

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
 Data File : BF110157.D
 Acq On : 25 Oct 2018 13:12
 Operator : JU/SJ
 Sample : J5618-06
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1018-S-DH-15

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-BF102318.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	2.334	37	42	60	rVB	403590	606832	16.64%	1.730%
2	3.610	257	259	268	rBV	17218	37355	1.02%	0.106%
3	5.210	526	531	541	rVB	120933	158357	4.34%	0.451%
4	5.593	589	596	599	rBV	3225185	3068001	84.11%	8.746%
5	6.593	760	766	770	rBV2	2940724	3447641	94.52%	9.828%
6	6.734	786	790	794	rBV	3171256	3256412	89.27%	9.283%
7	6.969	826	830	833	rBV	1036388	956567	26.22%	2.727%
8	7.122	852	856	859	rBV	2863200	2489405	68.25%	7.096%
9	7.528	920	925	928	rBV	2098824	2057875	56.42%	5.866%
10	8.251	1043	1048	1051	rBV	1383876	1260781	34.56%	3.594%
11	9.322	1225	1230	1234	rBV	3760060	3647705	100.00%	10.398%
12	9.716	1293	1297	1302	rBV	388736	321959	8.83%	0.918%
13	10.010	1343	1347	1351	rBV	1685705	1400134	38.38%	3.991%
14	10.798	1477	1481	1485	rBV	2223538	2160702	59.23%	6.159%
15	11.498	1597	1600	1603	rBV	1425096	1335718	36.62%	3.808%
16	11.522	1603	1604	1608	rVB	94141	64609	1.77%	0.184%
17	12.010	1683	1687	1690	rBV	255671	239761	6.57%	0.683%
18	12.716	1804	1807	1813	rBV	127108	105345	2.89%	0.300%
19	12.792	1816	1820	1827	rBV5	28431	40894	1.12%	0.117%
20	12.945	1841	1846	1852	rVB	103329	118453	3.25%	0.338%
21	13.086	1866	1870	1873	rBV	3109465	2673366	73.29%	7.621%
22	13.557	1946	1950	1954	rBV	161047	232240	6.37%	0.662%
23	13.586	1954	1955	1960	rVV	77994	74747	2.05%	0.213%
24	13.633	1960	1963	1967	rVB2	38903	52844	1.45%	0.151%
