

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
 Data File : BF114125.D
 Acq On : 10 May 2019 17:29
 Operator : JU/SJ
 Sample : K2762-12
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P021-SS002-1218-01

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-BF051019.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	2.146	5	10	56	rVB	1696651	3983067	54.37%	4.829%
2	5.481	572	577	580	rBV	7260811	6870196	93.79%	8.329%
3	6.487	743	748	751	rBV	7255785	7325444	100.00%	8.881%
4	6.622	767	771	775	rBV	7118107	7120253	97.20%	8.632%
5	6.851	806	810	813	rBV	2767712	2210239	30.17%	2.680%
6	7.010	832	837	840	rBV	6052306	5443273	74.31%	6.599%
7	7.410	900	905	908	rBV	4942024	4603573	62.84%	5.581%
8	7.451	908	912	916	rVB	186855	152647	2.08%	0.185%
9	8.128	1023	1027	1031	rBV	2163642	2011144	27.45%	2.438%
10	9.204	1205	1210	1213	rBV	5434880	5009769	68.39%	6.074%
11	9.592	1272	1276	1280	rBV	735350	671057	9.16%	0.814%
12	9.886	1320	1326	1329	rBV	2185474	2029971	27.71%	2.461%
13	10.086	1356	1360	1367	rVB2	55153	74234	1.01%	0.090%
14	10.669	1454	1459	1463	rBV	3463641	3286453	44.86%	3.984%
15	11.369	1574	1578	1581	rBV	2469140	2076177	28.34%	2.517%
16	11.898	1663	1668	1679	rVV	1279676	1455590	19.87%	1.765%
17	12.010	1683	1687	1690	rVB	210262	218473	2.98%	0.265%
18	12.604	1786	1788	1795	rVB6	57961	90654	1.24%	0.110%
19	12.680	1796	1801	1815	rVV	1194753	1324468	18.08%	1.606%
20	12.780	1815	1818	1821	rVB2	76991	80623	1.10%	0.098%
21	12.951	1843	1847	1850	rBV	4929777	4264389	58.21%	5.170%
22	13.868	1999	2003	2014	rVB	346593	526561	7.19%	0.638%
23	14.027	2025	2030	2033	rBV	1582561	1554981	21.23%	1.885%
