

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120719\
 Data File : BF118133.D
 Acq On : 7 Dec 2019 17:07
 Operator : JU
 Sample : K6174-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SOLID-COMP

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-BF120619.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	2.134	3	8	16	rVB	261785	337880	9.45%	1.097%
2	5.075	504	508	517	rBV	412750	521200	14.57%	1.693%
3	5.481	570	577	580	rBV	2638164	2579666	72.13%	8.377%
4	6.498	744	750	755	rBV	2652830	2729397	76.32%	8.863%
5	6.634	769	773	776	rBV	3177413	2938253	82.16%	9.542%
6	6.863	809	812	817	rBV	890643	721968	20.19%	2.345%
7	7.022	835	839	842	rBV	2803293	2313303	64.69%	7.512%
8	7.428	904	908	911	rBV	1824992	1633854	45.69%	5.306%
9	8.151	1025	1031	1037	rBV	1117537	953089	26.65%	3.095%
10	9.227	1210	1214	1218	rBV	3738012	3540069	98.99%	11.496%
11	9.622	1278	1281	1286	rBV	256438	231821	6.48%	0.753%
12	9.910	1326	1330	1341	rVB	1233255	1129399	31.58%	3.668%
13	10.704	1461	1465	1477	rBV	2714394	2432638	68.02%	7.900%
14	11.404	1580	1584	1591	rBV	1380158	1190166	33.28%	3.865%
15	11.927	1669	1673	1682	rBV	346742	335744	9.39%	1.090%
16	12.716	1803	1807	1814	rBV2	87577	103604	2.90%	0.336%
17	12.998	1850	1855	1858	rBV	4112479	3576186	100.00%	11.613%
18	13.563	1946	1951	1954	rBV2	40813	46643	1.30%	0.151%
19	13.886	2003	2006	2017	rBV	466620	534835	14.96%	1.737%
20	14.057	2031	2035	2041	rVB	826856	799420	22.35%	2.596%
21	14.210	2058	2061	2068	rBV	93956	94384	2.64%	0.307%