25	13.969	2014	2020	2028	rBV2	207407	267665	7.34%	0.763%
26	14.145	2046	2050	2053	rBV	863935	815016	22.34%	2.323%
27	14.239	2063	2066	2071	rBV3	41800	62048	1.70%	0.177%
28	14.286	2071	2074	2080	rVB	108796	109358	3.00%	0.312%
29	14.592	2120	2126	2134	rBV	267230	321203	8.81%	0.916%
30	14.916	2175	2181	2187	rBV	415351	491551	13.48%	1.401%
31	15.216	2228	2232	2235	rBV	37310	56970	1.56%	0.162%
32	15.268	2235	2241	2245	rVV	519423	626237	17.17%	1.785%
33	15.539	2284	2287	2294	rVB3	41517	64989	1.78%	0.185%
34	15.604	2294	2298	2302	rBV	29116	39428	1.08%	0.112%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.674	2303	2310	2322	rVV2	996897	1446011	39.64%	4.122%
36	16.133	2382	2388	2394	rBV	357730	551323	15.11%	1.572%
37	16.668	2473	2479	2488	rVB	158279	274151	7.52%	0.782%
38	17.304	2581	2587	2597	rVB2	61228	146120	4.01%	0.417%

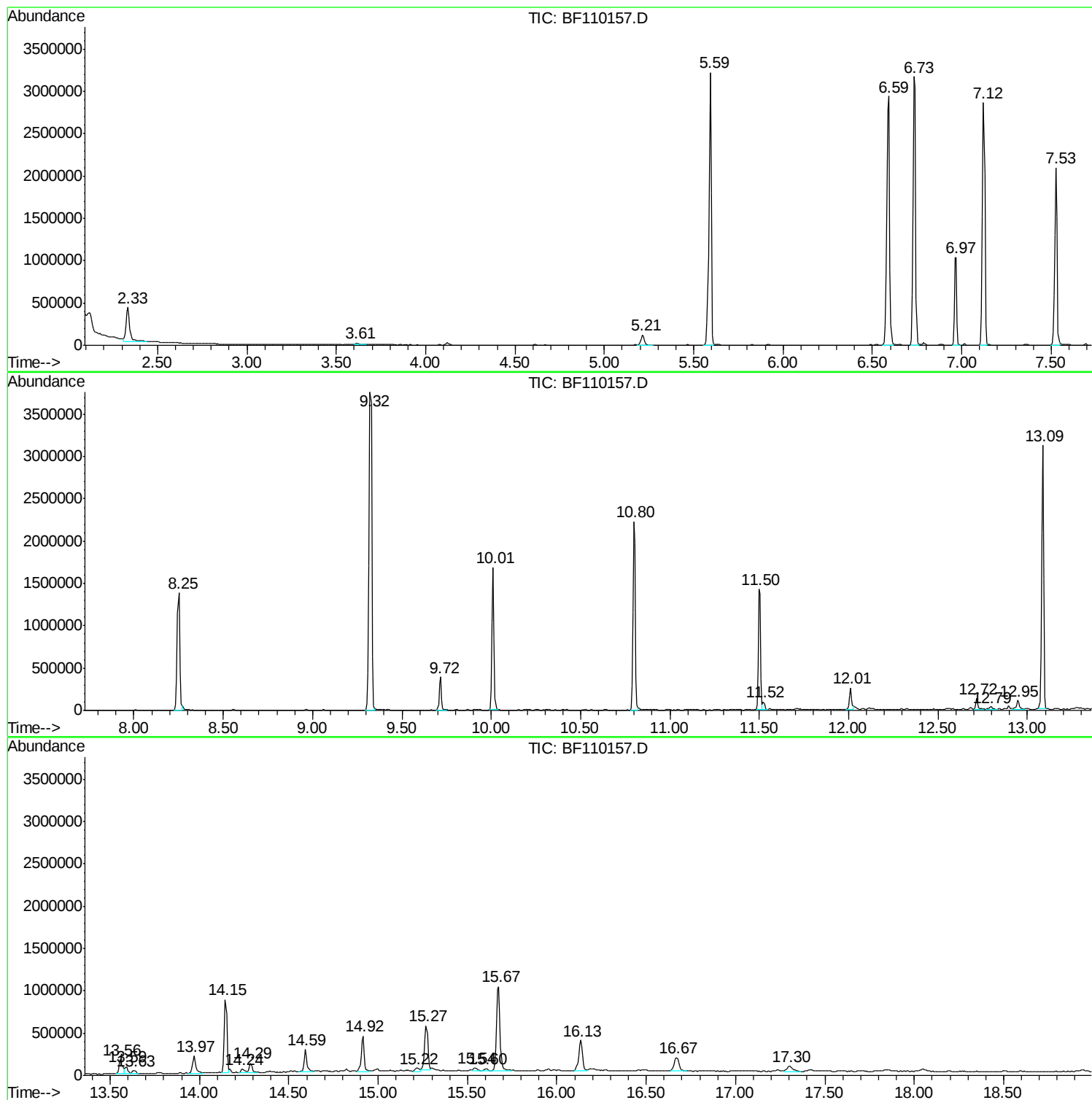
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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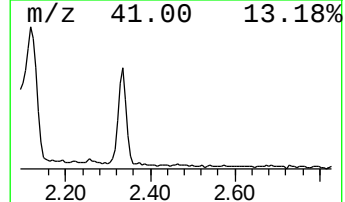
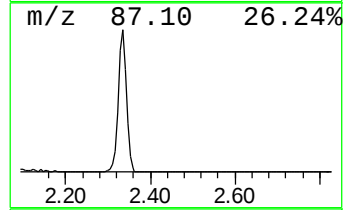
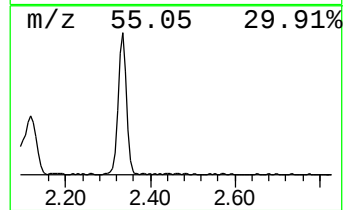
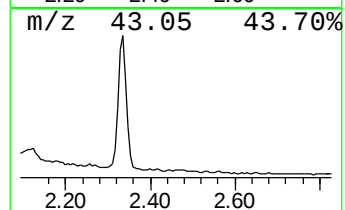
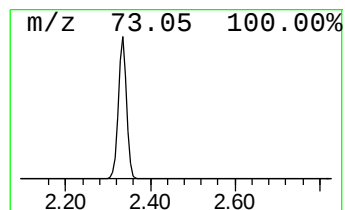
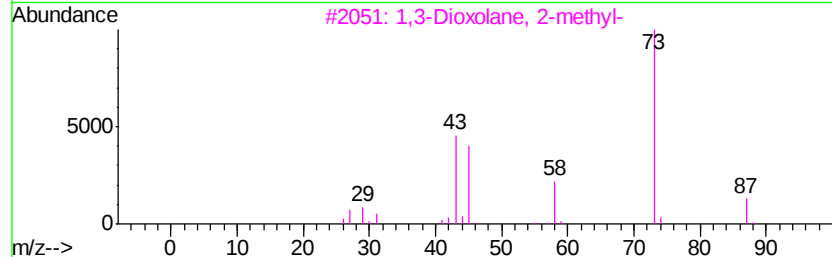
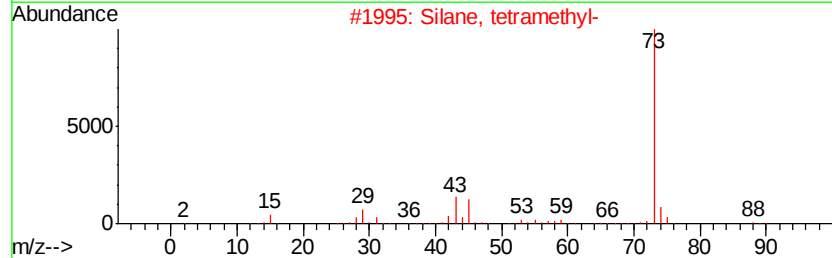
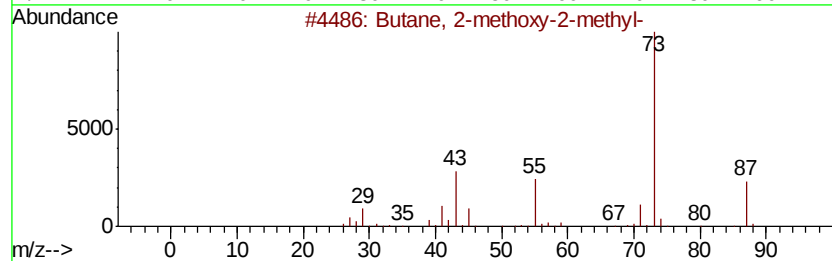
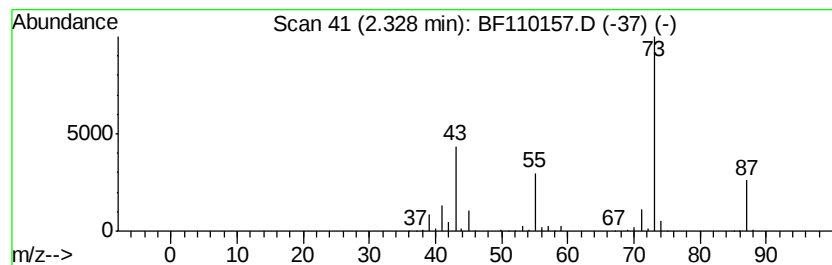
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	12.69 ng	606832	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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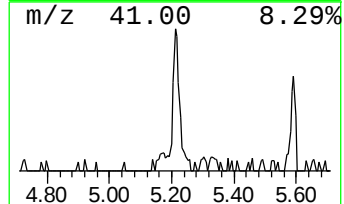
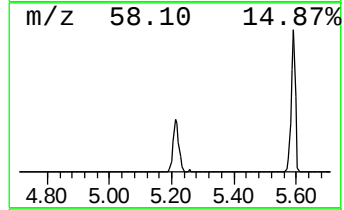
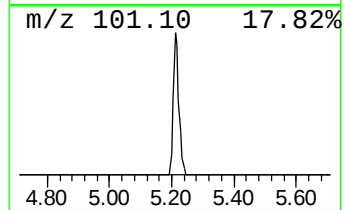
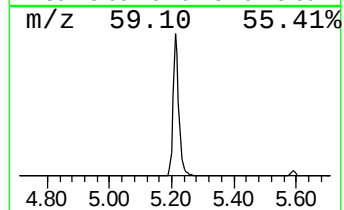