24	14.204	2055	2060	2065	rBV	481386	541487	7.39%	0.656%
25	14.527	2110	2115	2123	rVB	1345118	1534169	20.94%	1.860%
26	14.851	2163	2170	2174	rBV	3318093	3907597	53.34%	4.737%
27	14.927	2180	2183	2187	rVB	587339	551531	7.53%	0.669%
28	15.192	2223	2228	2237	rVB	3631886	4483899	61.21%	5.436%
29	15.539	2282	2287	2290	rBV	1810370	2397083	32.72%	2.906%
30	15.580	2290	2294	2302	rVB	2790679	3807246	51.97%	4.616%
31	16.015	2362	2368	2373	rBV	1232595	1823958	24.90%	2.211%
32	16.521	2449	2454	2461	rVB	454921	794493	10.85%	0.963%
33	17.115	2551	2555	2562	rVB2	122264	259723	3.55%	0.315%

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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P021-SS002-1218-01

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

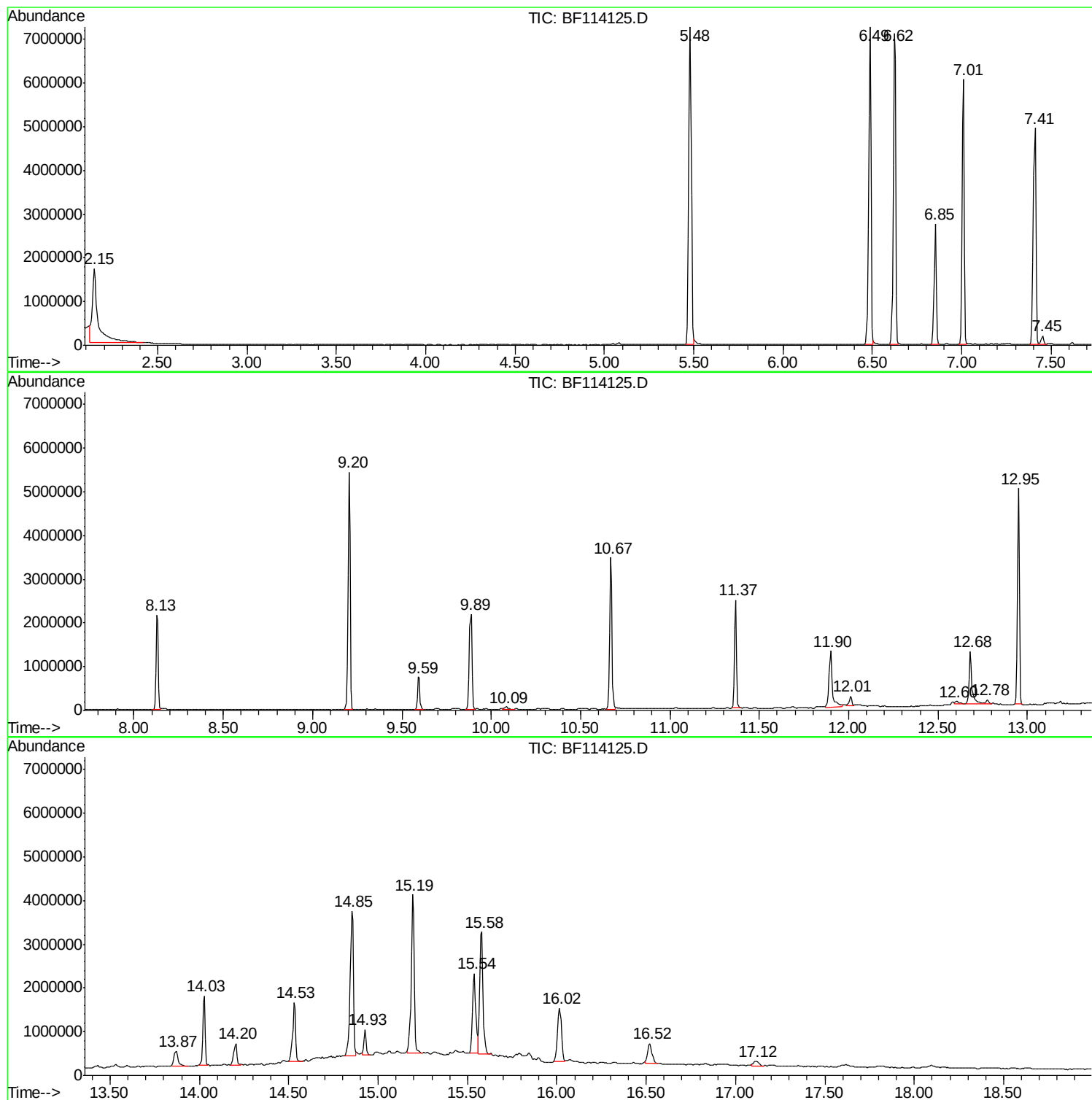
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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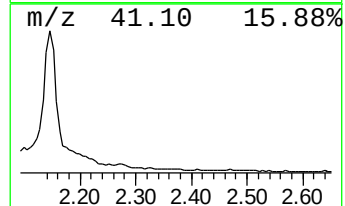
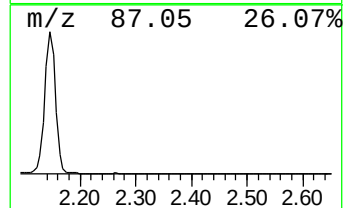
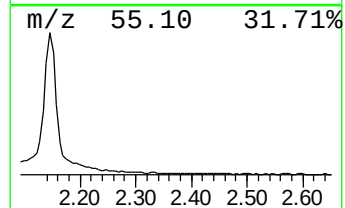
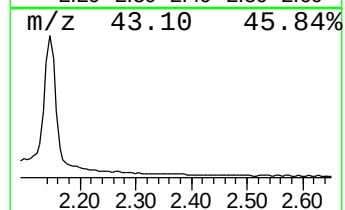
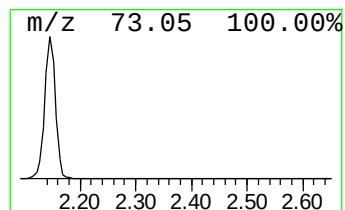
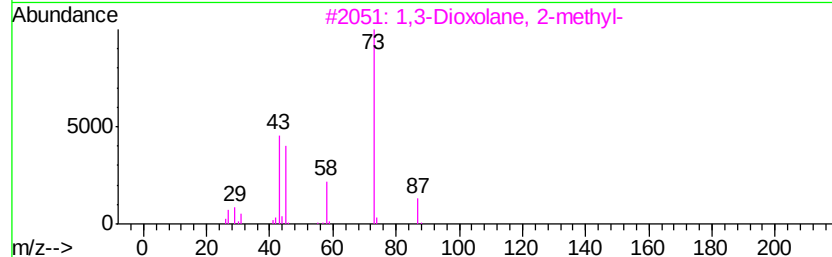
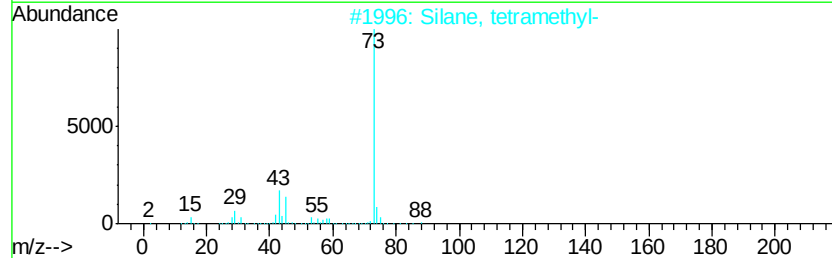
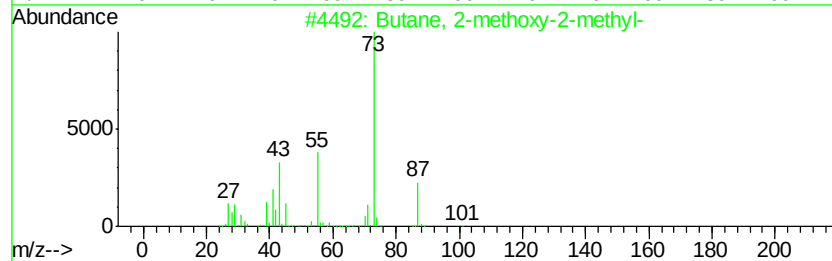
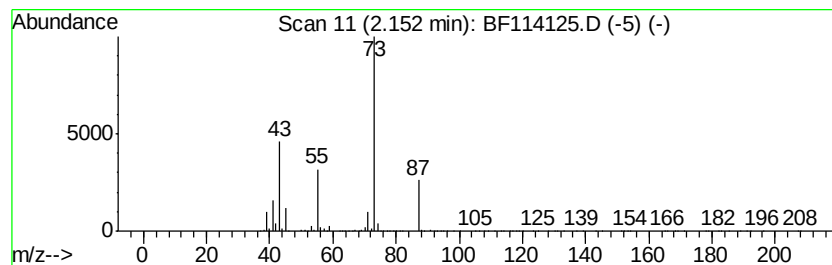
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.15	36.04 ng	3983070	1,4-Dichlorobenzene-d4	6.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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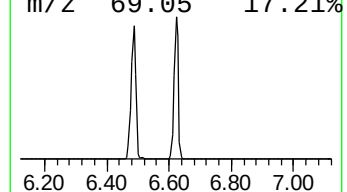
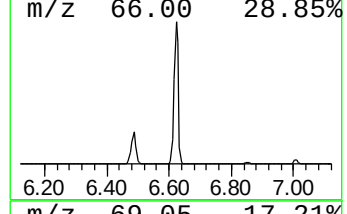
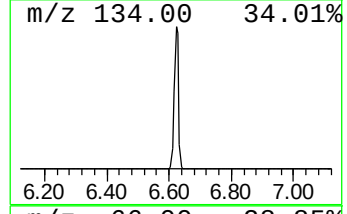
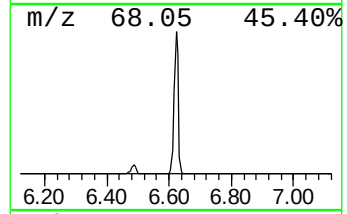