22	14.515	2109	2113	2120	rBV	130718	175272	4.90%	0.569%
23	14.827	2162	2166	2171	rBV	164856	177422	4.96%	0.576%
24	15.174	2221	2225	2229	rBV	176205	204119	5.71%	0.663%
25	15.545	2282	2288	2297	rBV	651784	1026434	28.70%	3.333%
26	16.009	2362	2367	2372	rBV	114228	168168	4.70%	0.546%
27	16.068	2372	2377	2385	rBV5	57882	117218	3.28%	0.381%
28	16.527	2450	2455	2461	rBV3	65041	118390	3.31%	0.384%
29	17.139	2554	2559	2566	rVB4	31102	63303	1.77%	0.206%

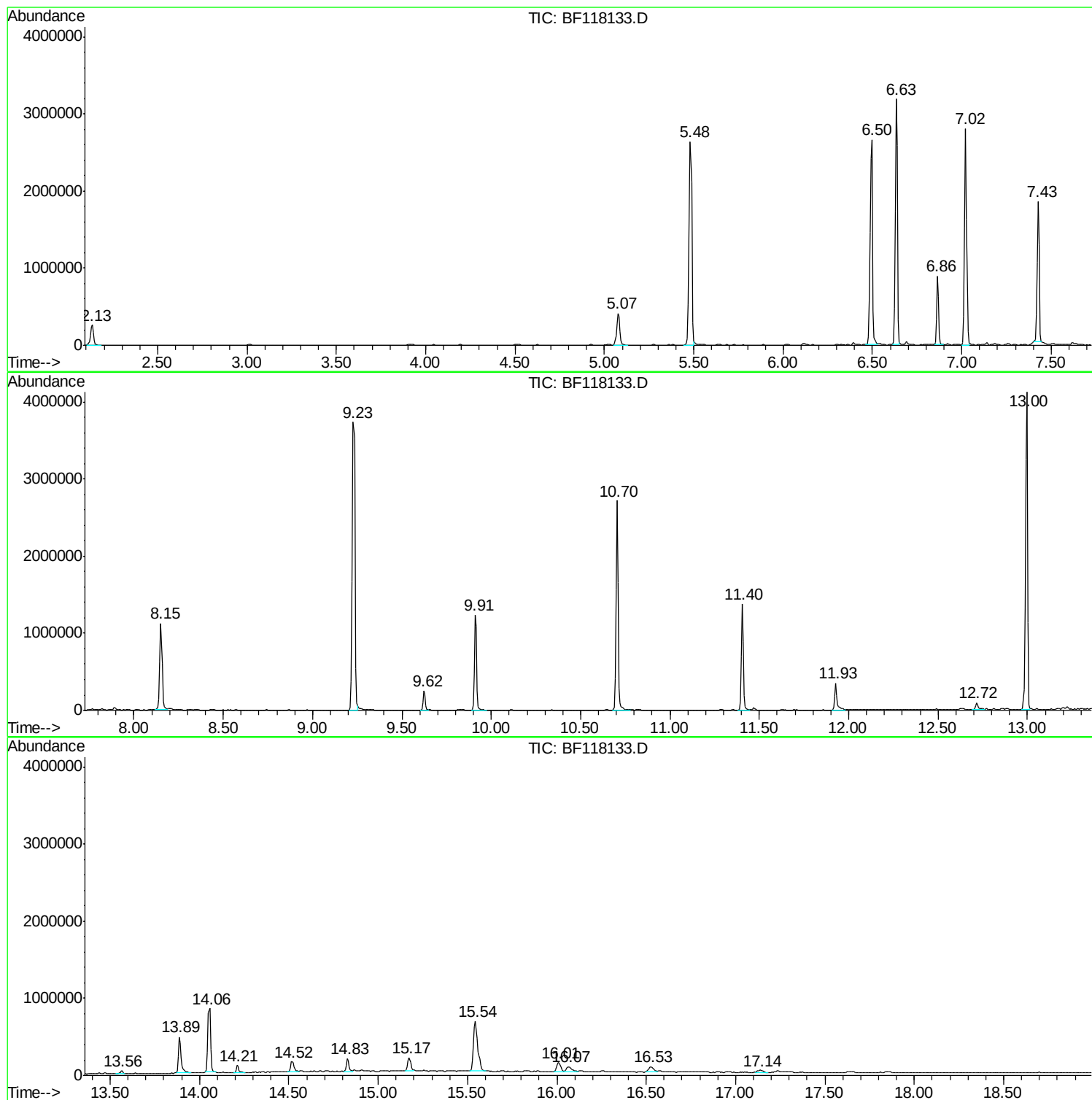
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOLID-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.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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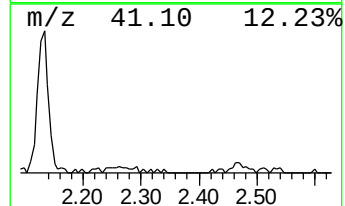
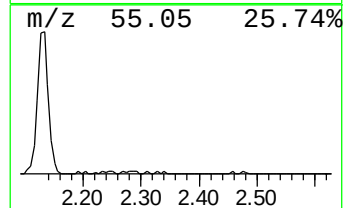
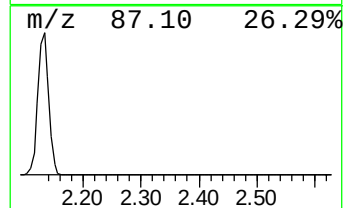
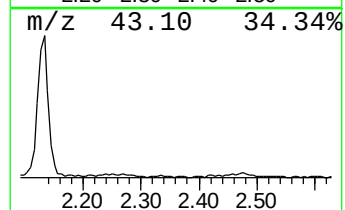
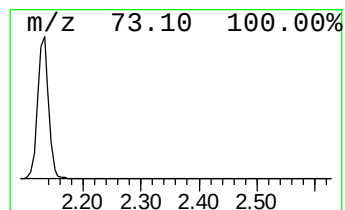
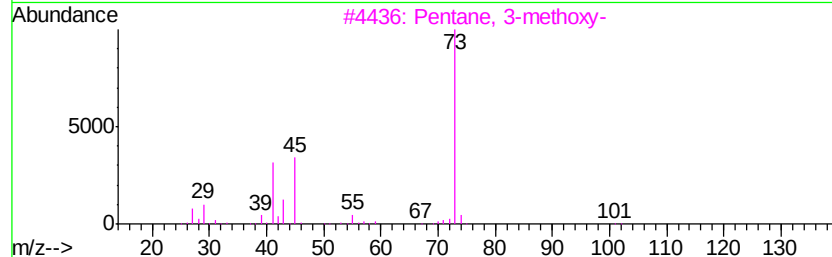
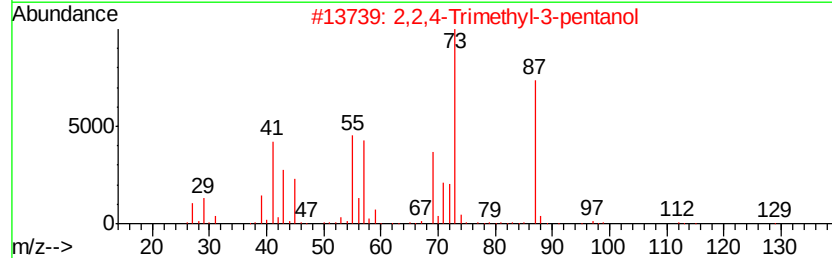
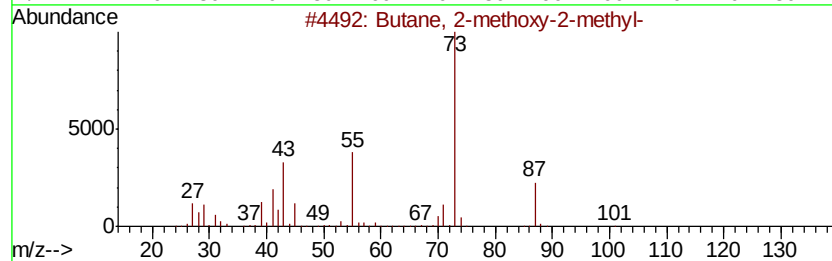
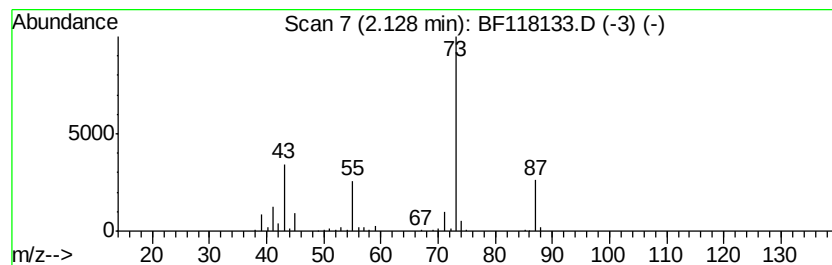
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	9.36 ng	337880	1,4-Dichlorobenzene-d4	6.86

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		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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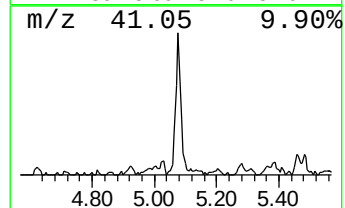
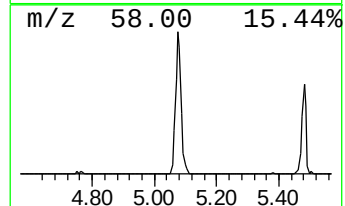