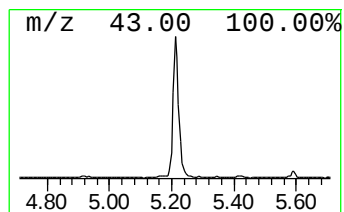
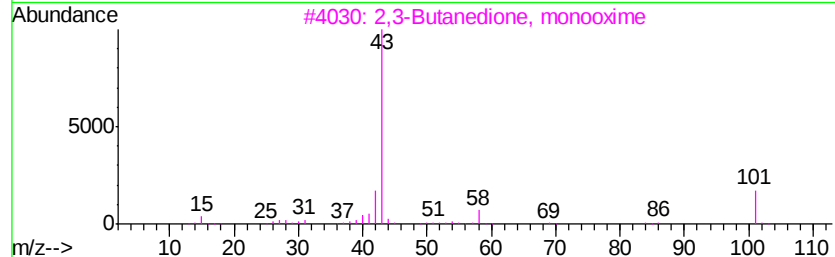
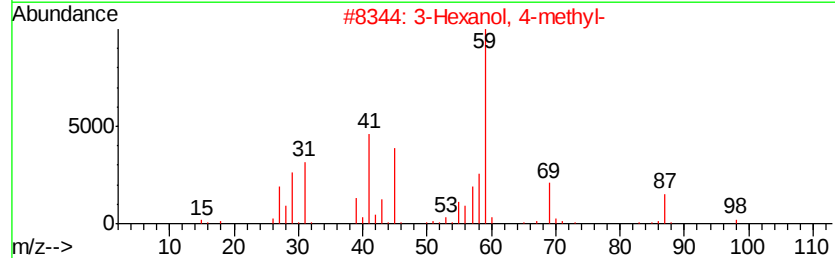
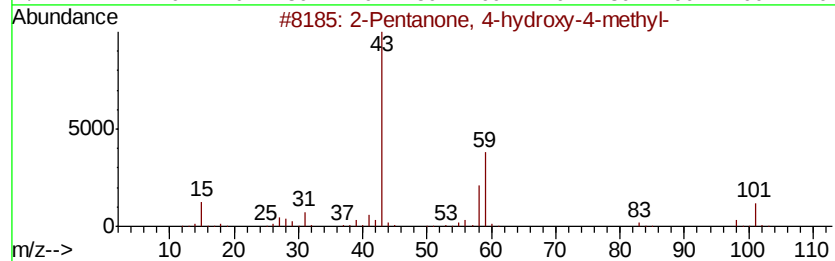
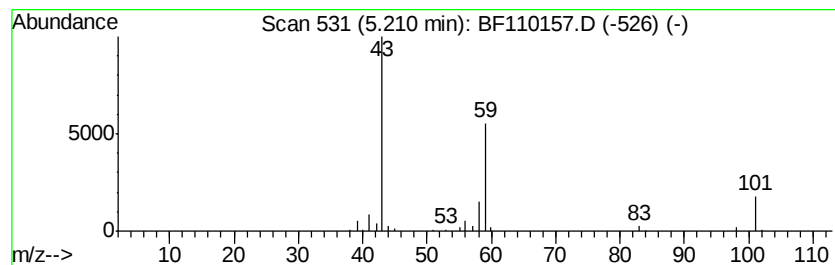
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	3.31 ng	158357	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4			Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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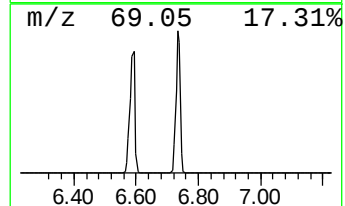
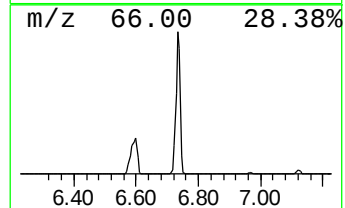
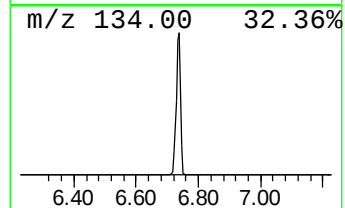
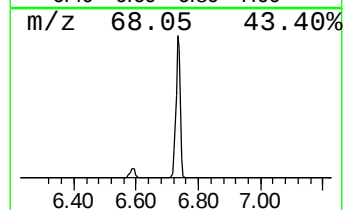
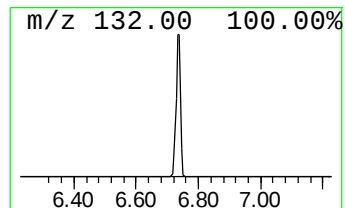
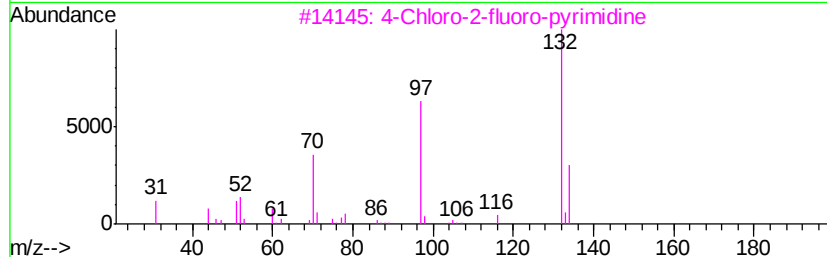
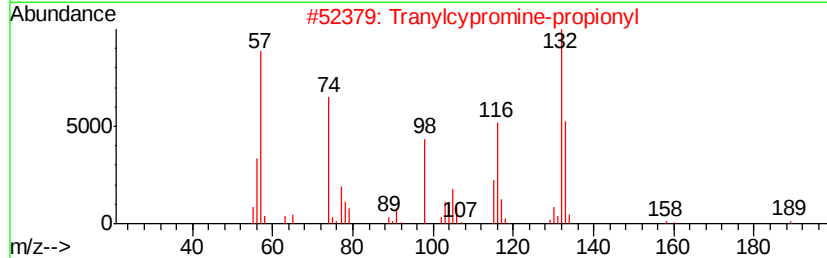
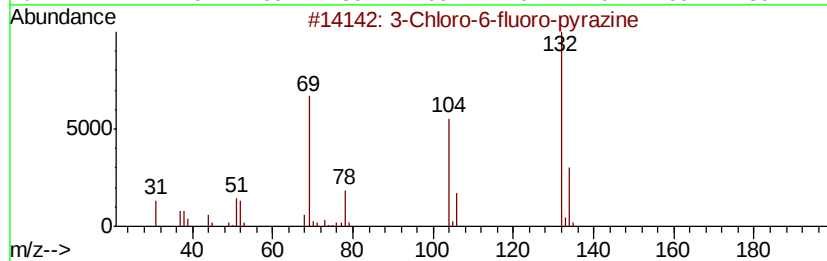
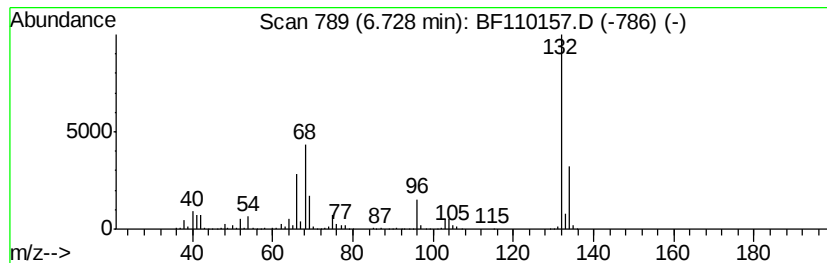
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	68.09 ng	3256410	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	10
3	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9
4	4-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-60-2	9
5	Imidazole, 4,5-dicyano-1-methyl-			132	C6H4N4	019485-35-9	9



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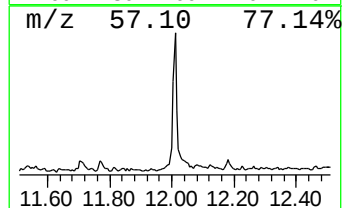
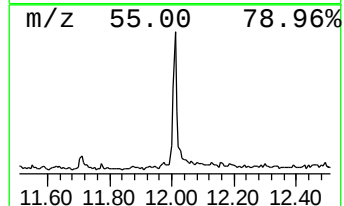
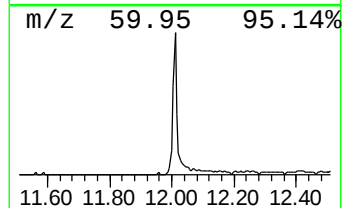
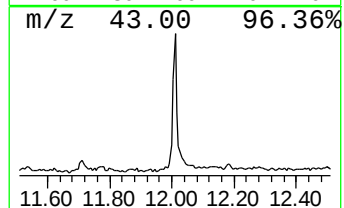
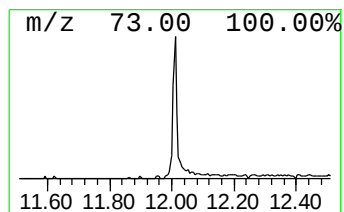
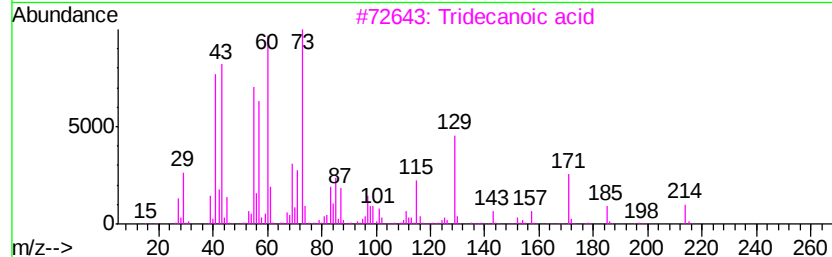
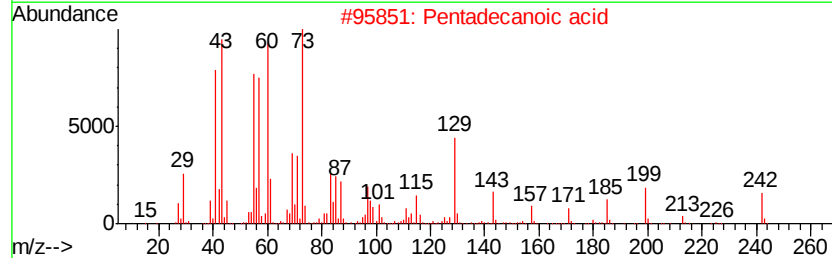
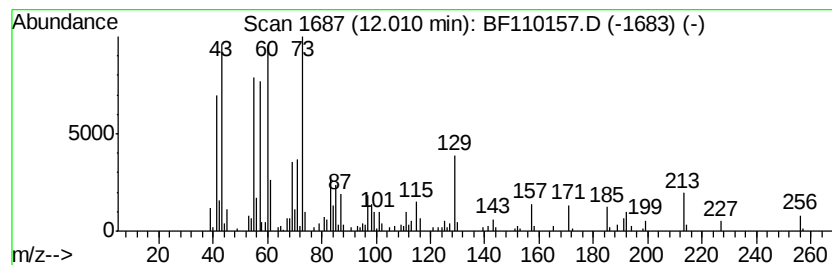
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	3.59 ng	239761	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



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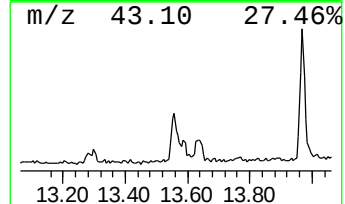