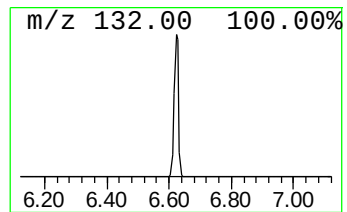
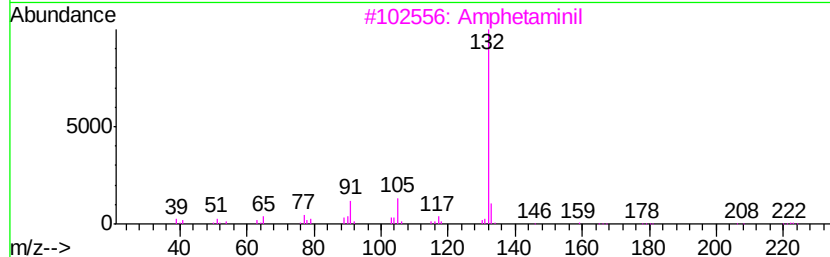
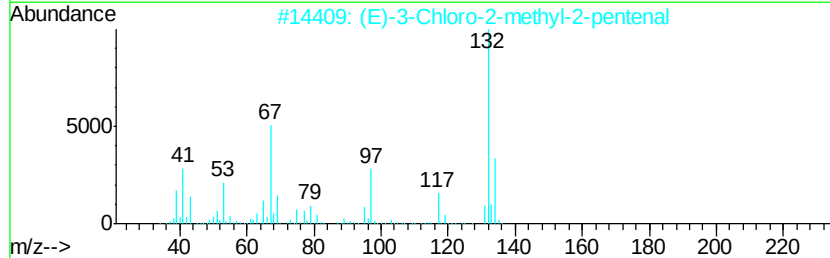
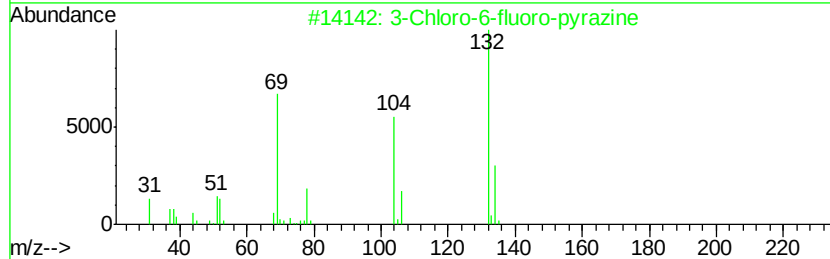
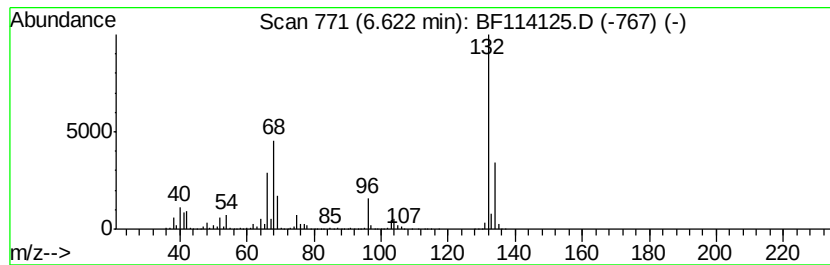
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	64.43 ng	7120250	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Amphetaminil	250	C17H18N2	017590-01-1	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Xenon	132	Xe	007440-63-3	9



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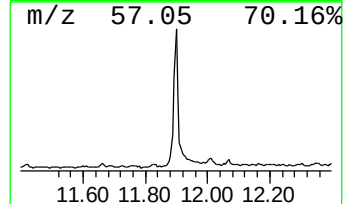
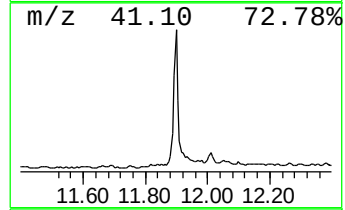
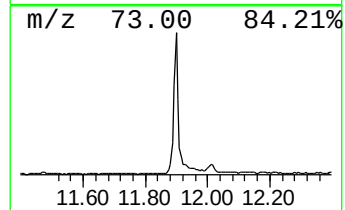
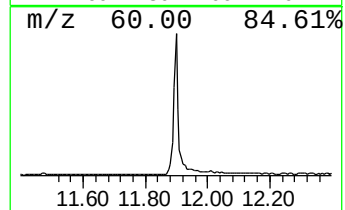
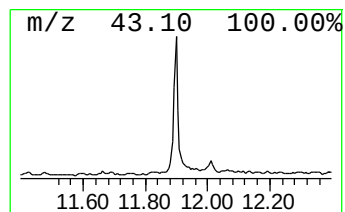
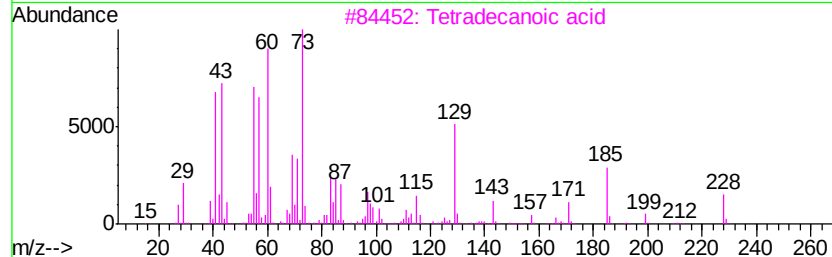
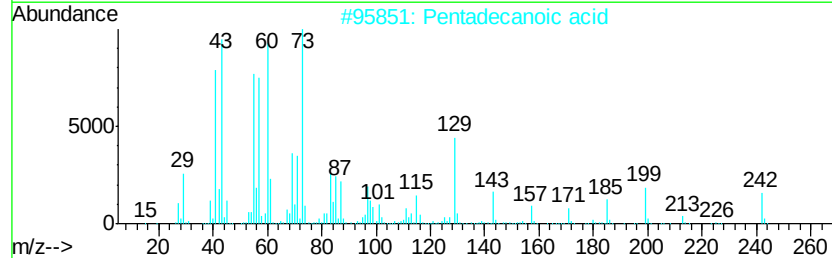
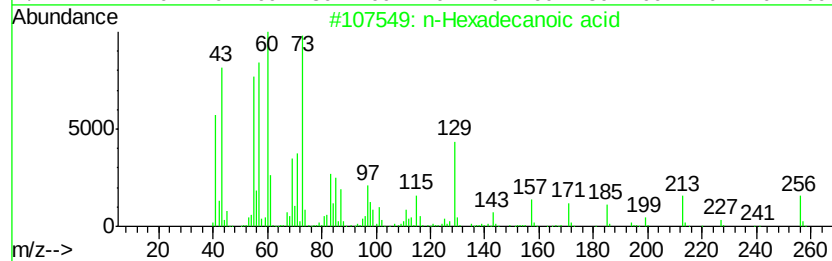
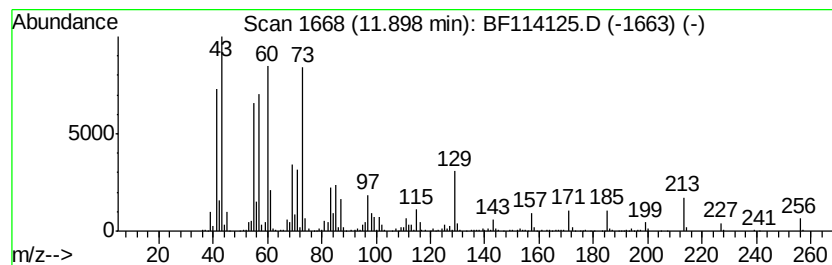
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	14.02 ng	1455590	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Tridecanoic acid	214	C13H26O2	000638-53-9	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



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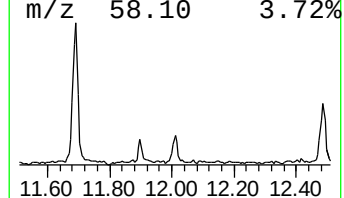
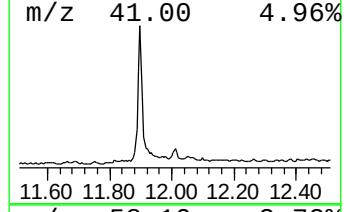
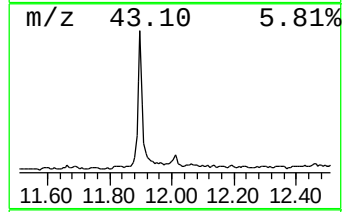
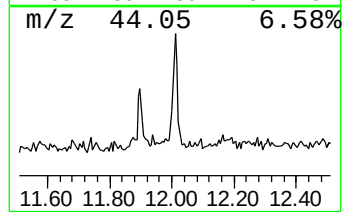
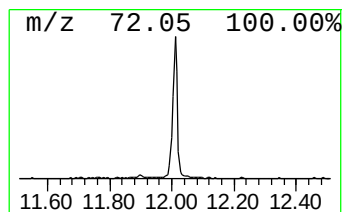
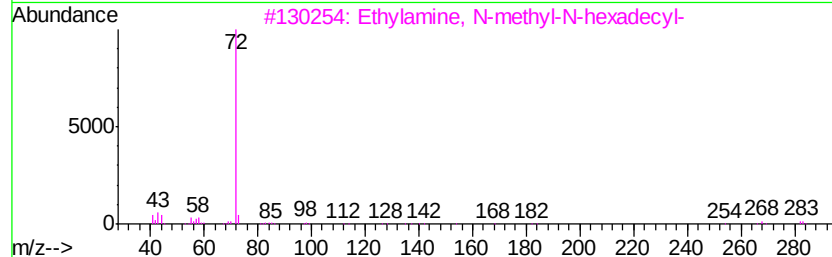
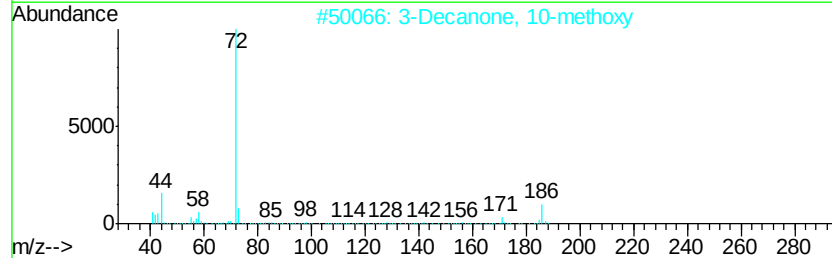
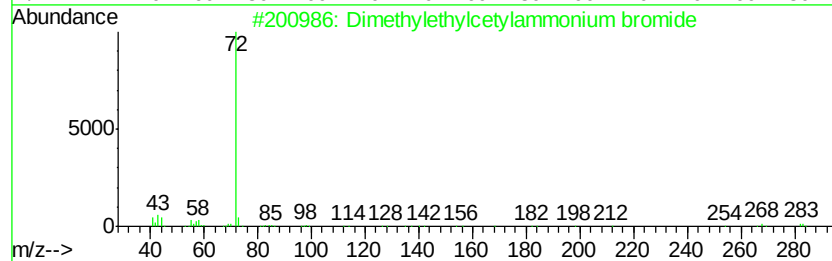
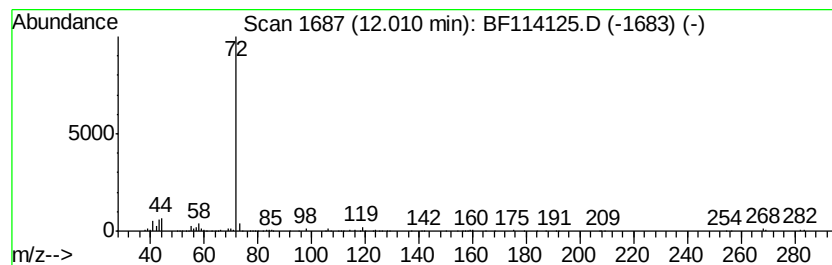