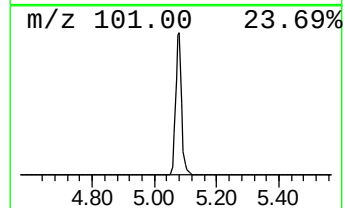
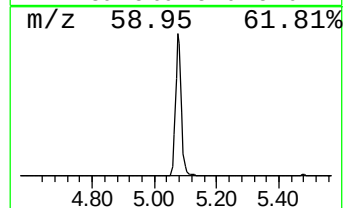
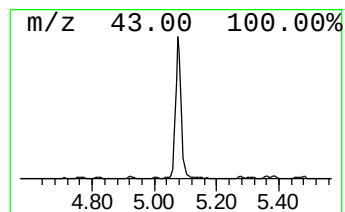
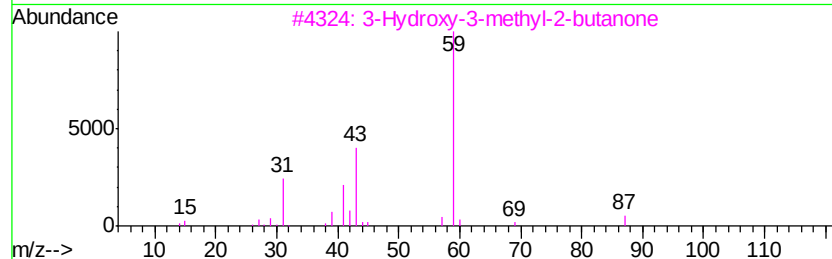
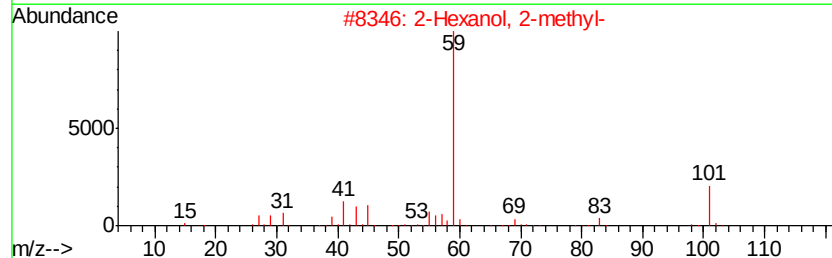
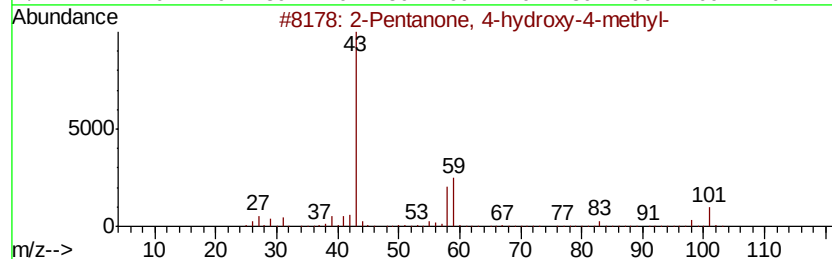
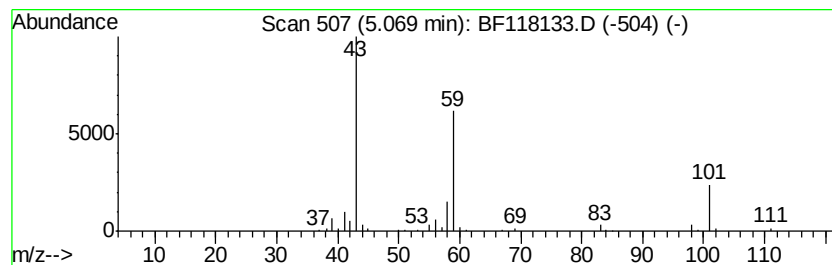
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	14.44 ng	521200	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	27
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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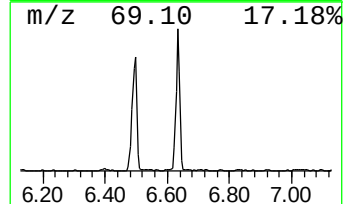
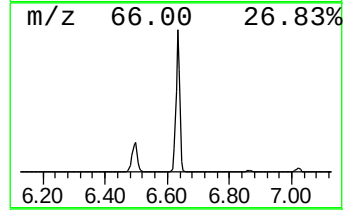
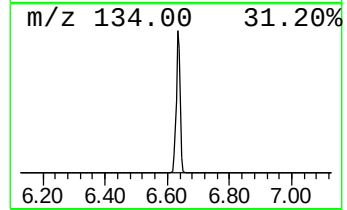
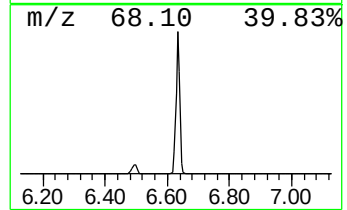
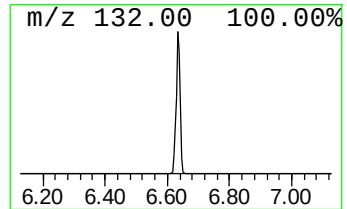
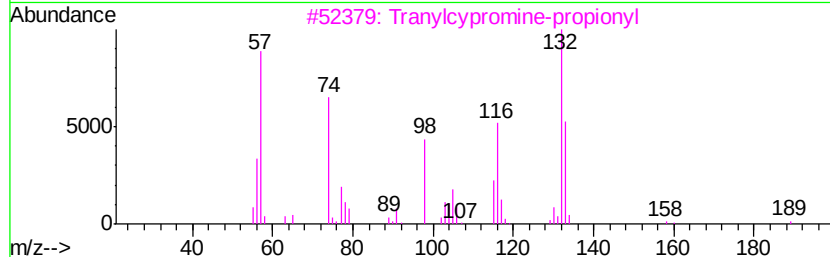
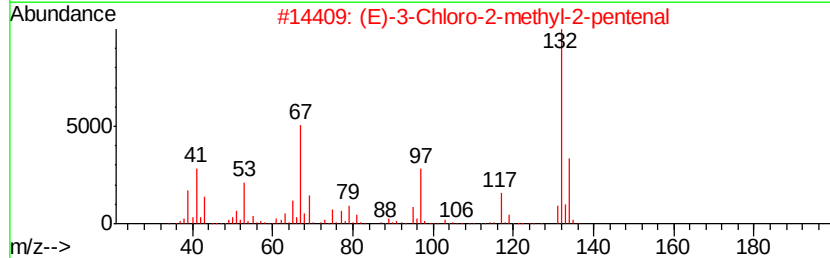
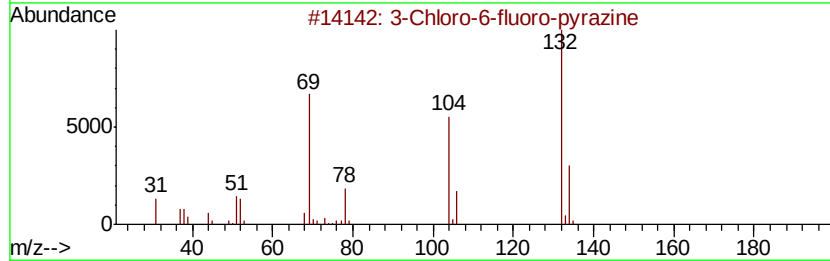
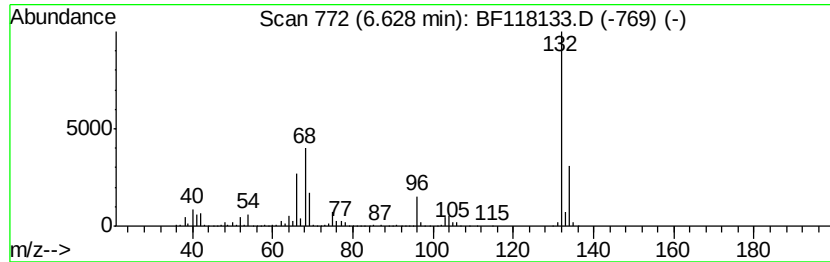
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	81.40 ng	2938250	1,4-Dichlorobenzene-d4	6.86

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	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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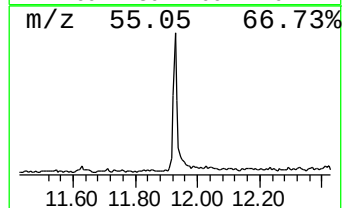
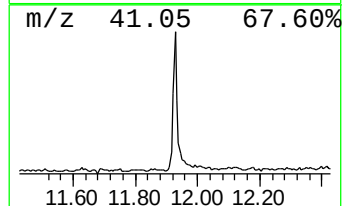
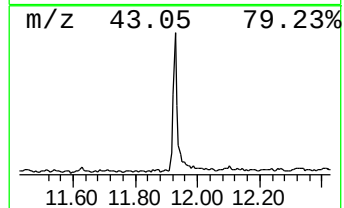
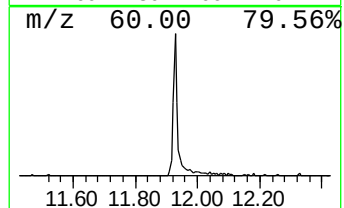
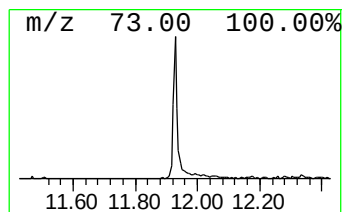
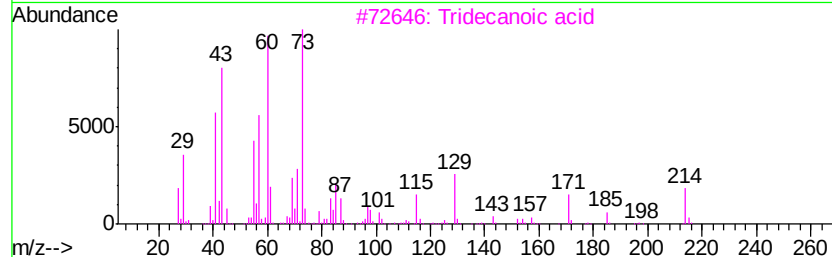
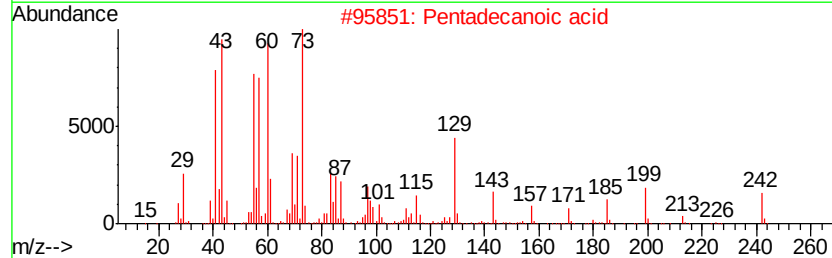
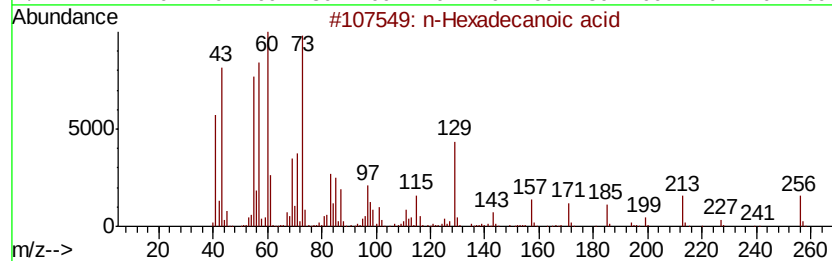