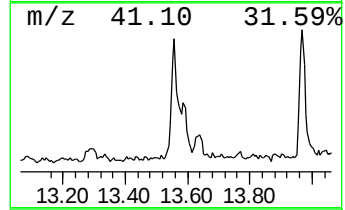
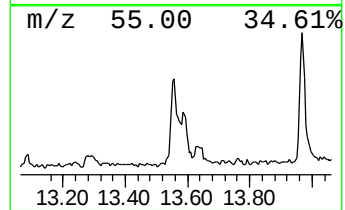
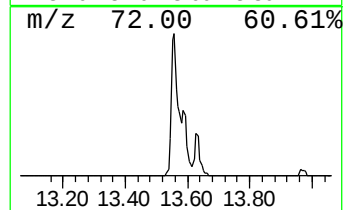
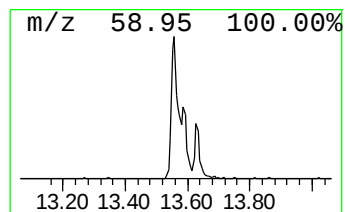
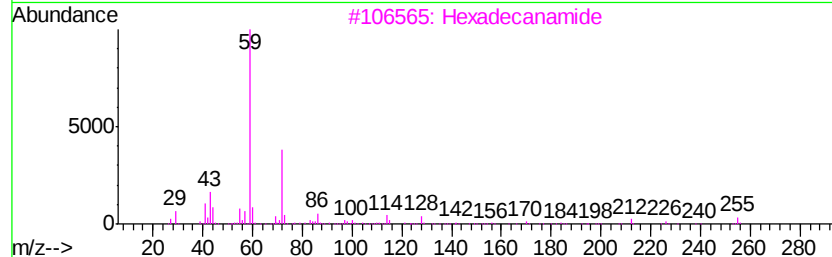
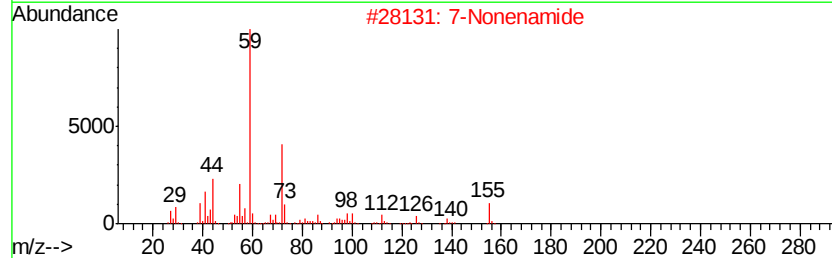
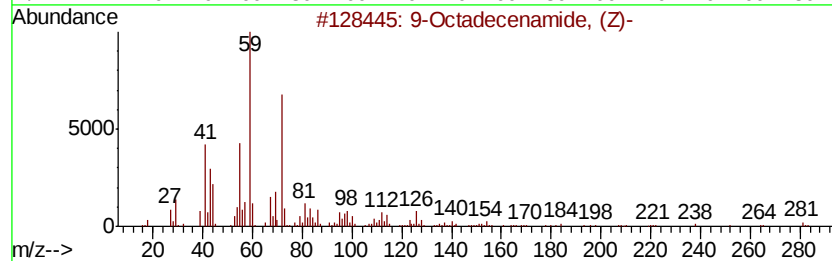
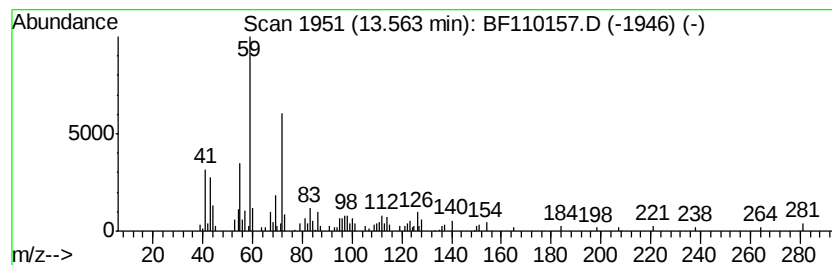
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	5.70 ng	232240	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		7-Nonenamide	155	C9H17NO	090949-53-4	83
3		Hexadecanamide	255	C16H33NO	000629-54-9	72
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
5		Octanamide	143	C8H17NO	000629-01-6	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110157.D
Acq On : 25 Oct 2018 13:12
Operator : JU/SJ
Sample : J5618-06
Misc :
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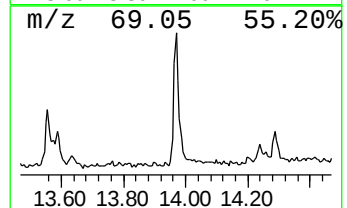
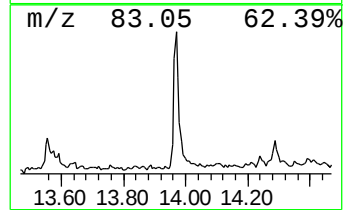
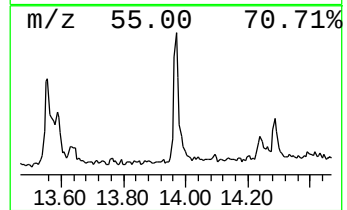
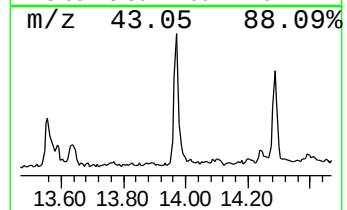
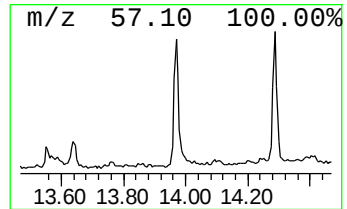
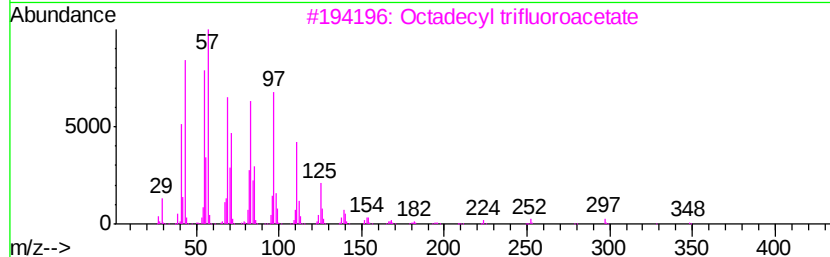
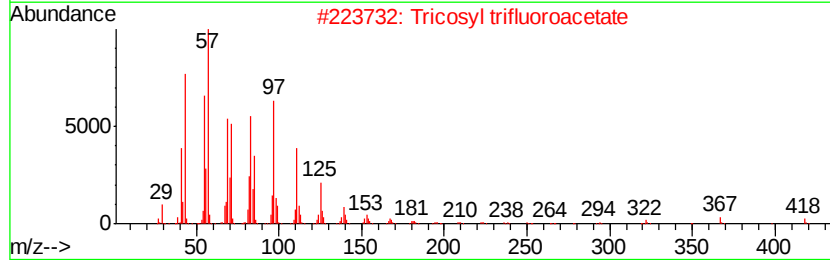
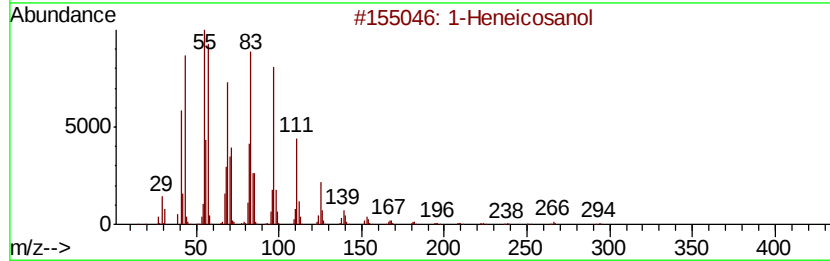
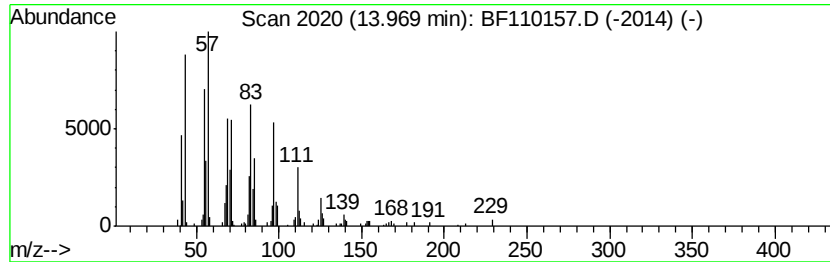
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ClientSampleId :
SSSI-1018-S-DH-15

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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-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	6.57 ng	267665	Chrysene-d12	14.15
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heneicosanol	312 C21H44O	015594-90-8 93
2		Tricosyl trifluoroacetate	436 C25H47F3O2	1000351-75-1 91
3		Octadecyl trifluoroacetate	366 C20H37F3O2	079392-43-1 91