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dimethylethylcetylammmonium ... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.10 ng	218473	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dimethylethylcetylammmonium bromide	377	C20H44BrN	000124-03-8	80
2		3-Decanone, 10-methoxy	186	C11H22O2	1000130-73-5	64
3		Ethylamine, N-methyl-N-hexadecyl-	283	C19H41N	066997-40-8	41
4		3-Buten-1-amine, N-ethyl-N-methyl-	113	C7H15N	061308-10-9	39
5		N,N-dimethyl-4-tert-butylampheta...	219	C15H25N	1000378-90-5	39



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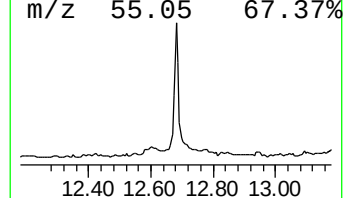
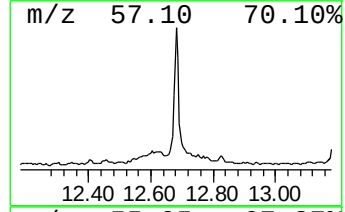
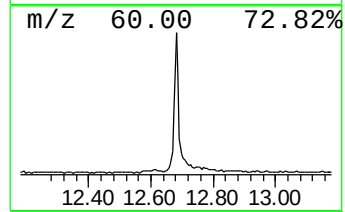
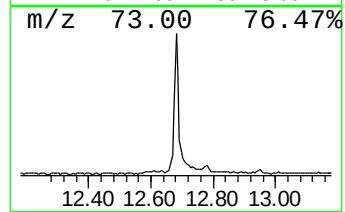
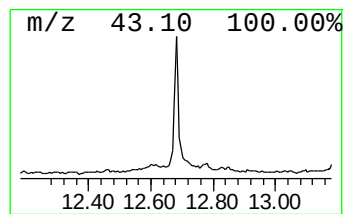
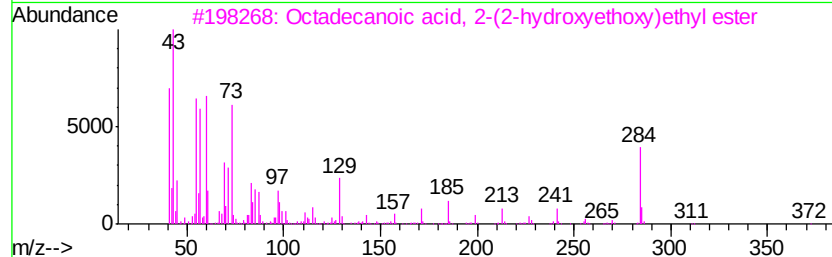
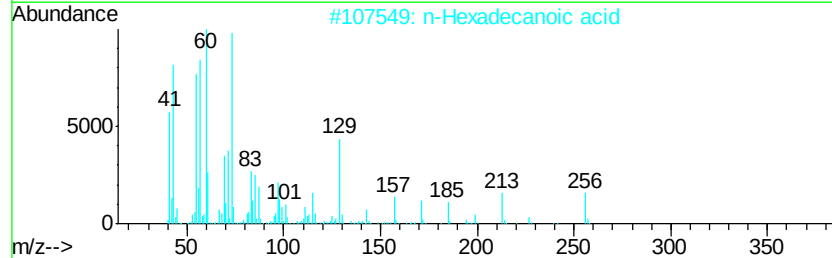
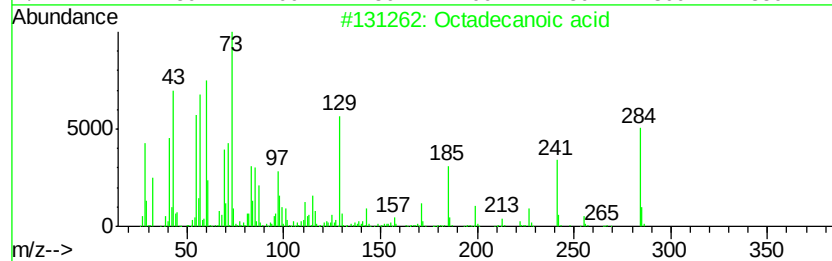
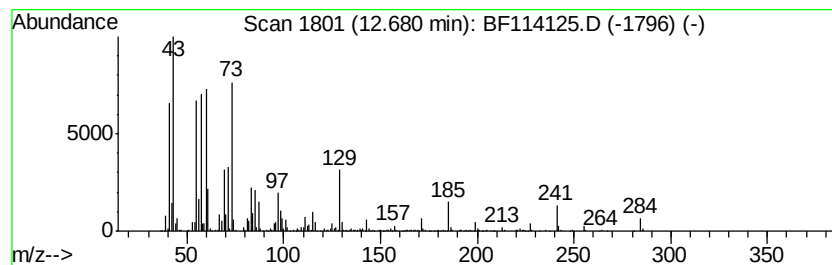
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.68	12.76 ng	1324470	Phenanthrene-d10		11.37	
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	93
3		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5		Tridecanoic acid	214	C13H26O2	000638-53-9	68



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Misc :
ALS Vial : 3 Sample Multiplier: 1

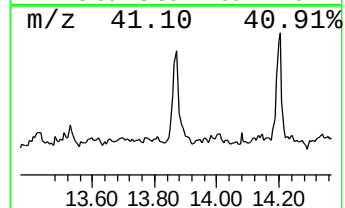
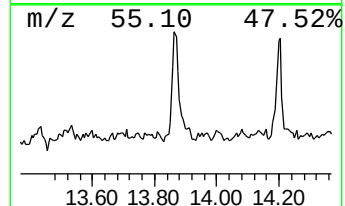
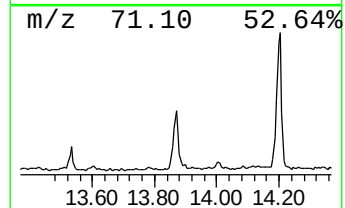
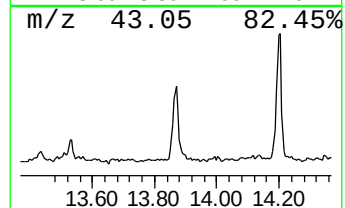
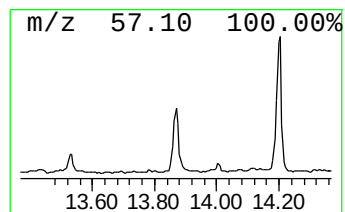
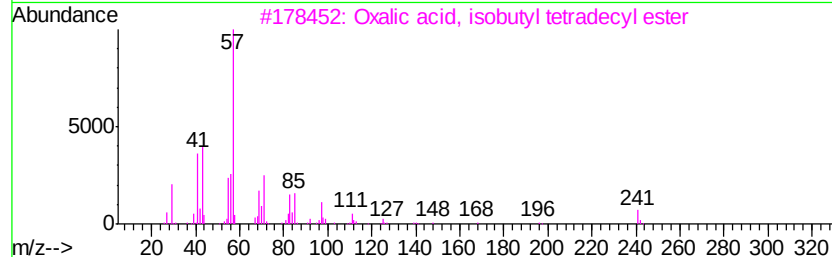
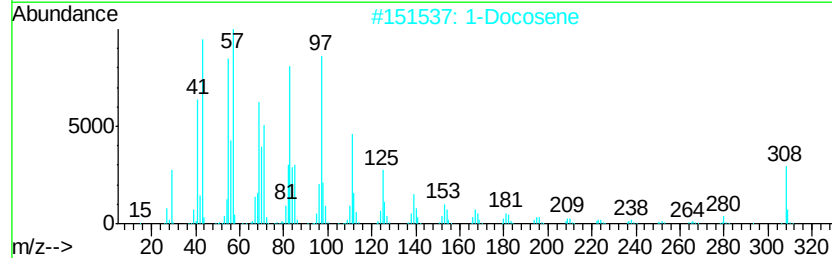
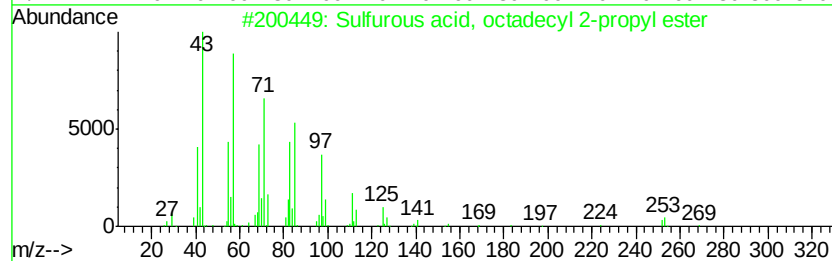
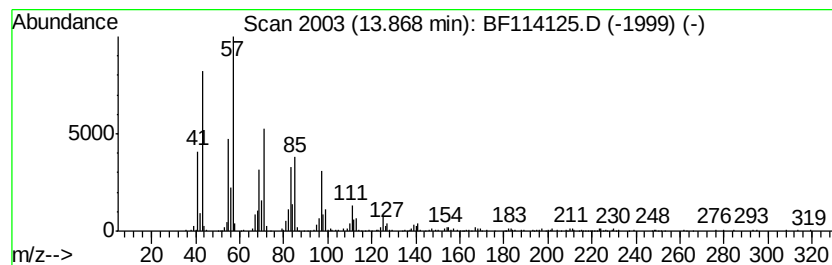
