Instrument :
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ClientSampleId :
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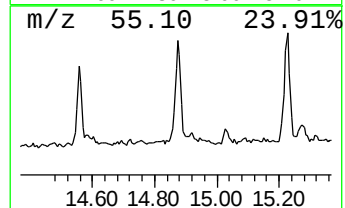
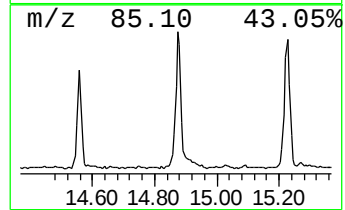
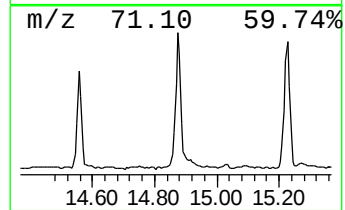
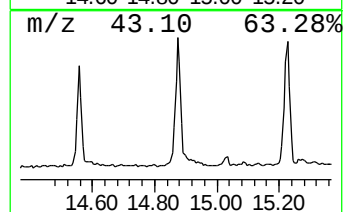
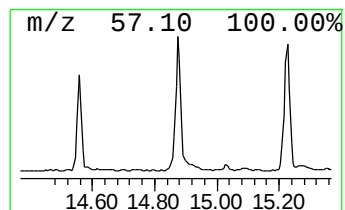
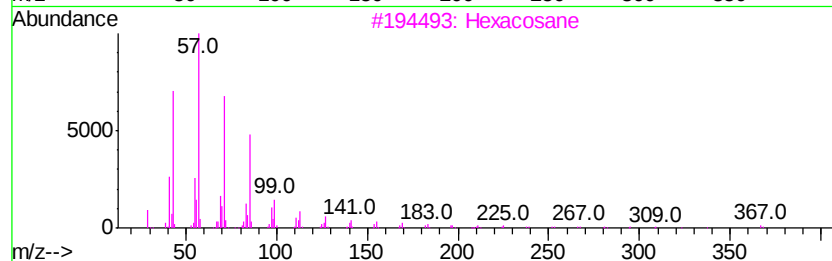
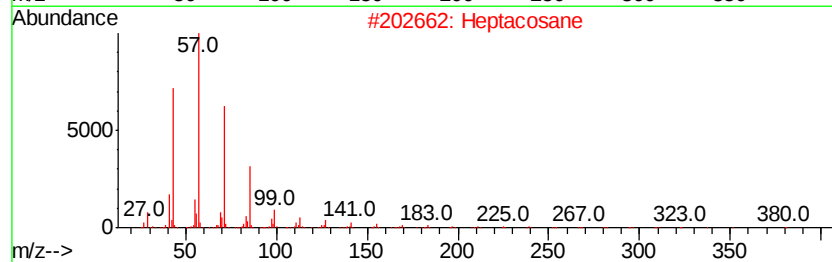
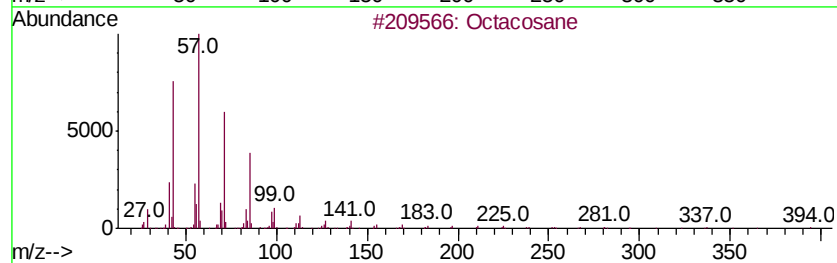
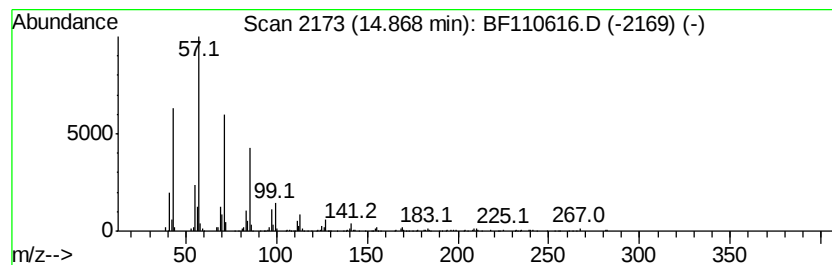
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	19.79 ng	490444	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heneicosane	296	C21H44	000629-94-7	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110616.D
Acq On : 9 Nov 2018 10:04
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Sample : J5813-03
Misc :