4		Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1 91
5		Docosyl pentafluoropropionate	472 C25H45F5O2	1000351-80-9 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110157.D
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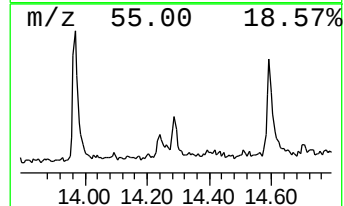
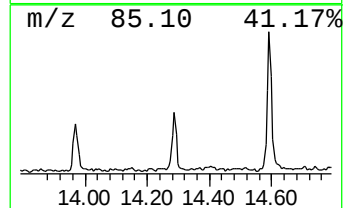
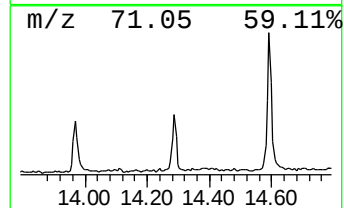
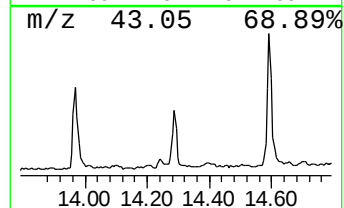
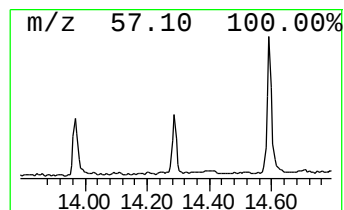
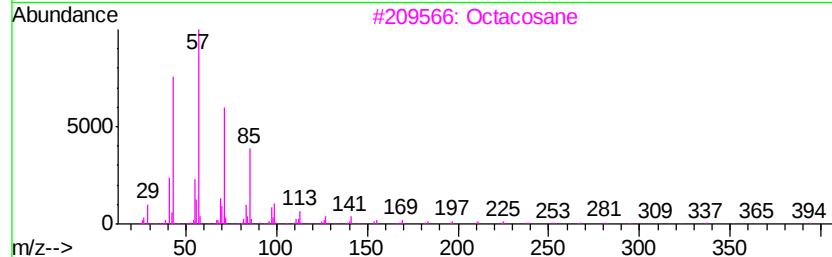
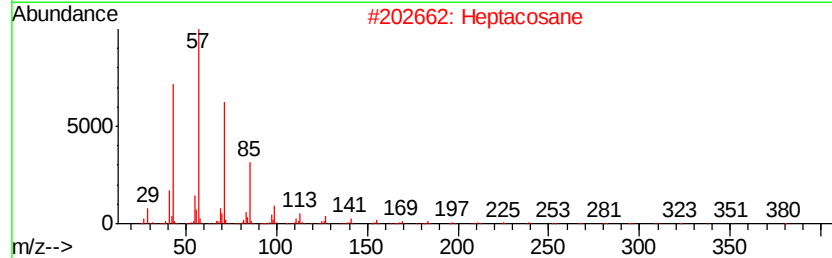
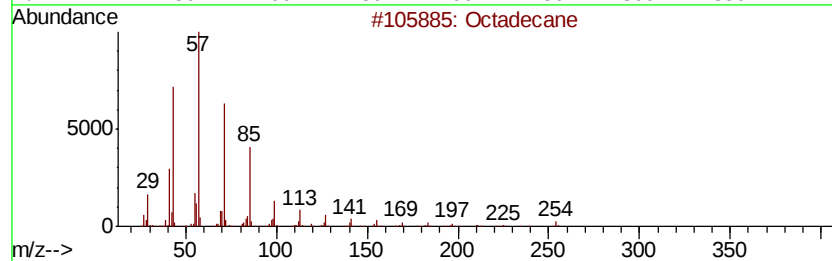
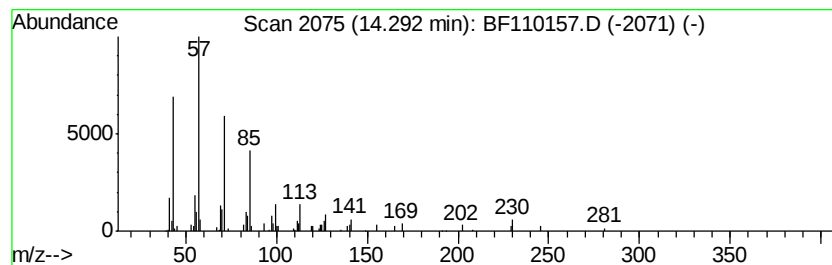
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.68 ng	109358	Chrysene-d12	14.15
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	91
2	Heptacosane	380 C27H56	000593-49-7	91
3	Octacosane	394 C28H58	000630-02-4	90
4	triacontane	422 C30H62	000638-68-6	90
5	Tridecanol, 2-ethyl-2-methyl-	242 C16H34O	1000115-66-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110157.D
Acq On : 25 Oct 2018 13:12
Operator : JU/SJ
Sample : J5618-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

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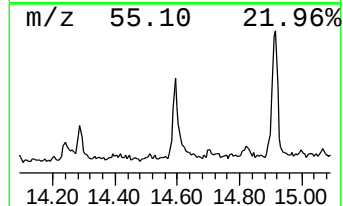
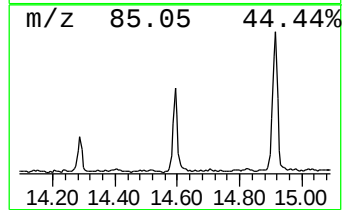
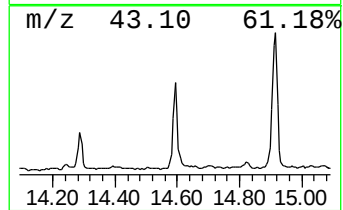
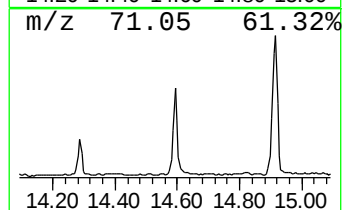
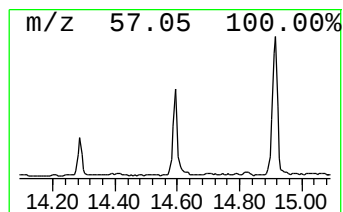
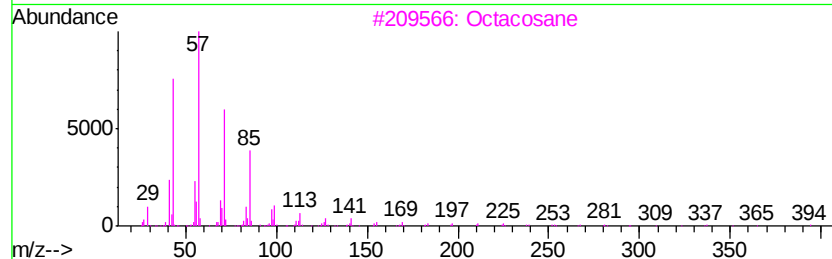
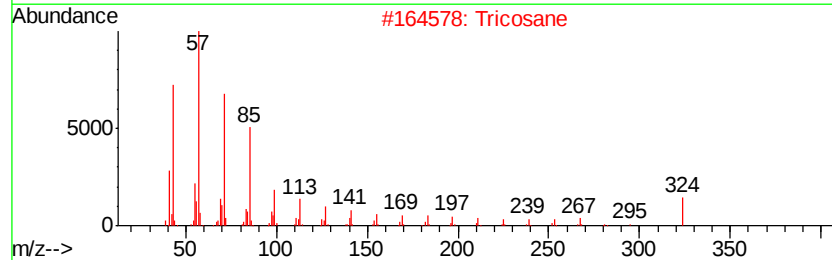
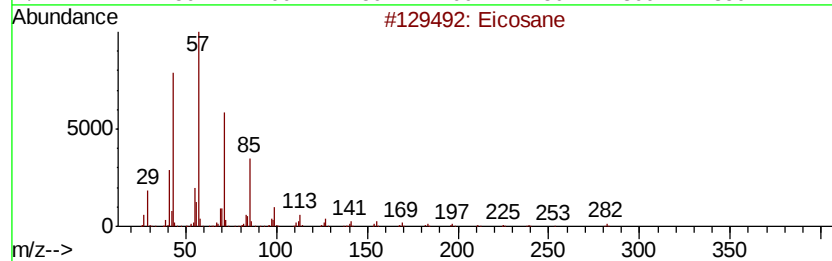
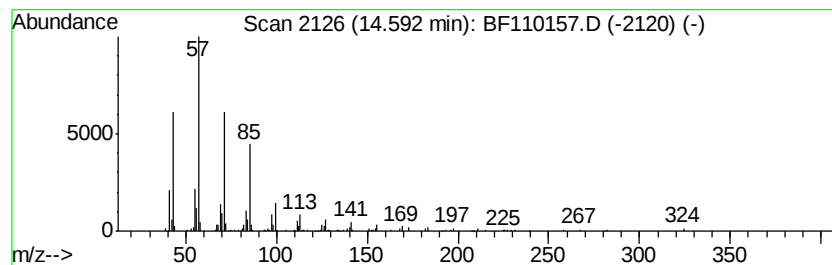
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	7.88 ng	321203	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	96