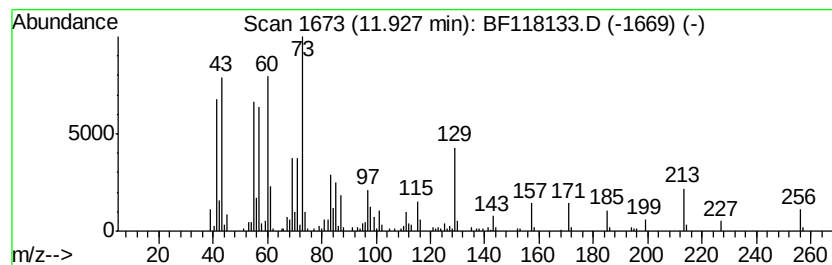
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.93	5.64 ng	335744	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58



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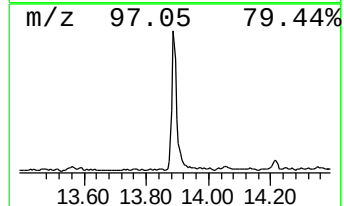
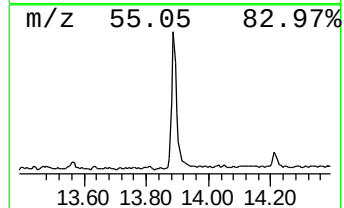
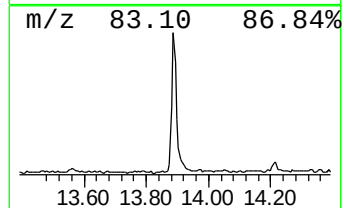
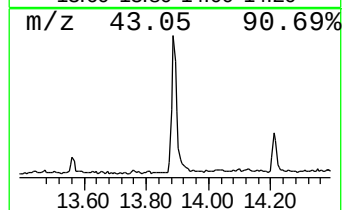
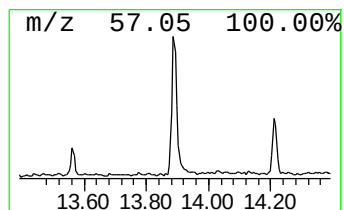
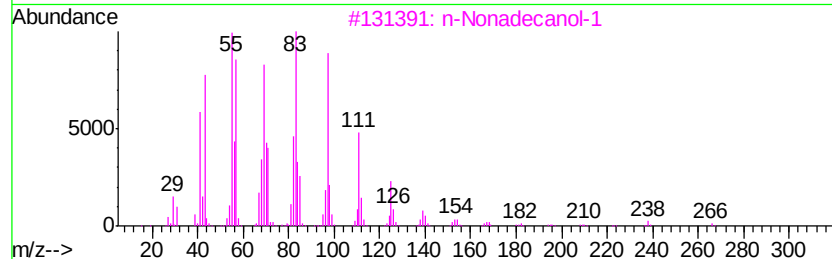
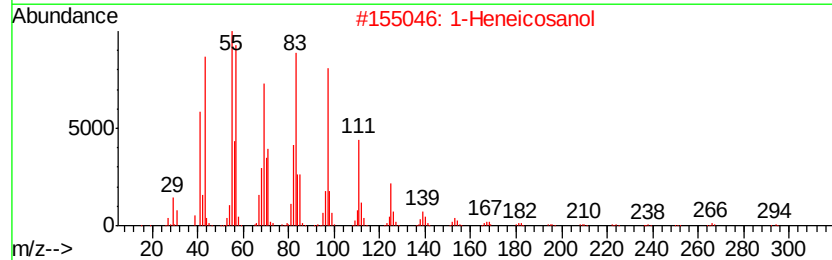
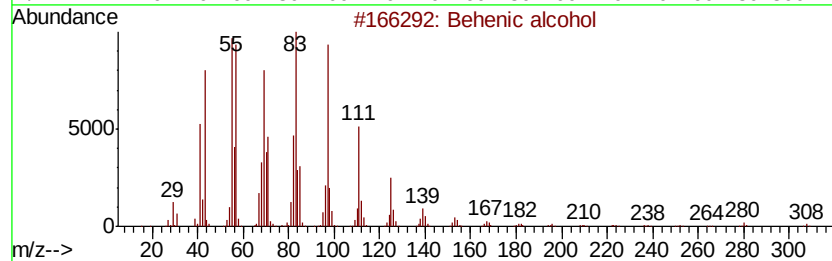
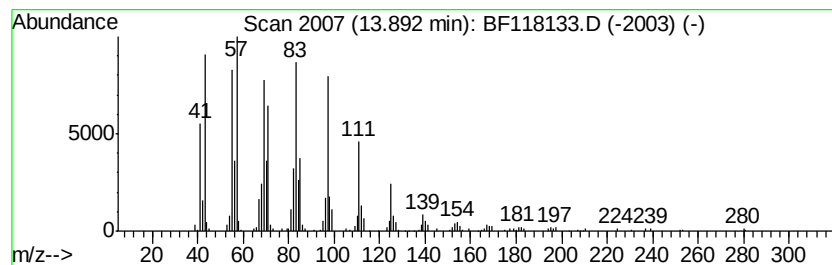
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	13.38 ng	534835	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



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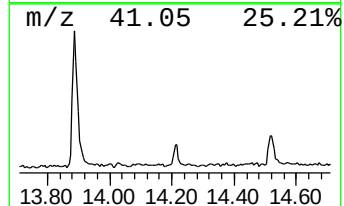
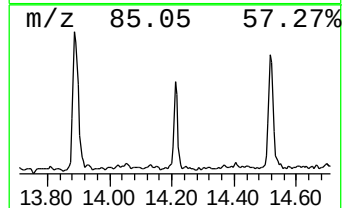
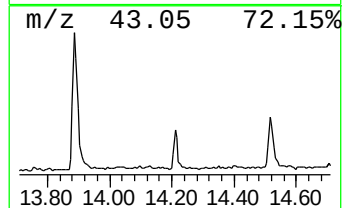
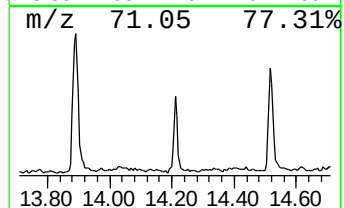
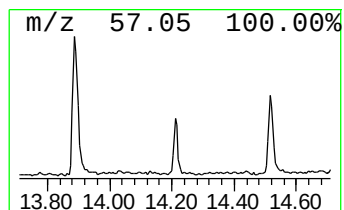
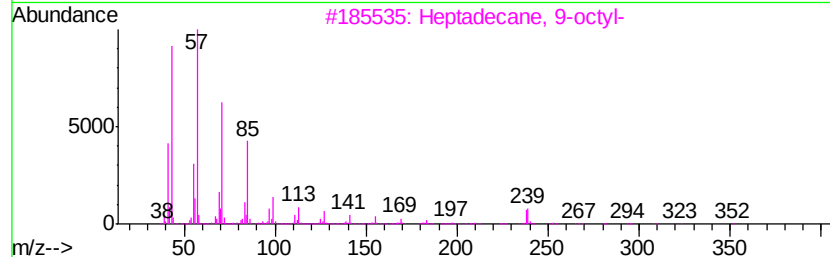
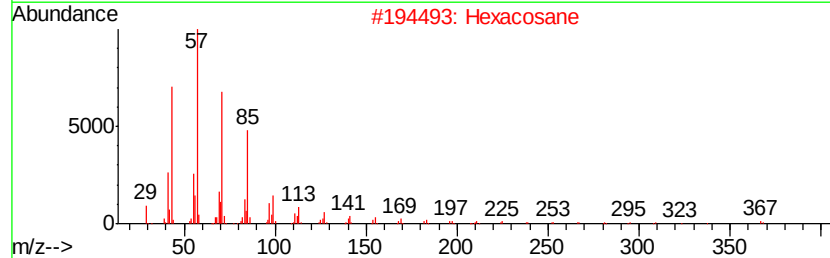
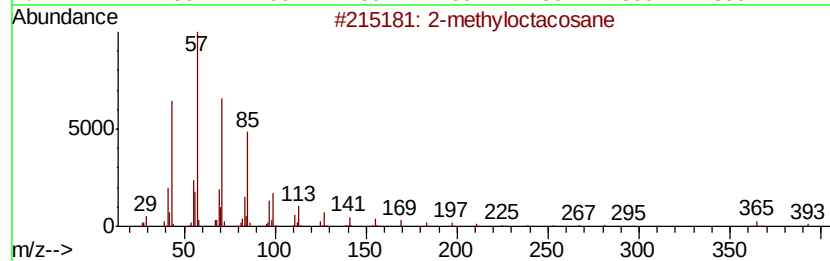
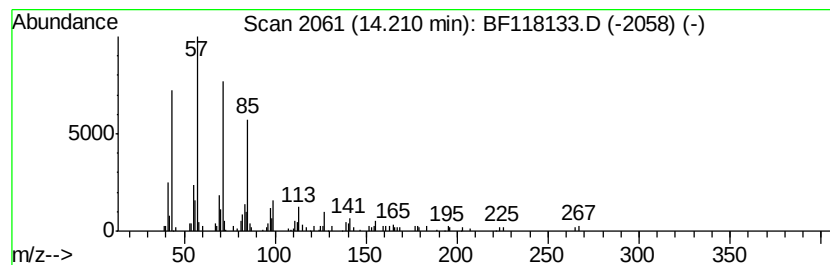
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyloctacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	2.36 ng	94384	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Hentriacontane	437	C31H64	000630-04-6	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
Data File : BF118133.D
Acq On : 7 Dec 2019 17:07