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Instrument :
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ClientSampleId :
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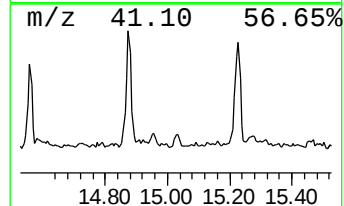
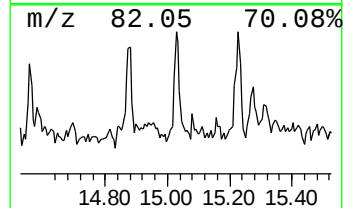
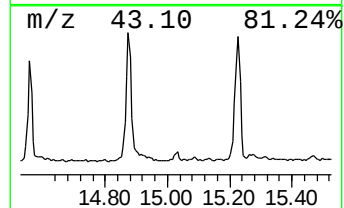
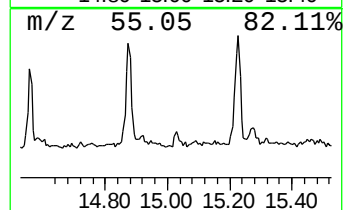
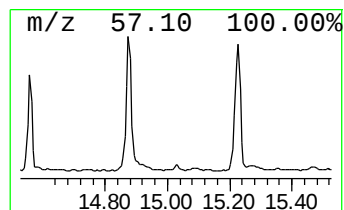
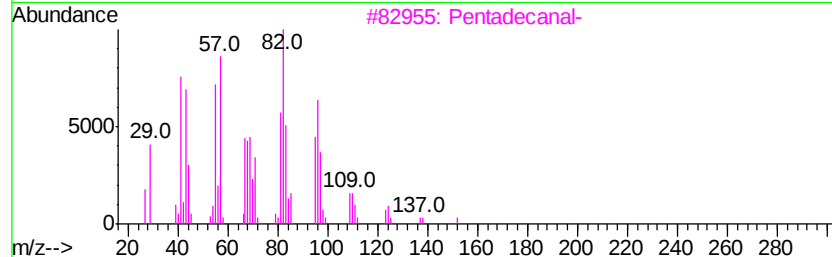
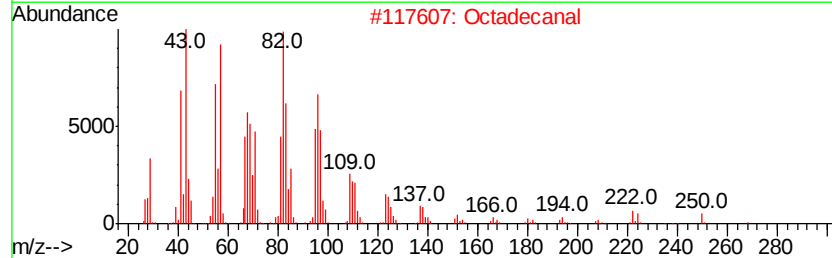
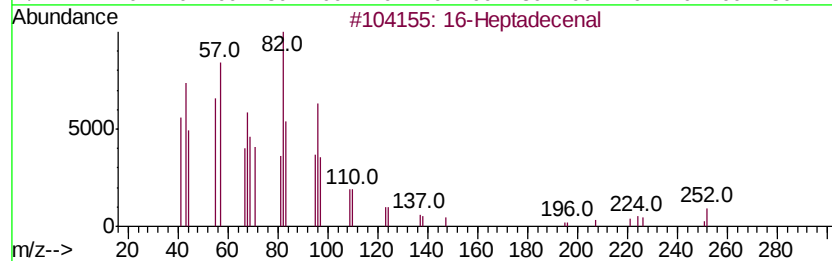
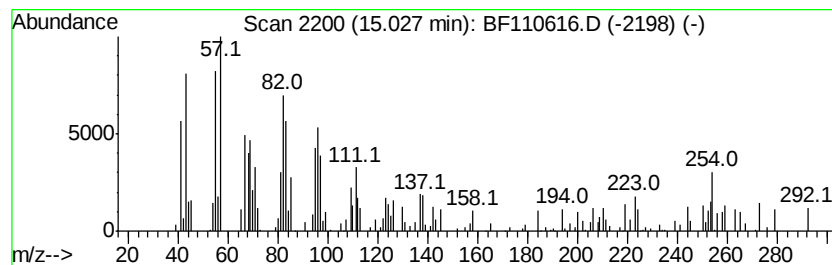
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 16-Heptadecenal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	2.88 ng	47122	Perylene-d12	15.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			16-Heptadecenal	252	C17H32O	1000144-57-9	55
2			Octadecanal	268	C18H36O	000638-66-4	53