2		Tricosane	324	C23H48	000638-67-5	95
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110157.D
Acq On : 25 Oct 2018 13:12
Operator : JU/SJ
Sample : J5618-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

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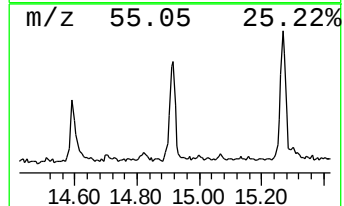
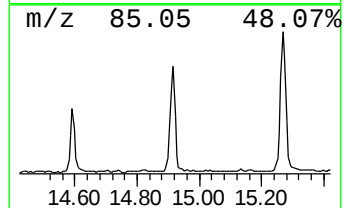
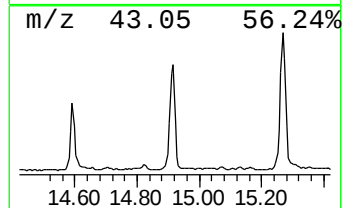
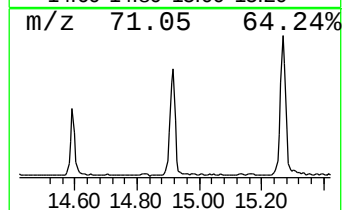
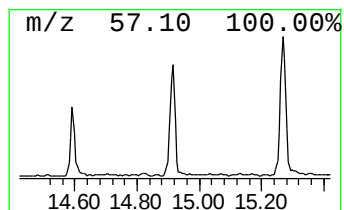
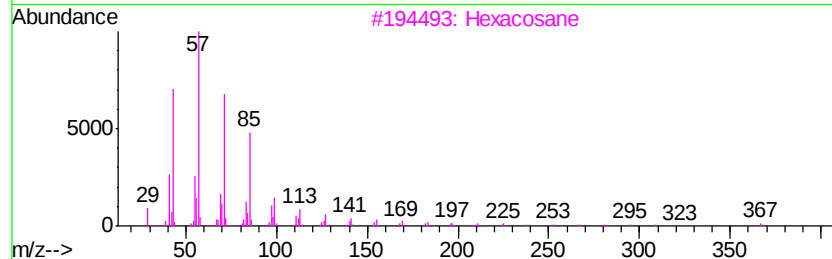
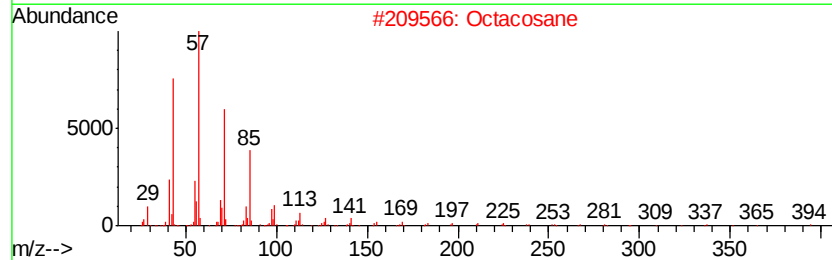
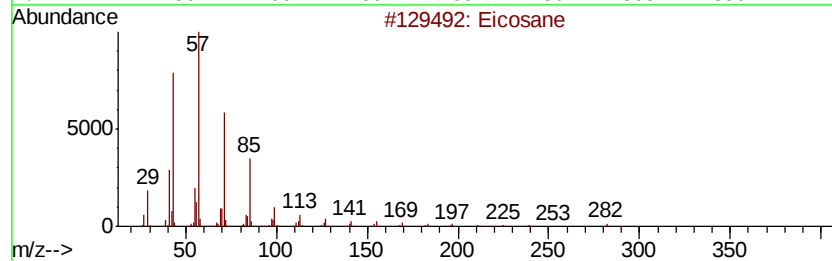
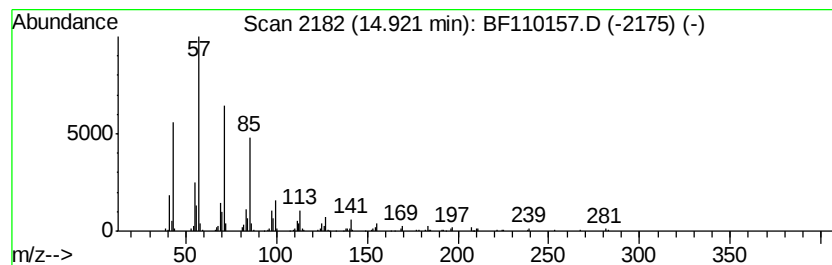
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	6.80 ng	491551	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		Octacosane	394	C28H58	000630-02-4	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
 Data File : BF110157.D
 Acq On : 25 Oct 2018 13:12
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Instrument :
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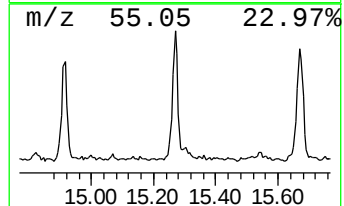
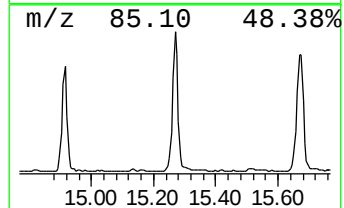
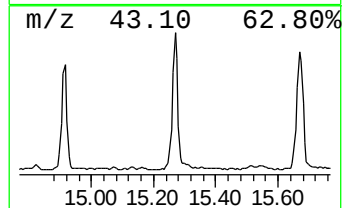
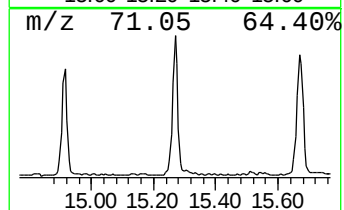
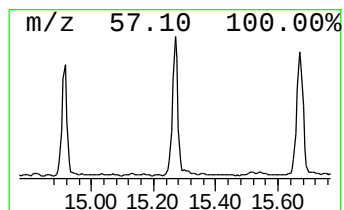
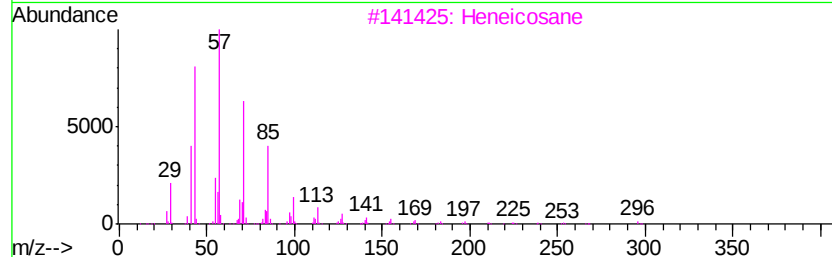
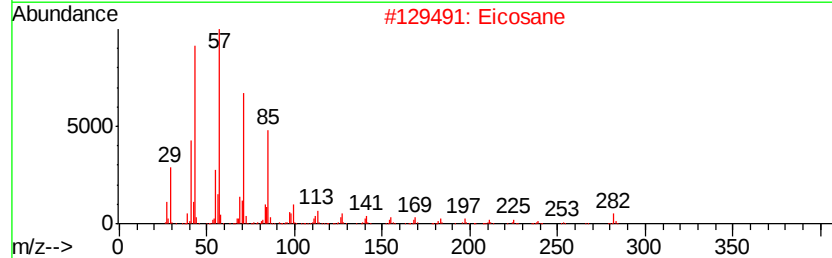
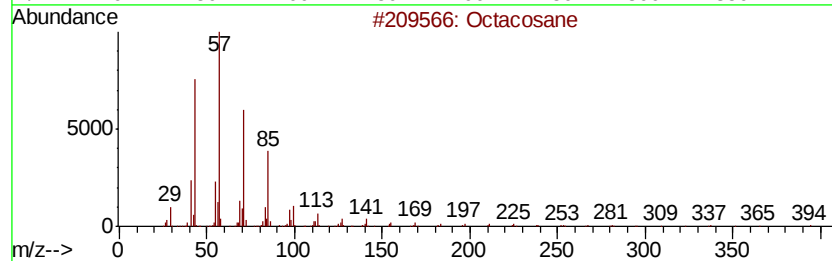
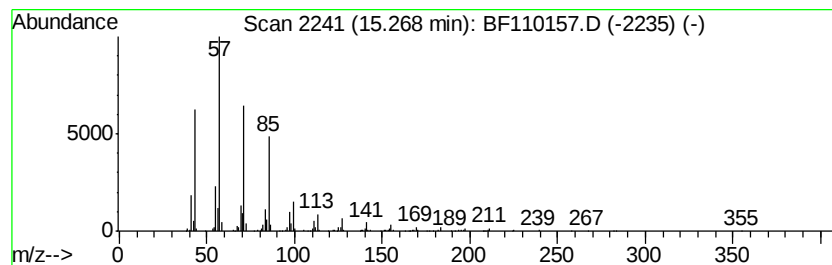
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	8.66 ng	626237	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Eicosane	282	C20H42	000112-95-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Octadecane	254	C18H38	000593-45-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110157.D