Operator : JU
Sample : K6174-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOLID-COMP

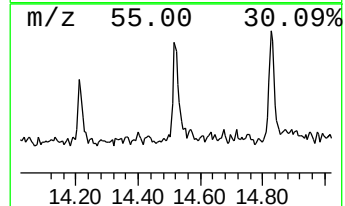
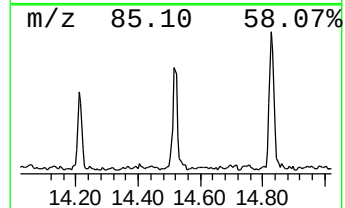
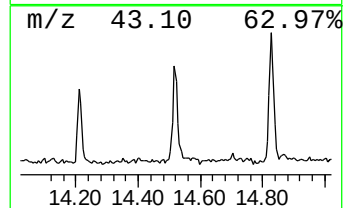
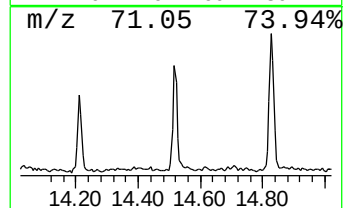
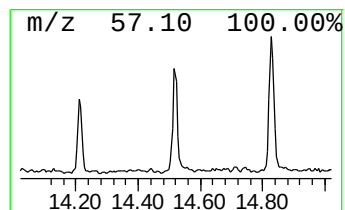
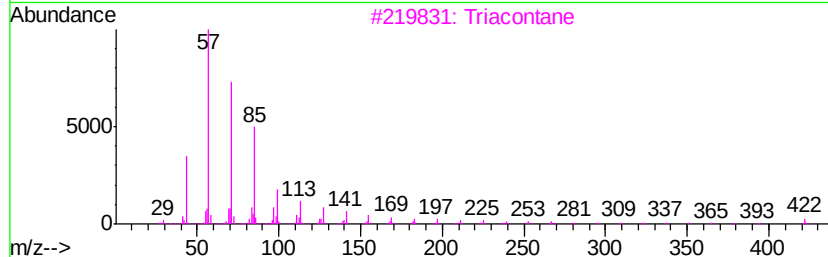
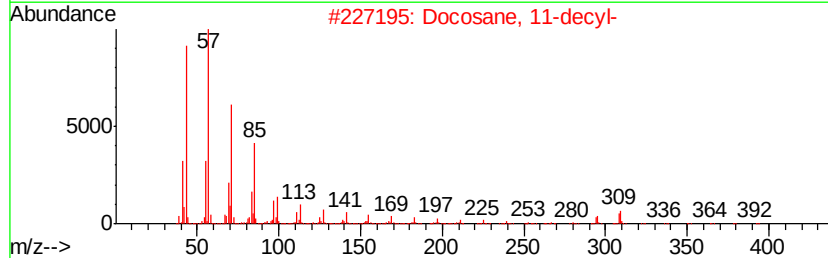
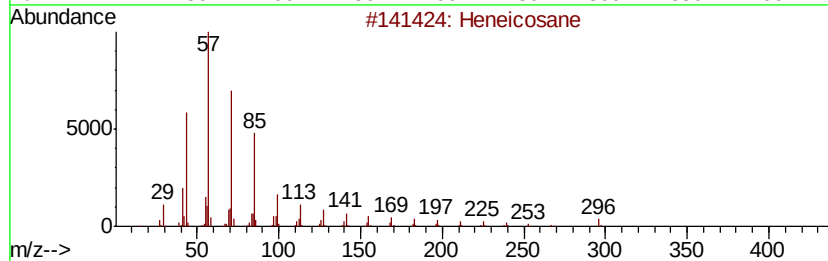
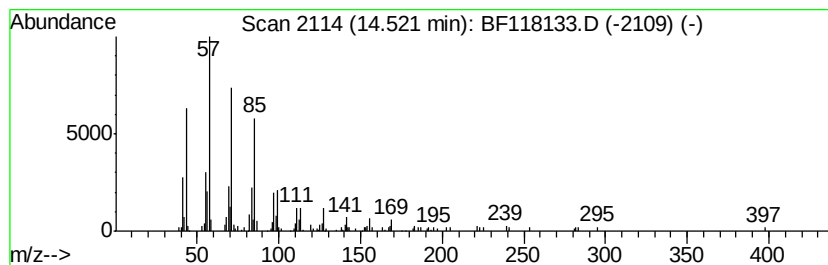
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	4.38 ng	175272	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Docosane, 11-decyl-		451	C32H66	055401-55-3	91
3	Triacontane		422	C30H62	000638-68-6	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Octacosane		394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
Data File : BF118133.D
Acq On : 7 Dec 2019 17:07
Operator : JU
Sample : K6174-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOLID-COMP

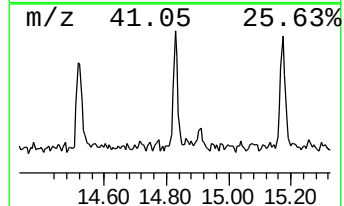
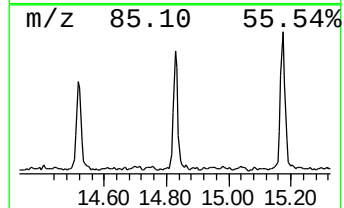
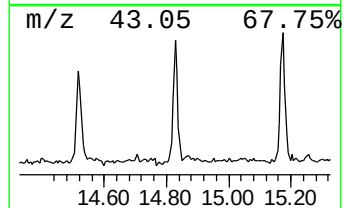
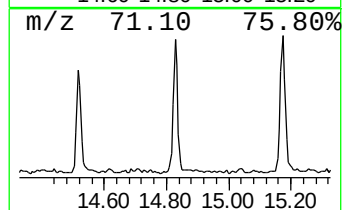
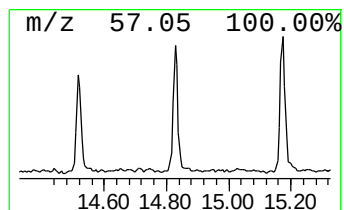
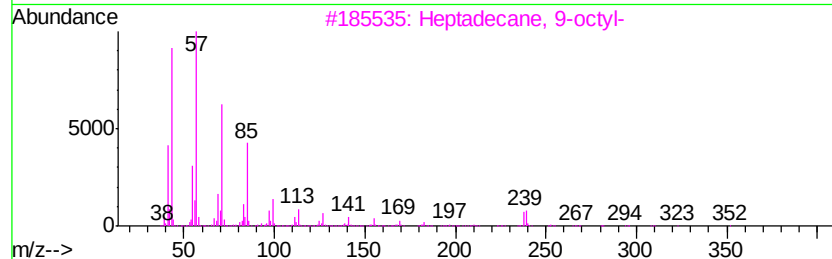
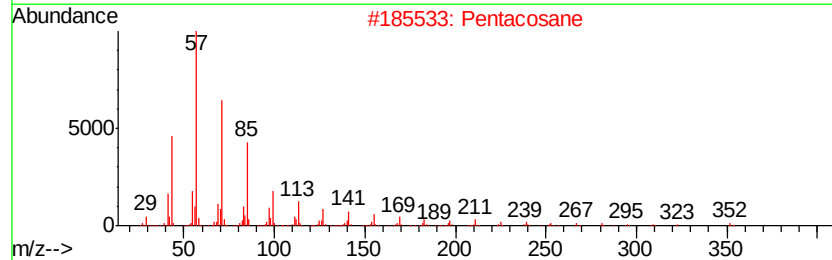
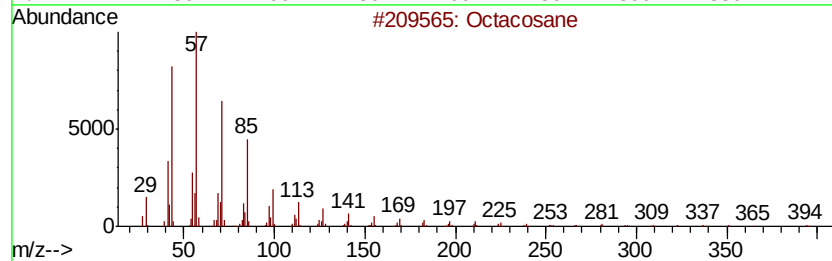
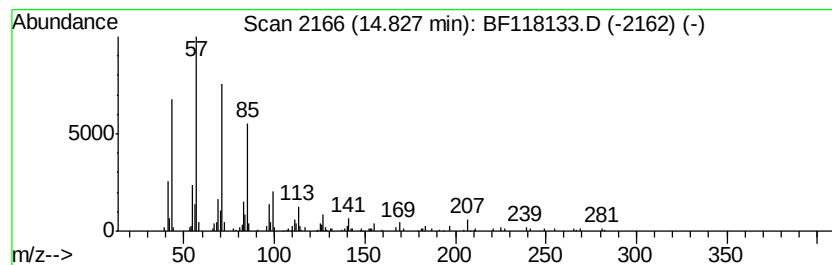
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.46 ng	177422	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	91