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, octadecyl 2... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.87	6.77 ng	526561	Chrysene-d12	14.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	90
2	1-Docosene	308	C22H44	001599-67-3	90
3	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	87
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	68
5	Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
 Data File : BF114125.D
 Acq On : 10 May 2019 17:29
 Operator : JU/SJ
 Sample : K2762-12
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

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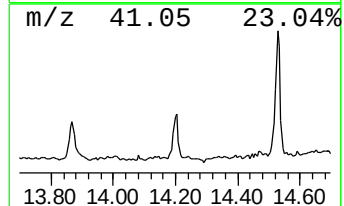
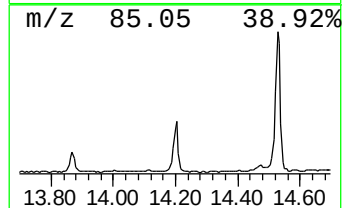
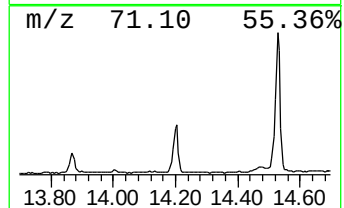
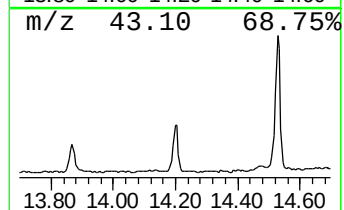
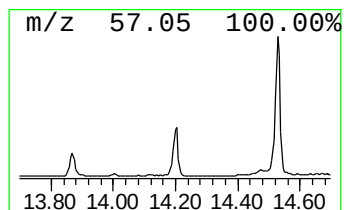
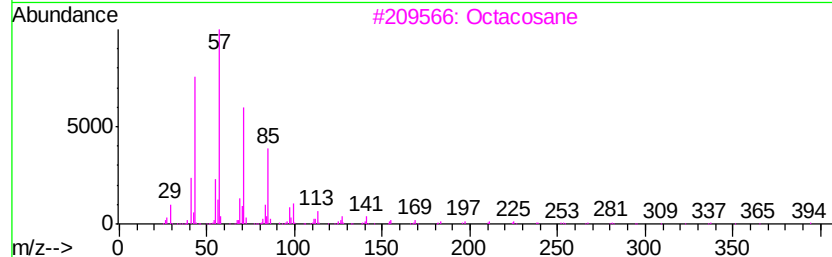
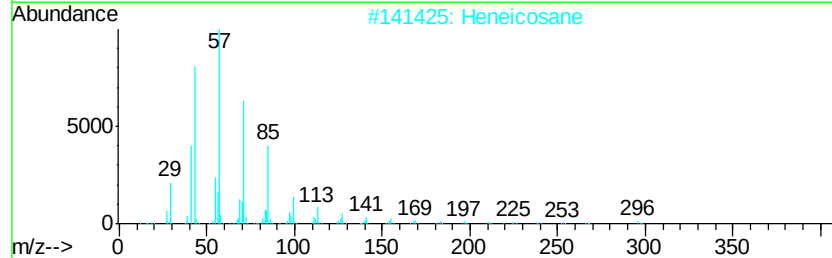
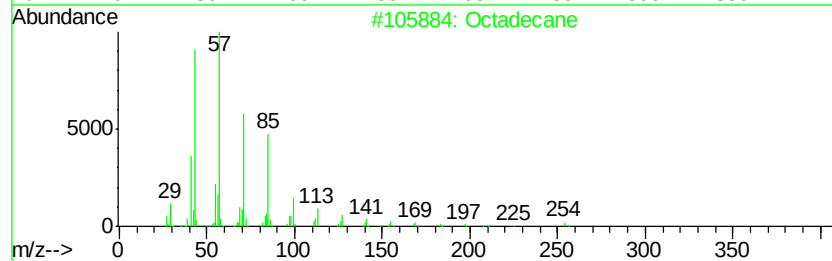
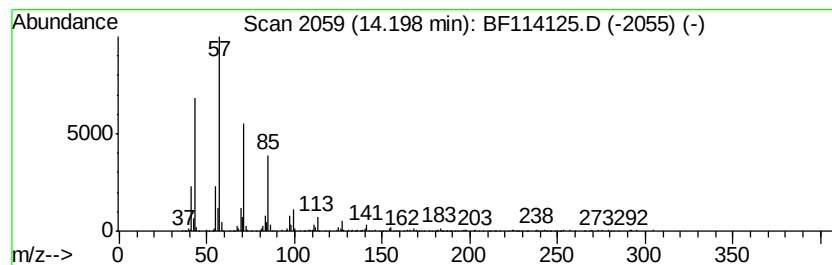
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	6.96 ng	541487	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Octacosane		394	C28H58	000630-02-4	91
4	Hexacosane		366	C26H54	000630-01-3	91
5	Heptadecane		240	C17H36	000629-78-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
Data File : BF114125.D
Acq On : 10 May 2019 17:29
Operator : JU/SJ
Sample : K2762-12
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P021-SS002-1218-01

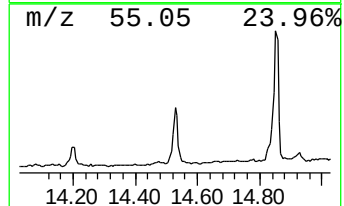
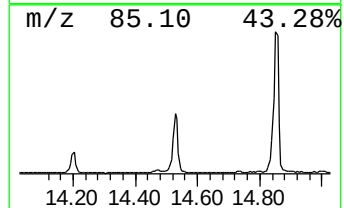
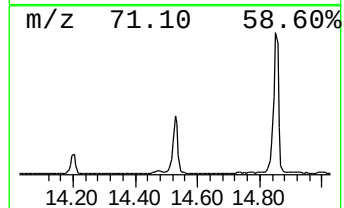
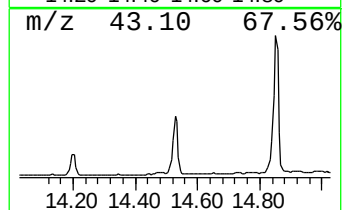
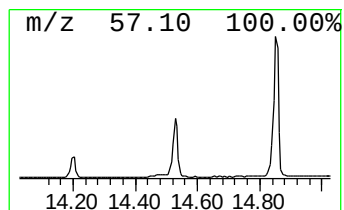
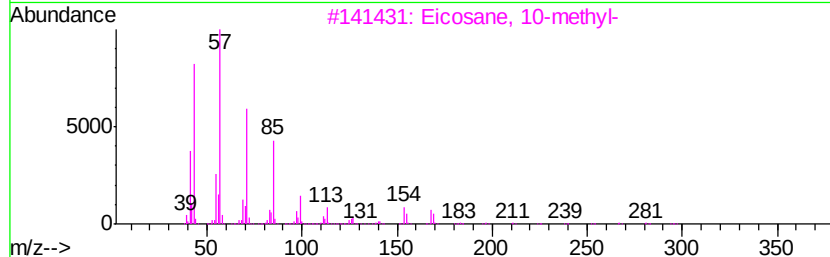
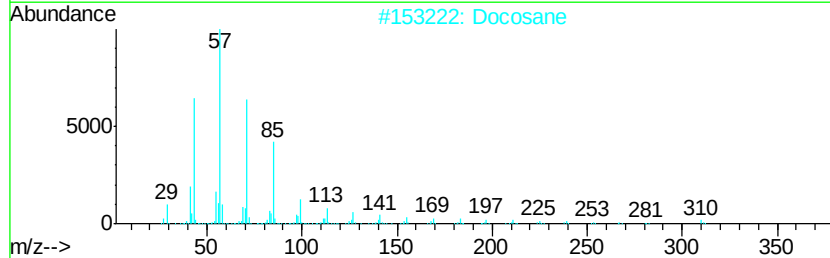