Acq On : 25 Oct 2018 13:12
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Misc :
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ClientSampleId :
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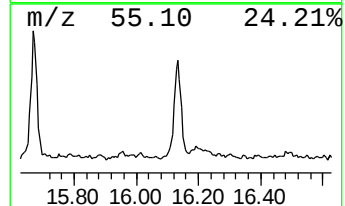
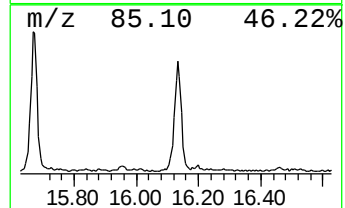
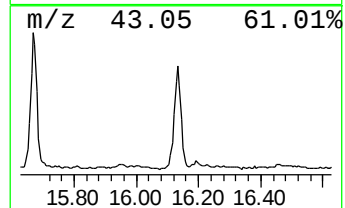
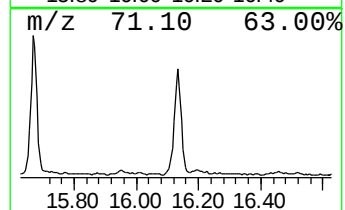
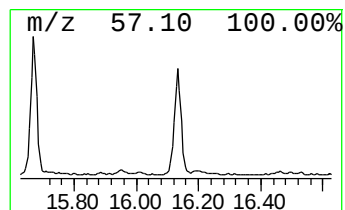
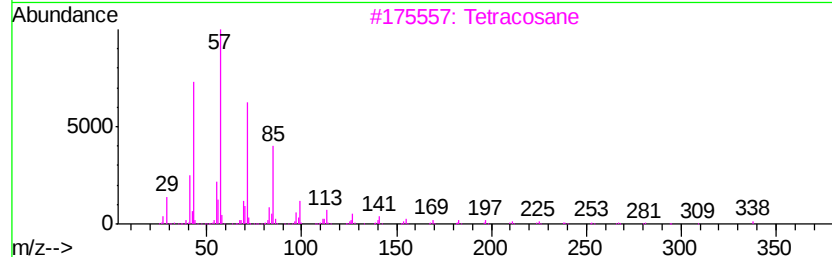
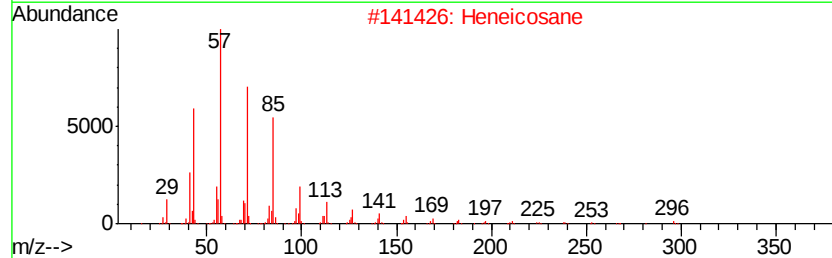
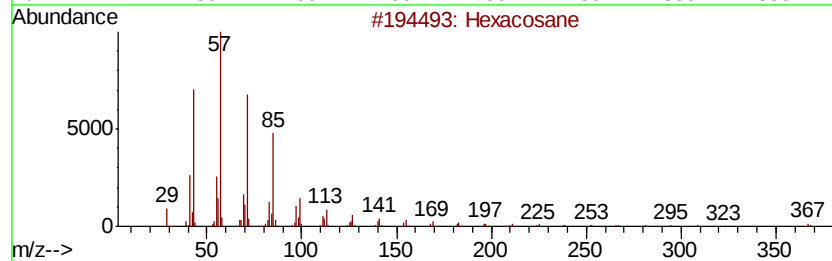
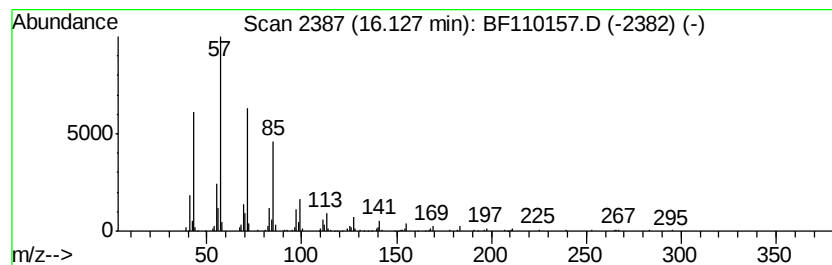
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane, 11-(1-ethylpro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	7.63 ng	551323	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5		Nonadecane	268	C19H40	000629-92-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110157.D
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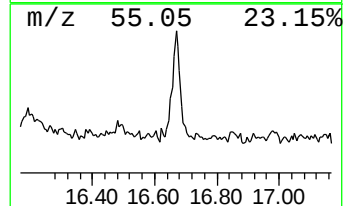
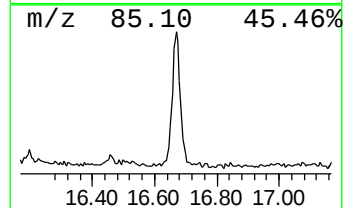
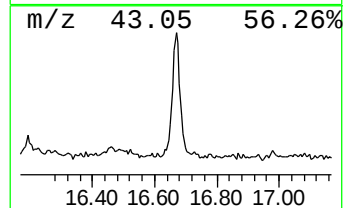
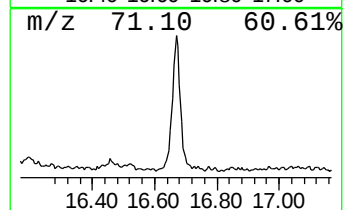
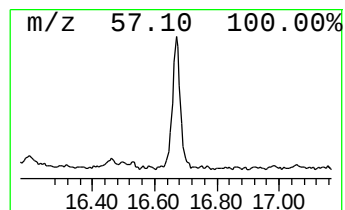
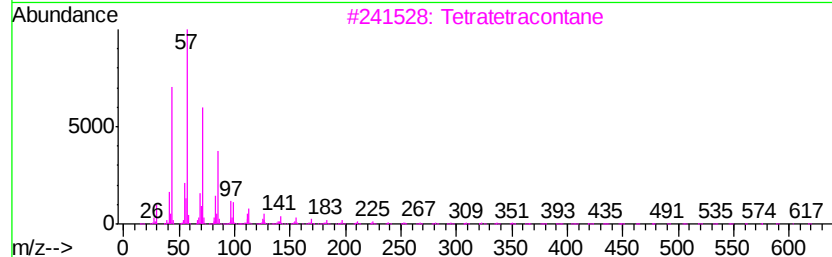
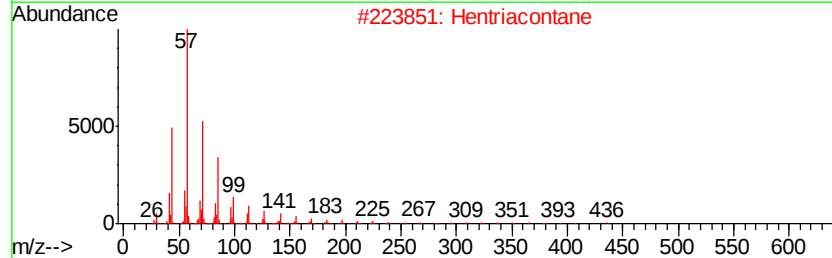
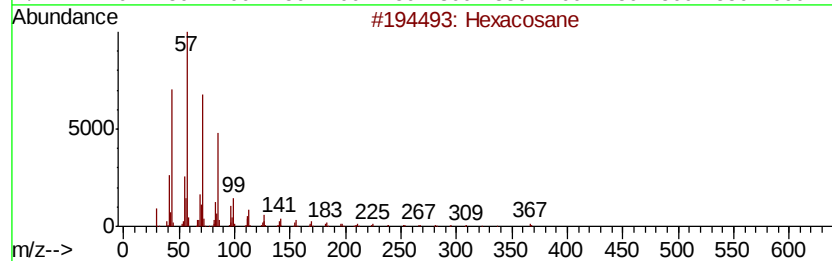
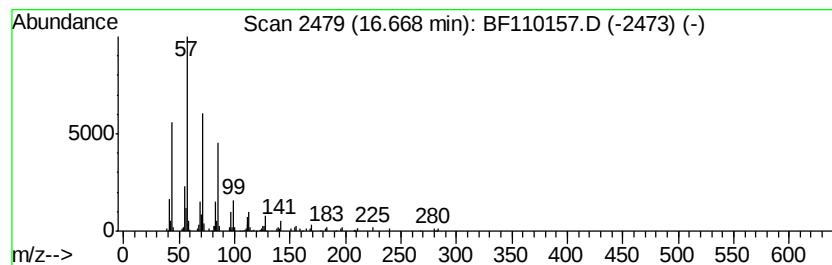
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	3.79 ng	274151	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110157.D
Acq On : 25 Oct 2018 13:12
Operator : JU/SJ
Sample : J5618-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SSSI-1018-S-DH-15

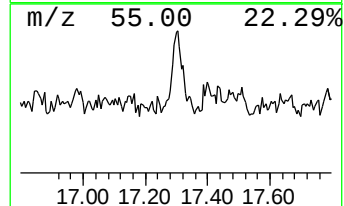
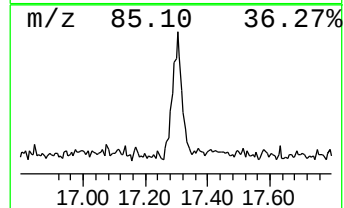
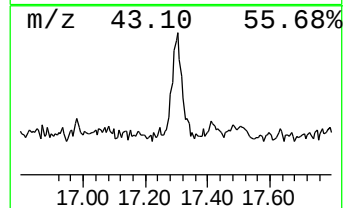