2		Pentacosane	352	C25H52	000629-99-2	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4		Eicosane	282	C20H42	000112-95-8	90
5		triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
Data File : BF118133.D
Acq On : 7 Dec 2019 17:07
Operator : JU
Sample : K6174-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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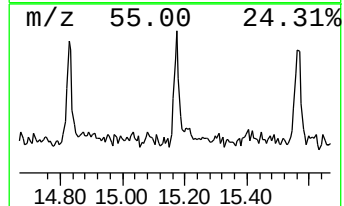
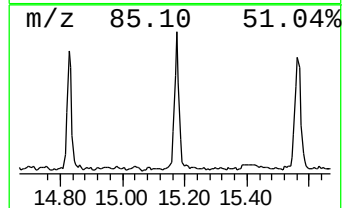
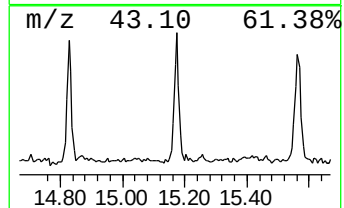
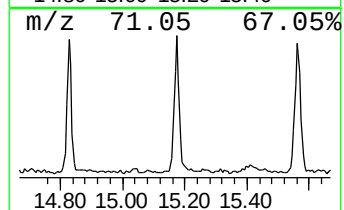
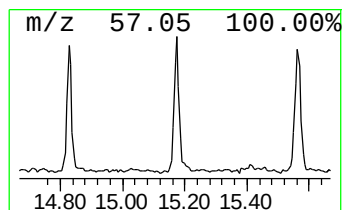
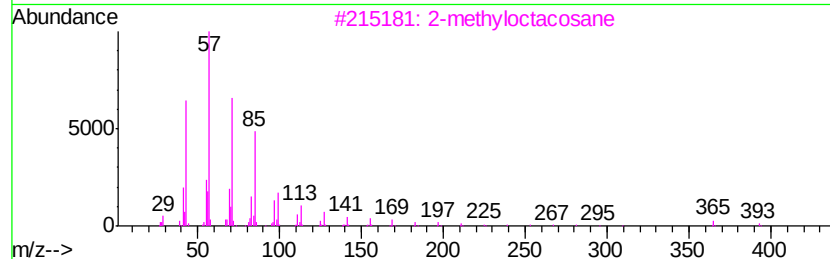
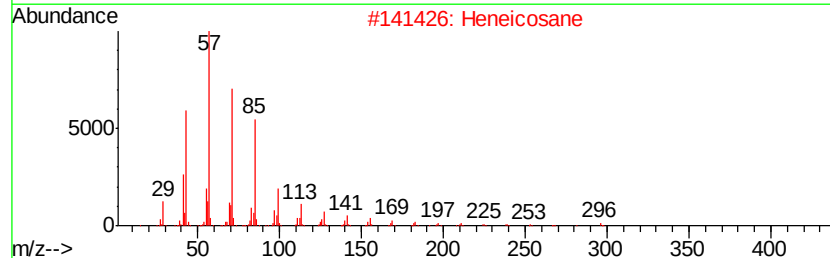
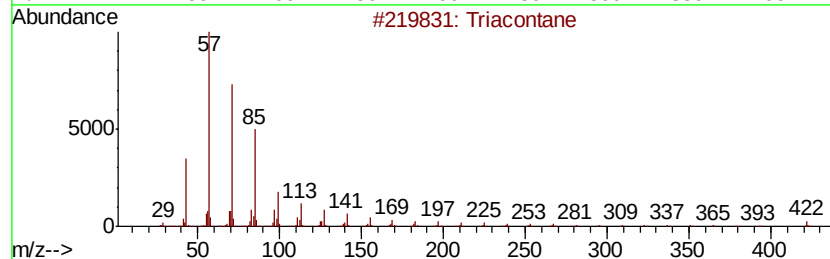
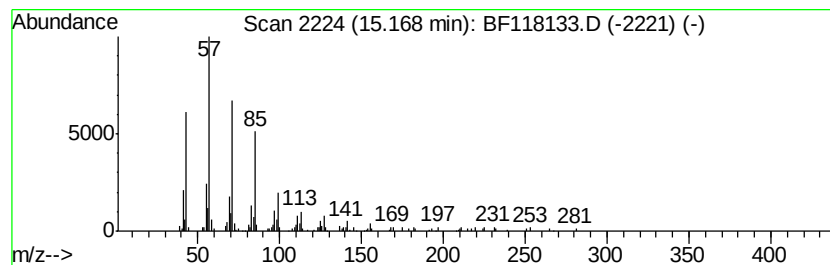
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	3.98 ng	204119	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
Data File : BF118133.D
Acq On : 7 Dec 2019 17:07
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Sample : K6174-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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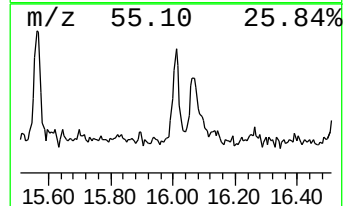
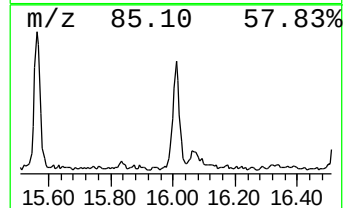
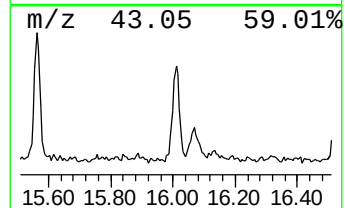
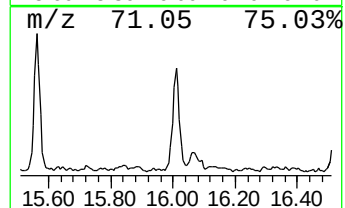
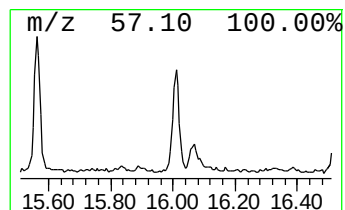
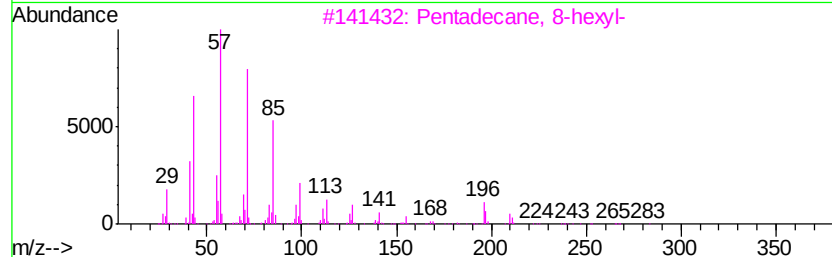
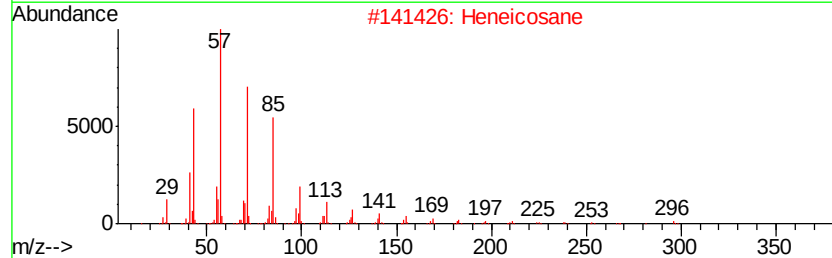
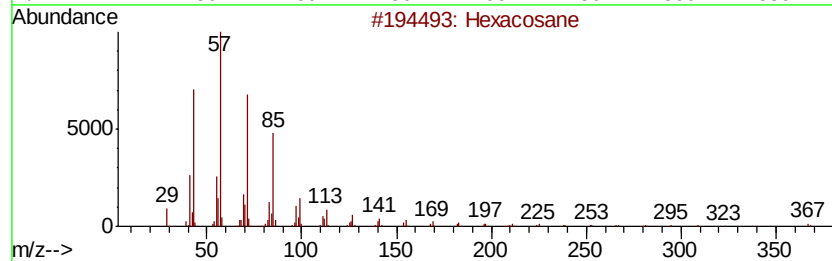
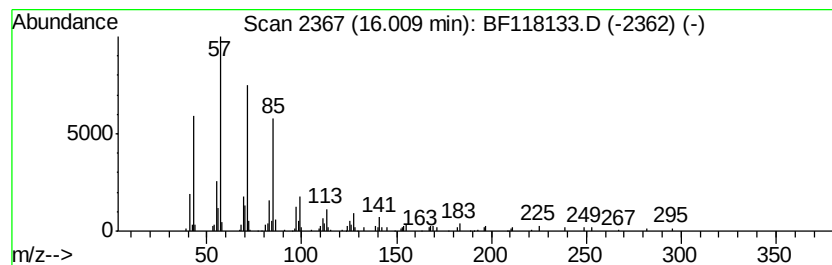