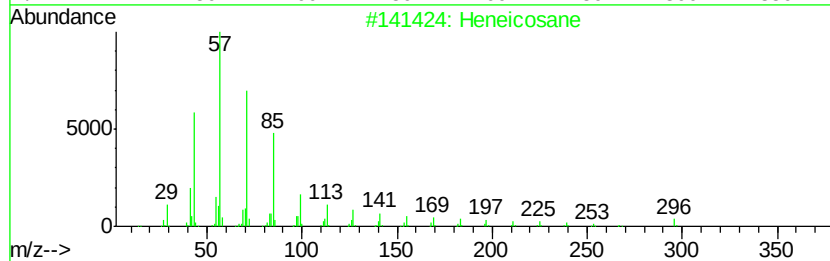
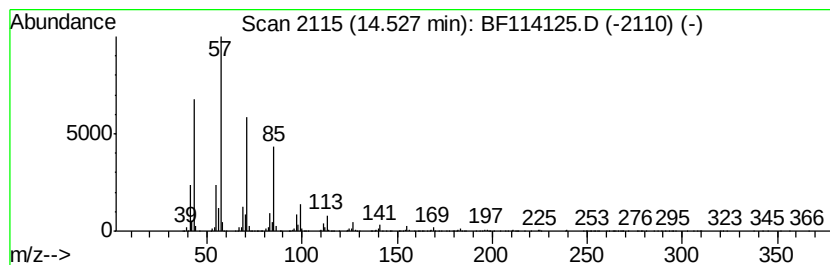
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	19.73 ng	1534170	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	94
2		Docosane	310	C22H46	000629-97-0	94
3		Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
4		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	94
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
Data File : BF114125.D
Acq On : 10 May 2019 17:29
Operator : JU/SJ
Sample : K2762-12
Misc :
ALS Vial : 3 Sample Multiplier: 1

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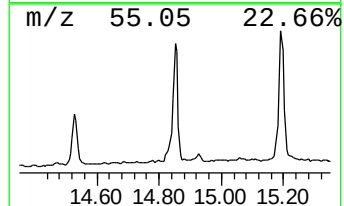
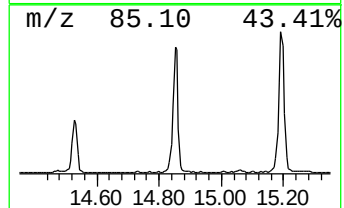
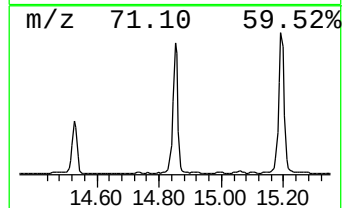
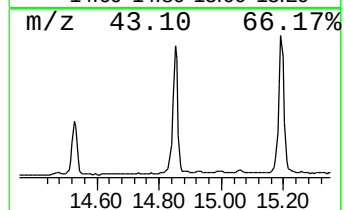
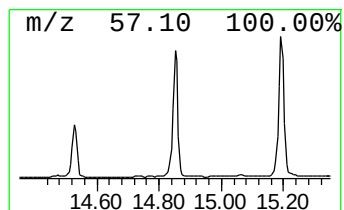
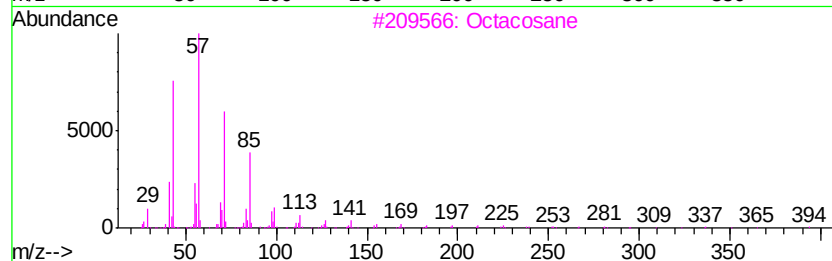
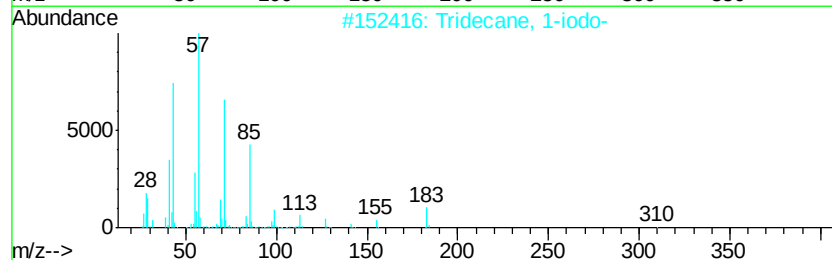
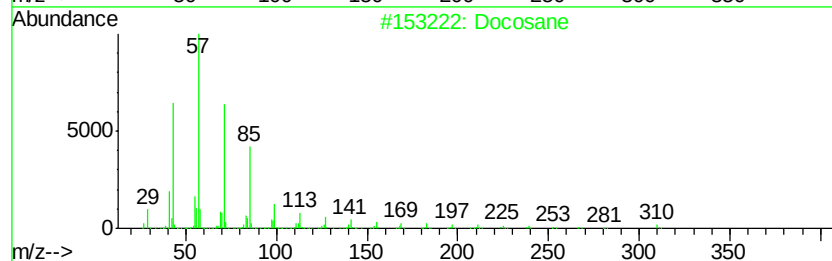
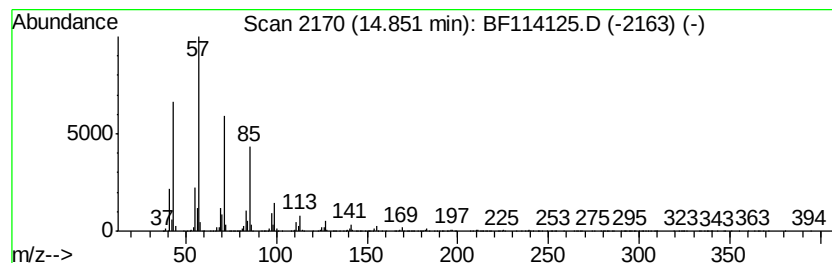
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	32.60 ng	3907600	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	93
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3		Octacosane	394	C28H58	000630-02-4	91
4		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	91
5		Eicosane	282	C20H42	000112-95-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
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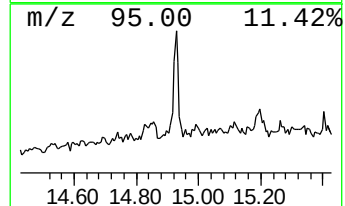
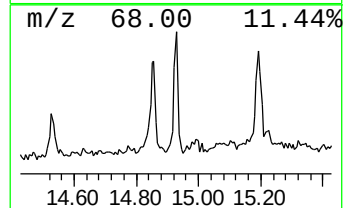
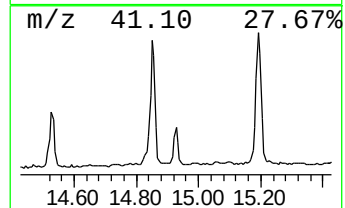
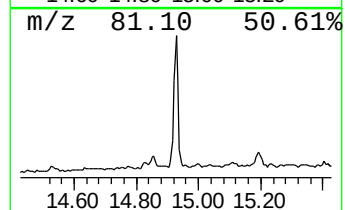
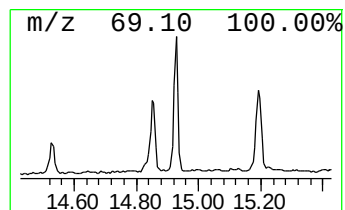
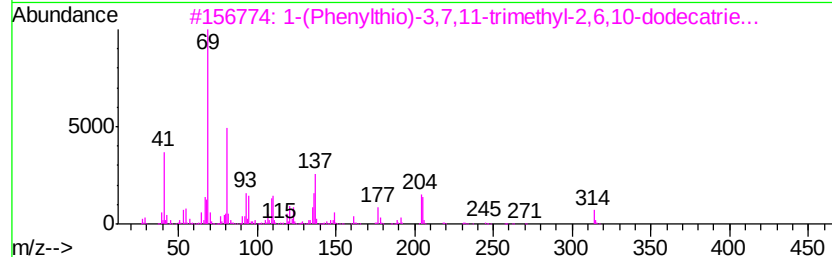
