

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
 Data File : BF115767.D
 Acq On : 25 Jul 2019 19:34
 Operator : HP/JU
 Sample : K3990-10
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-5-B

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-BF071219.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	4	10	21	rVB	508154	662608	19.19%	2.294%
2	5.087	506	510	521	rVB	54301	73592	2.13%	0.255%
3	5.492	575	579	593	rBV	2230621	2137758	61.92%	7.401%
4	6.498	745	750	770	rBV	2364831	2323657	67.31%	8.045%
5	6.639	770	774	777	rBV	2710295	2338694	67.75%	8.097%
6	6.869	809	813	817	rBV	903072	714719	20.70%	2.475%
7	7.028	836	840	843	rBV	2084718	1814129	52.55%	6.281%
8	7.428	903	908	919	rBV	1549636	1457561	42.22%	5.046%
9	8.151	1027	1031	1050	rBV	963038	919062	26.62%	3.182%
10	9.222	1209	1213	1229	rBV	2699835	2820100	81.69%	9.764%
11	9.339	1229	1233	1243	rVB	66960	80902	2.34%	0.280%
12	9.616	1276	1280	1291	rBV	581912	551060	15.96%	1.908%
13	9.904	1325	1329	1344	rBV	1323656	1148690	33.27%	3.977%
14	10.692	1459	1463	1481	rBV	1897322	1873523	54.27%	6.487%
15	11.386	1578	1581	1589	rBV	1198728	1232453	35.70%	4.267%
16	11.639	1617	1624	1647	rBV3	103395	469642	13.60%	1.626%
17	11.910	1667	1670	1675	rBV	112604	131934	3.82%	0.457%
18	12.474	1757	1766	1769	rBV	52777	71798	2.08%	0.249%
19	12.698	1800	1804	1812	rBV4	26165	53626	1.55%	0.186%
20	12.974	1846	1851	1854	rBV	3734961	3452186	100.00%	11.952%
21	13.204	1886	1890	1893	rBV	46483	43985	1.27%	0.152%
22	13.545	1942	1948	1950	rBV2	45618	45059	1.31%	0.156%
23	13.868	2000	2003	2005	rBV	62128	65696	1.90%	0.227%
24	13.904	2005	2009	2024	rVV3	97837	372615	10.79%	1.290%
25	14.027	2026	2030	2041	rVB	1215636	1199297	34.74%	4.152%
26	14.186	2053	2057	2063	rBV	129577	116337	3.37%	0.403%
27	14.492	2105	2109	2113	rBV	220004	188621	5.46%	0.653%
28	14.798	2157	2161	2168	rVB	301270	272182	7.88%	0.942%
29	15.139	2214	2219	2223	rBV	274763	322758	9.35%	1.117%
30	15.498	2274	2280	2295	rBV2	727544	1377996	39.92%	4.771%
31	15.951	2352	2357	2368	rBV	188718	296568	8.59%	1.027%
32	16.456	2437	2443	2451	rBV2	103316	184431	5.34%	0.639%
33	17.051	2538	2544	2550	rBV3	33495	69720	2.02%	0.241%

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ClientSampleId :
TP-5-B

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-BF071219.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