3			Pentadecanal-	226	C15H30O	002765-11-9	49
4			1,19-Eicosadiene	278	C20H38	014811-95-1	49
5			E-7-Tetradecen-1-ol acetate	254	C16H30O2	1000130-79-2	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110616.D
Acq On : 9 Nov 2018 10:04
Operator : JU/SJ
Sample : J5813-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

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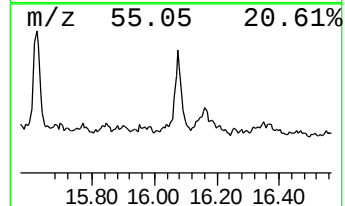
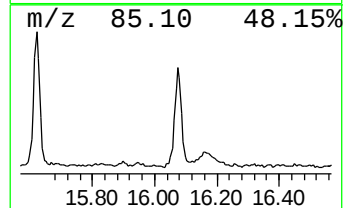
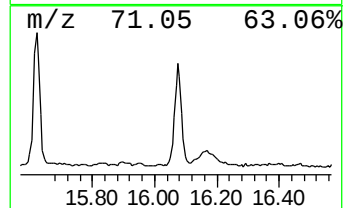
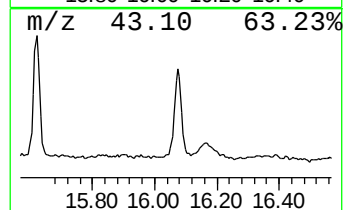
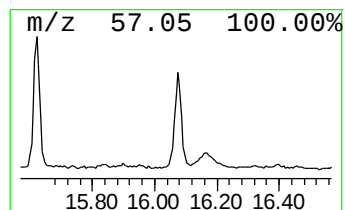
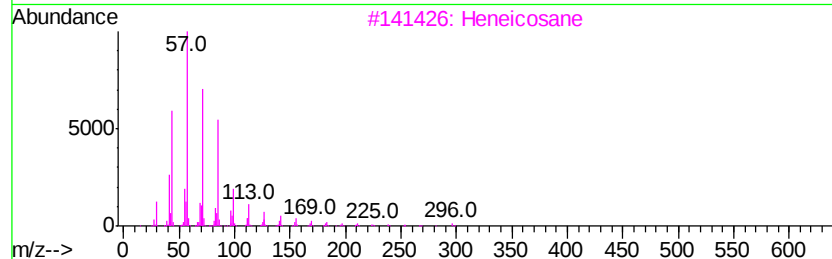
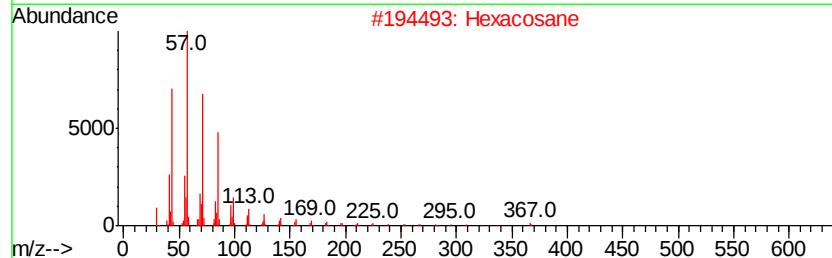
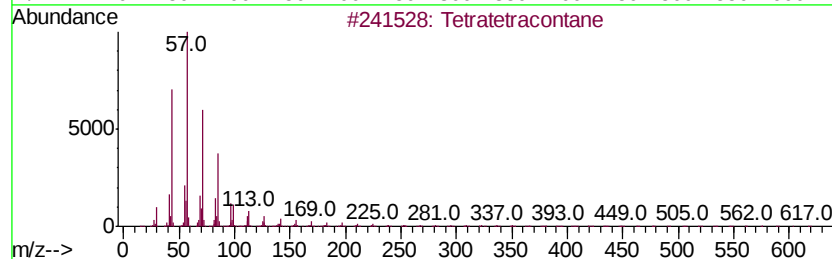
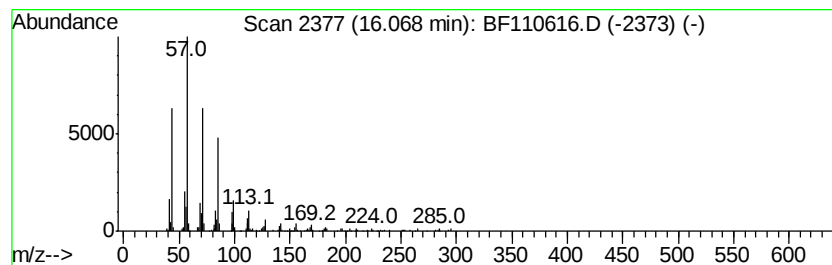
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	18.80 ng	307489	Perylene-d12	15.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110616.D