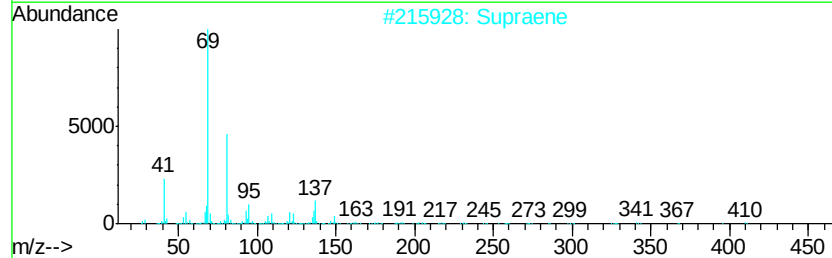
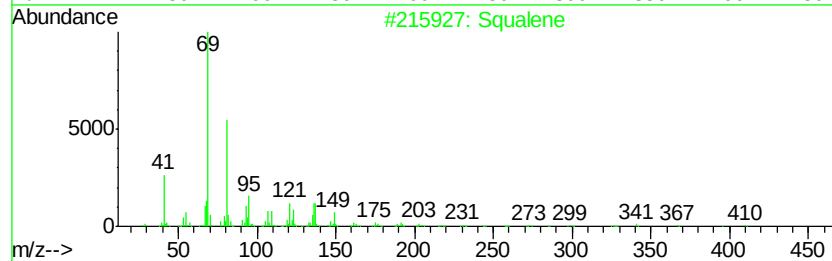
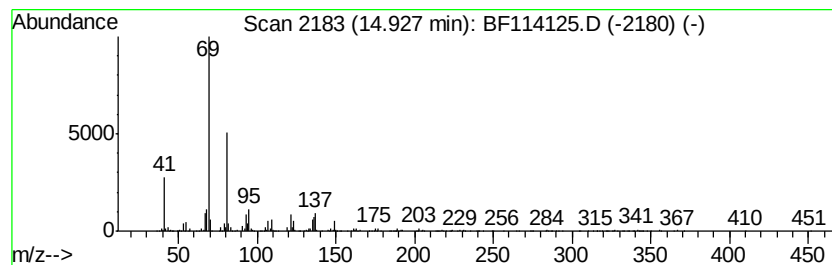
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 Squalene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	4.60 ng	551531	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	94
2	Supraene	410 C30H50	007683-64-9	91
3	1-(Phenylthio)-3,7,11-trimethyl-...	314 C21H30S	028413-57-2	78
4	4,8,12-Tetradecatrienal, 5,9,13-...	248 C17H28O	066408-55-7	72
5	(.+/-)-Lavandulol, pentafluorop...	300 C13H17F5O2	1000352-63-1	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
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 Acq On : 10 May 2019 17:29
 Operator : JU/SJ
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 ALS Vial : 3 Sample Multiplier: 1

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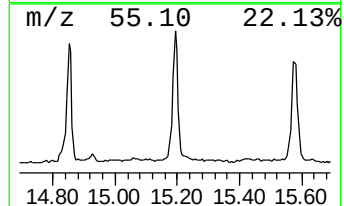
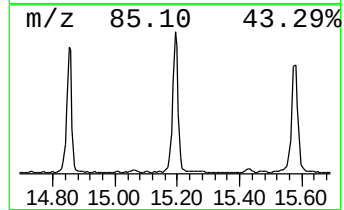
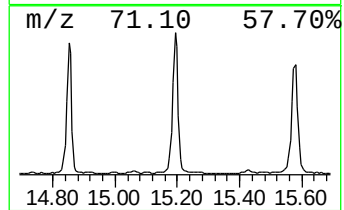
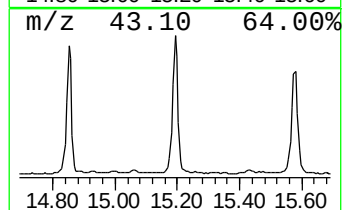
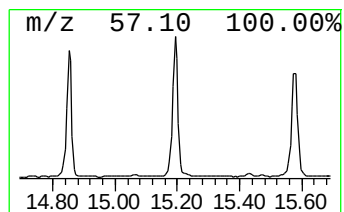
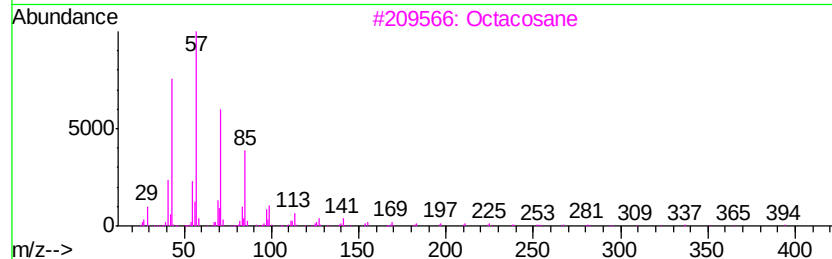
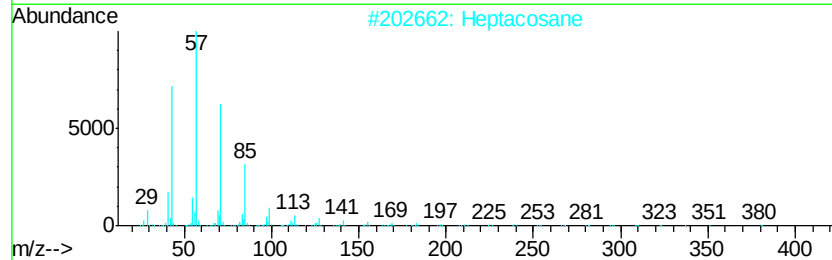
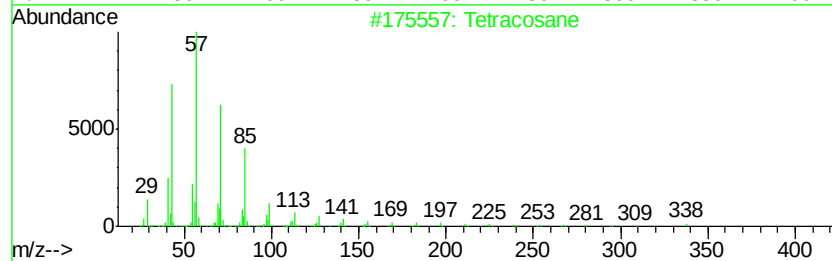
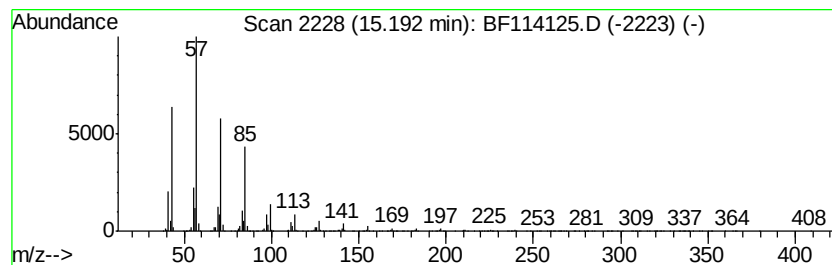
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 12 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	37.41 ng	4483900	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	93
2		Heptacosane	380	C27H56	000593-49-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heneicosane	296	C21H44	000629-94-7	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
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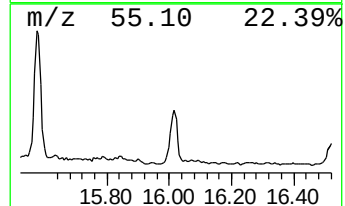