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	3.28 ng	168168	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
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Acq On : 7 Dec 2019 17:07
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Sample : K6174-01
Misc :
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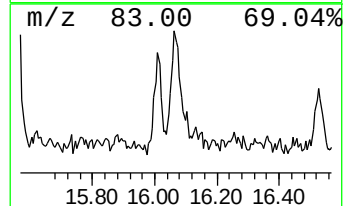
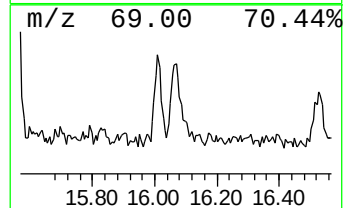
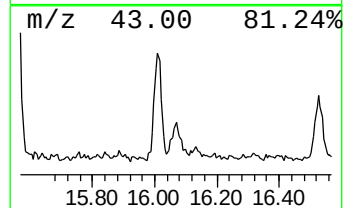
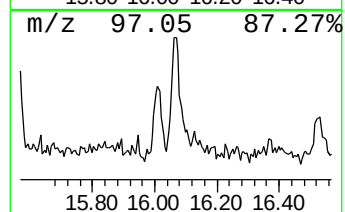
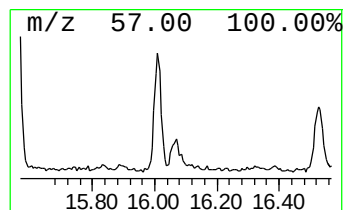
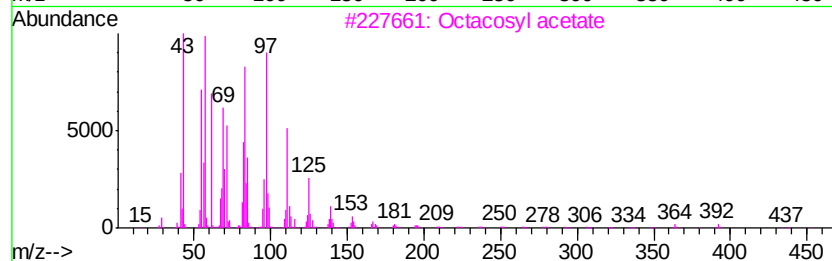
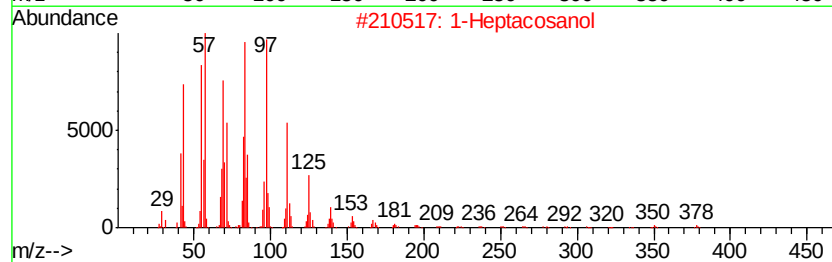
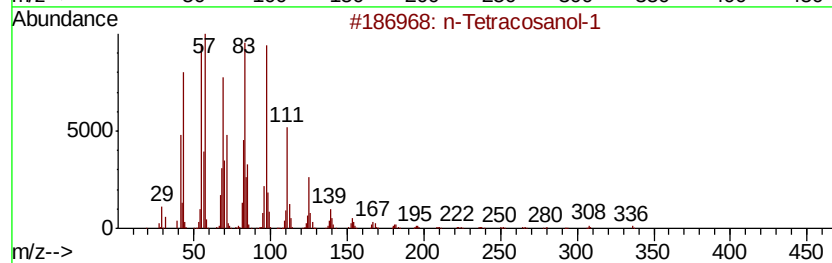
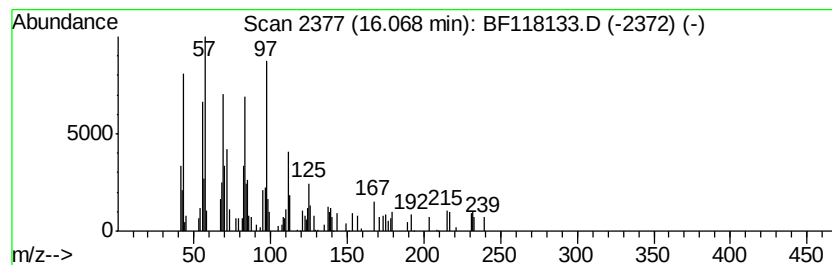
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Tetracosanol-1 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	2.28 ng	117218	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Tetracosanol-1	354 C24H50O	000506-51-4	93
2	1-Heptacosanol	396 C27H56O	002004-39-9	93
3	Octacosyl acetate	452 C30H60O2	018206-97-8	93
4	Octacosanol	410 C28H58O	000557-61-9	90
5	Octadecyl trifluoroacetate	366 C20H37F3O2	079392-43-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
Data File : BF118133.D
Acq On : 7 Dec 2019 17:07
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Sample : K6174-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SOLID-COMP

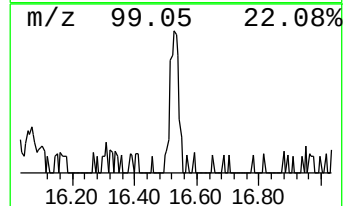
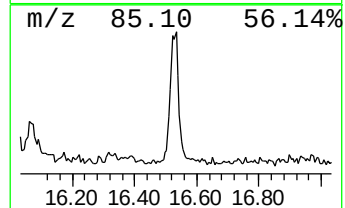
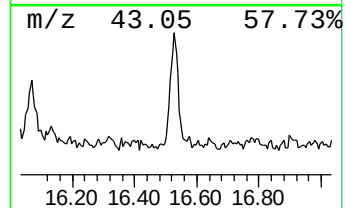