Acq On : 9 Nov 2018 10:04
Operator : JU/SJ
Sample : J5813-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

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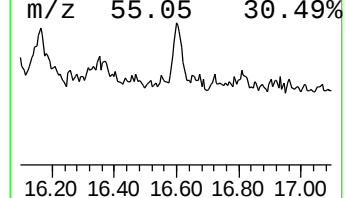
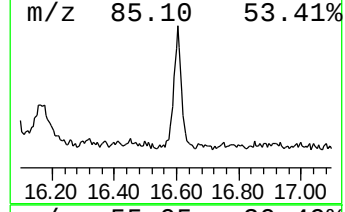
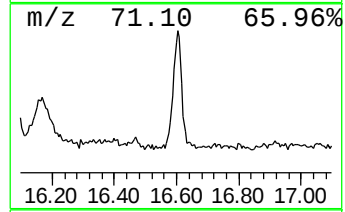
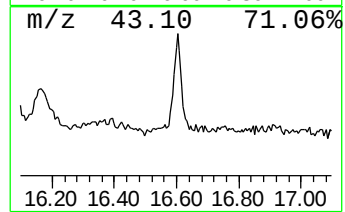
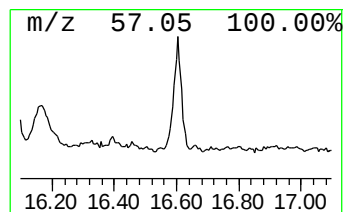
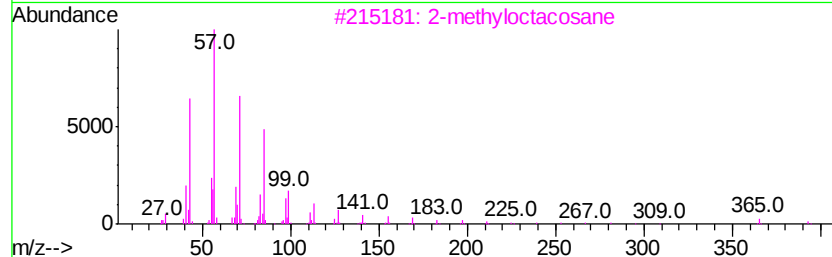
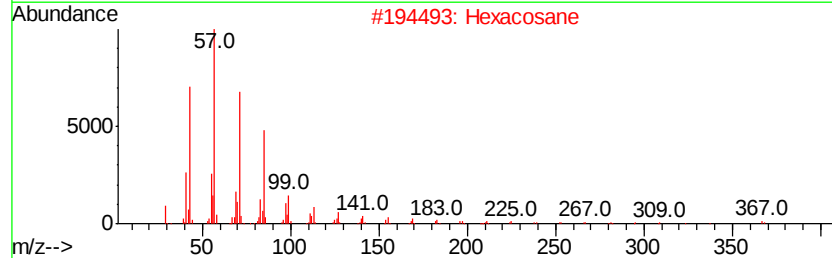
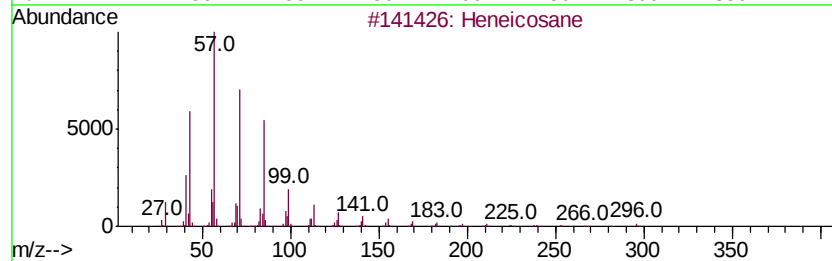
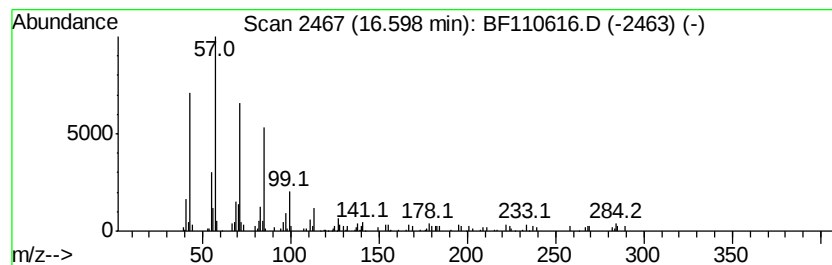
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	9.43 ng	154317	Perylene-d12	15.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	86
2		Hexacosane	366	C26H54	000630-01-3	83
3		2-methyloctacosane	408	C29H60	1000376-72-8	80
4		Tetratetracontane	619	C44H90	007098-22-8	70
5		Tetracosane	338	C24H50	000646-31-1	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
Data File : BF110616.D
Acq On : 9 Nov 2018 10:04
Operator : JU/SJ
Sample : J5813-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.72	6.72	80.5 ng		1857680	1	6.95	461427	20.0
n-Hexadecanoic acid	12.00	75.2 ng		2030100	4	11.47	539828	20.0
Octadecanoic acid	12.78	61.1 ng		1649550	4	11.47	539828	20.0
Pentadecane	13.61	2.7 ng		67805	5	14.13	495545	20.0
1-Dodecanol, 2-oc...	13.94	7.1 ng		175821	5	14.13	495545	20.0
Heptacosane	14.26	5.2 ng		127916	5	14.13	495545	20.0
Octacosane	14.87	19.8 ng		490444	5	14.13	495545	20.0
16-Heptadecenal	15.03	2.9 ng		47122	6	15.65	327168	20.0
Tetratetracontane	16.07	18.8 ng		307489	6	15.65	327168	20.0
Heneicosane	16.60	9.4 ng		154317	6	15.65	327168	20.0