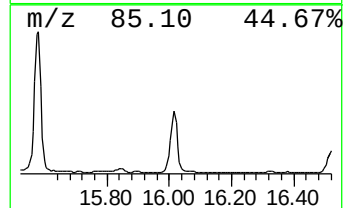
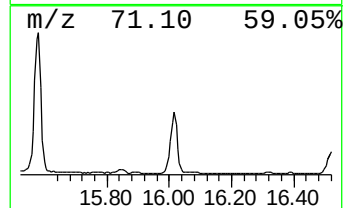
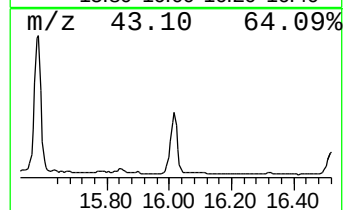
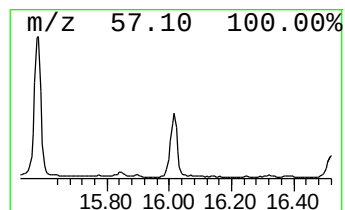
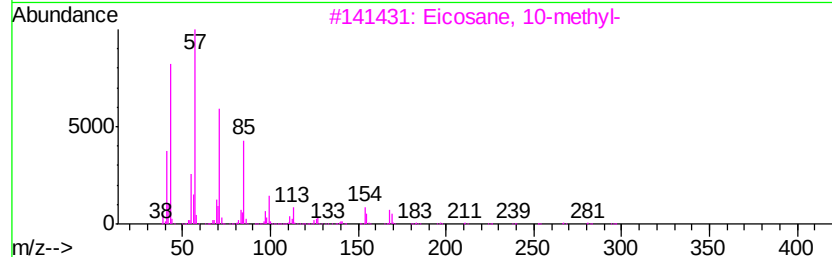
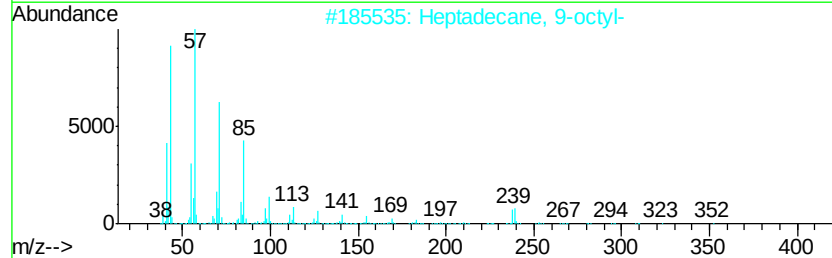
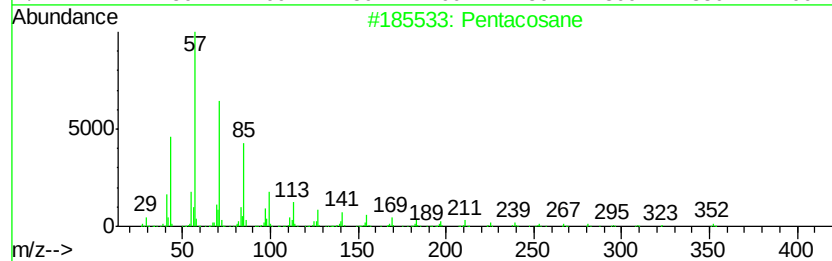
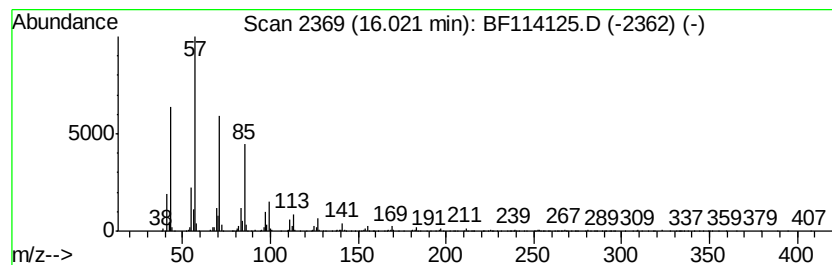
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	15.22 ng	1823960	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane	352 C25H52	000629-99-2	97
2	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	95
3	Eicosane, 10-methyl-	296 C21H44	054833-23-7	93
4	Heptacosane	380 C27H56	000593-49-7	91
5	Hexacosane	366 C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
Data File : BF114125.D
Acq On : 10 May 2019 17:29
Operator : JU/SJ
Sample : K2762-12
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P021-SS002-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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...	2.15	36.0	ng	3983070	1	6.85	2210240	20.0
unknown6.62	6.62	64.4	ng	7120250	1	6.85	2210240	20.0
n-Hexadecanoic acid	11.90	14.0	ng	1455590	4	11.37	2076180	20.0
Dimethylethylcety...	12.01	2.1	ng	218473	4	11.37	2076180	20.0
Octadecanoic acid	12.68	12.8	ng	1324470	4	11.37	2076180	20.0
Sulfurous acid, o...	13.87	6.8	ng	526561	5	14.03	1554980	20.0
Octadecane	14.20	7.0	ng	541487	5	14.03	1554980	20.0
Heneicosane	14.53	19.7	ng	1534170	5	14.03	1554980	20.0
Docosane	14.85	32.6	ng	3907600	6	15.54	2397080	20.0
Squalene	14.93	4.6	ng	551531	6	15.54	2397080	20.0
Tetracosane	15.19	37.4	ng	4483900	6	15.54	2397080	20.0
Pentacosane	16.02	15.2	ng	1823960	6	15.54	2397080	20.0