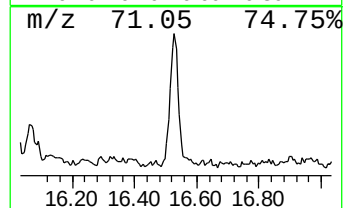
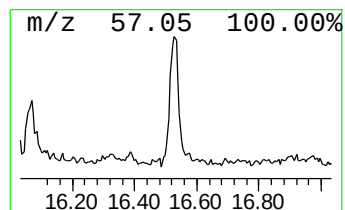
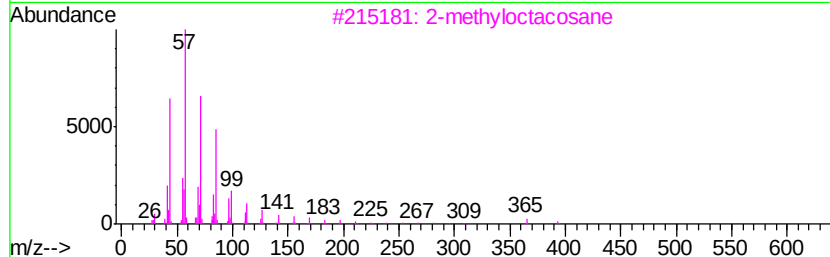
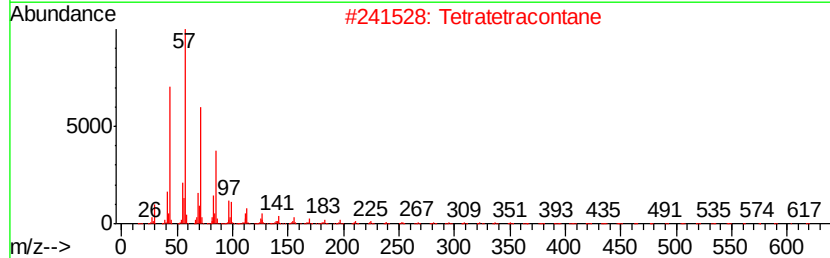
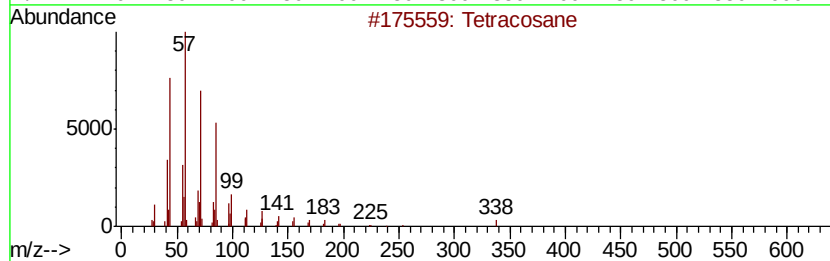
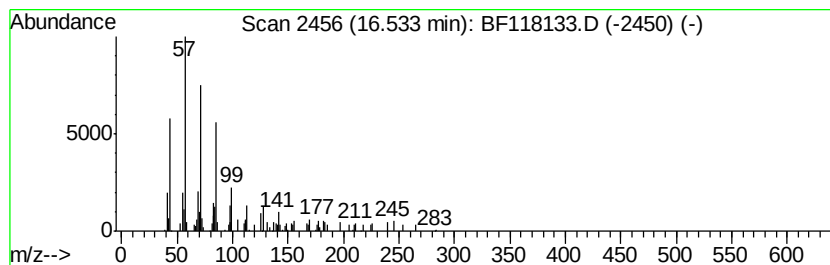
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.31 ng	118390	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	87
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		2-methyloctacosane	408	C29H60	1000376-72-8	87
4		Heneicosane	296	C21H44	000629-94-7	86
5		Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120719\
Data File : BF118133.D
Acq On : 7 Dec 2019 17:07
Operator : JU
Sample : K6174-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOLID-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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...	2.13	9.4	ng	337880	1	6.86	721968	20.0
2-Pentanone, 4-hy...	5.07	14.4	ng	521200	1	6.86	721968	20.0
unknown6.63	6.63	81.4	ng	2938250	1	6.86	721968	20.0
n-Hexadecanoic acid	11.93	5.6	ng	335744	4	11.40	1190170	20.0
Behenic alcohol	13.89	13.4	ng	534835	5	14.06	799420	20.0
2-methyloctacosane	14.21	2.4	ng	94384	5	14.06	799420	20.0
Heneicosane	14.52	4.4	ng	175272	5	14.06	799420	20.0
Pentacosane	14.83	3.5	ng	177422	6	15.54	1026430	20.0
triacontane	15.17	4.0	ng	204119	6	15.54	1026430	20.0
Hexacosane	16.01	3.3	ng	168168	6	15.54	1026430	20.0
n-Tetracosanol-1	16.07	2.3	ng	117218	6	15.54	1026430	20.0
Tetratetracontane	16.53	2.3	ng	118390	6	15.54	1026430	20.0