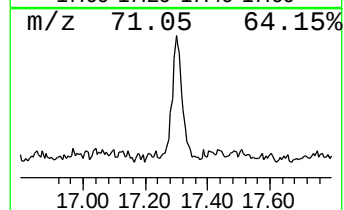
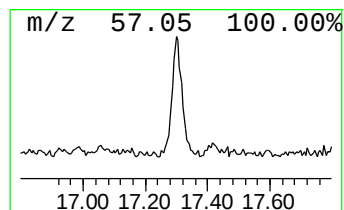
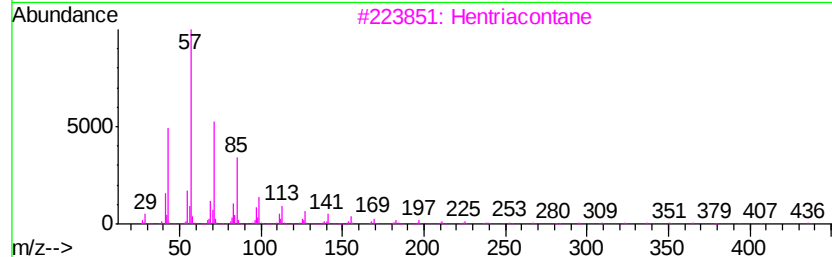
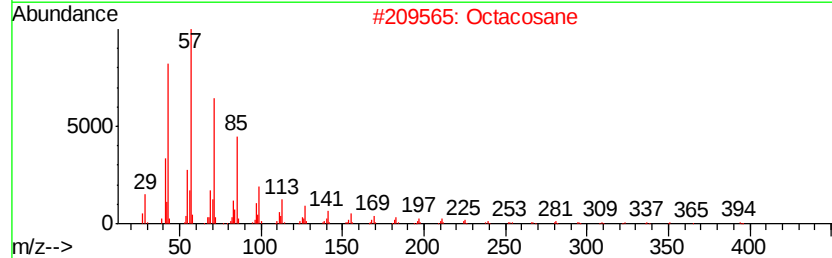
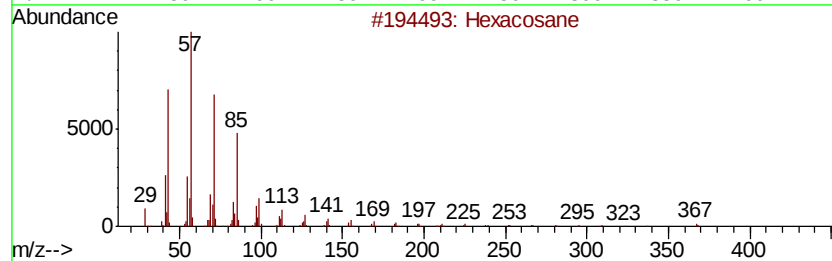
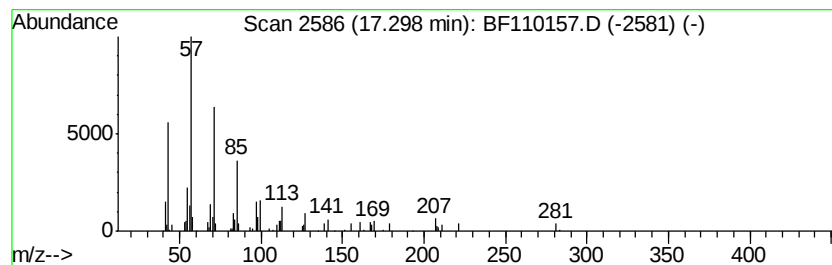
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tetratetracontane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	2.02 ng	146120	Perylene-d12	15.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	90
2	Octacosane		394	C28H58	000630-02-4	87
3	Hentriacontane		437	C31H64	000630-04-6	87
4	Tetratetracontane		619	C44H90	007098-22-8	87
5	Pentacosane		352	C25H52	000629-99-2	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102518\
 Data File : BF110157.D
 Acq On : 25 Oct 2018 13:12
 Operator : JU/SJ
 Sample : J5618-06
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1018-S-DH-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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
Butane, 2-methoxy...	2.33	12.7	ng	606832	1	6.97	956567	20.0
2-Pentanone, 4-hy...	5.21	3.3	ng	158357	1	6.97	956567	20.0
unknown6.73	6.73	68.1	ng	3256410	1	6.97	956567	20.0
n-Hexadecanoic acid	12.01	3.6	ng	239761	4	11.50	1335720	20.0
9-Octadecenamide,...	13.56	5.7	ng	232240	5	14.15	815016	20.0
1-Heneicosanol	13.97	6.6	ng	267665	5	14.15	815016	20.0
Octadecane	14.29	2.7	ng	109358	5	14.15	815016	20.0
Eicosane	14.59	7.9	ng	321203	5	14.15	815016	20.0
Hexacosane	14.92	6.8	ng	491551	6	15.67	1446010	20.0
Octacosane	15.27	8.7	ng	626237	6	15.67	1446010	20.0
Heneicosane, 11-(...	16.13	7.6	ng	551323	6	15.67	1446010	20.0
Hentriacontane	16.67	3.8	ng	274151	6	15.67	1446010	20.0
Tetratetracontane	17.30	2.0	ng	146120	6	15.67	1446010	20.0