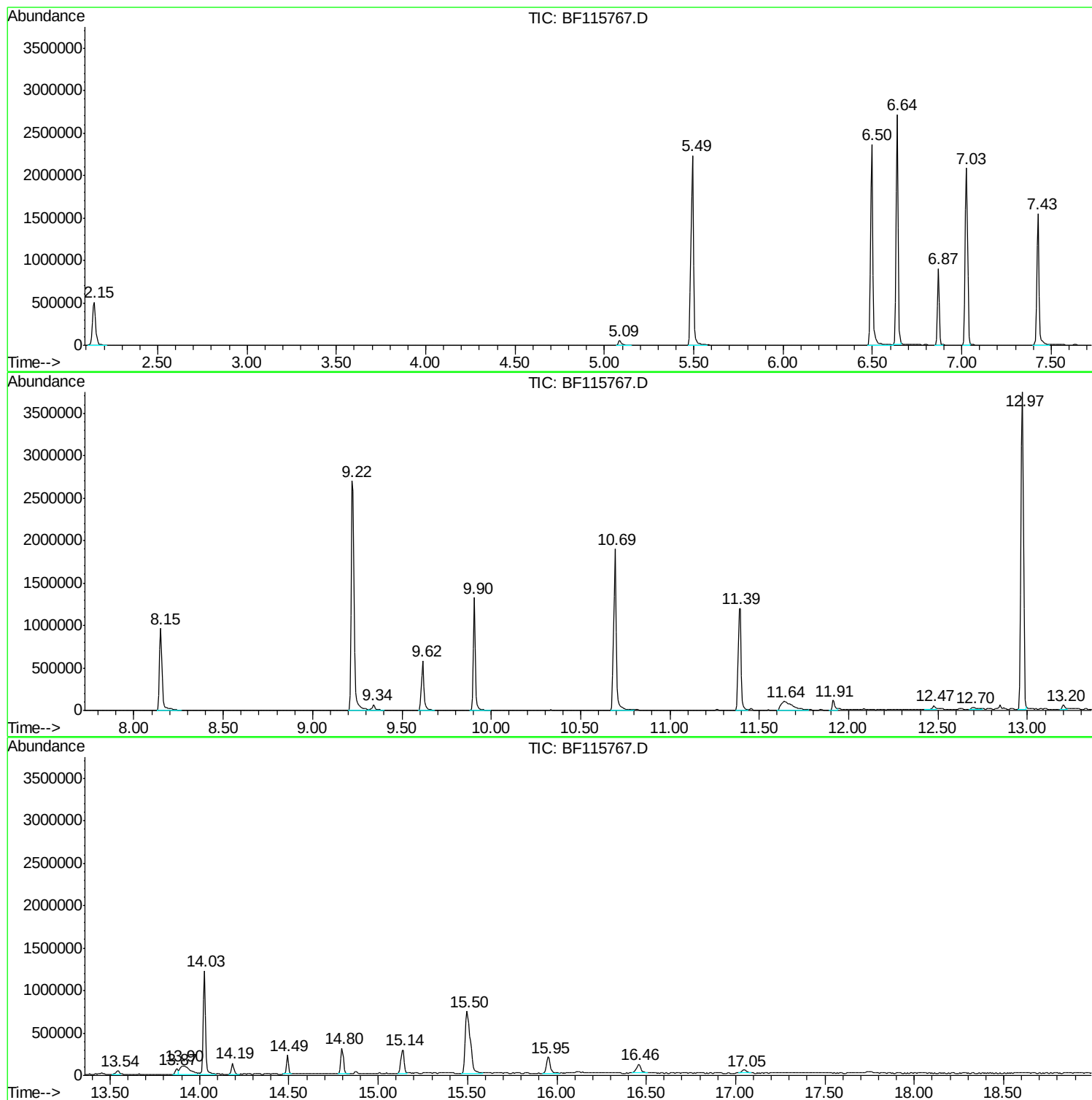
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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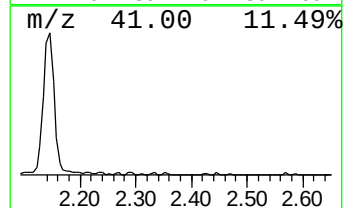
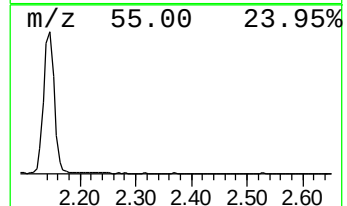
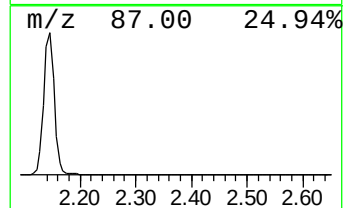
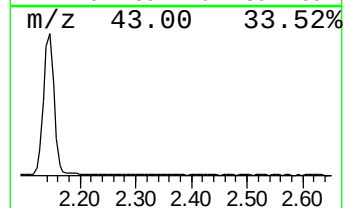
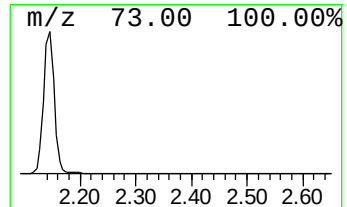
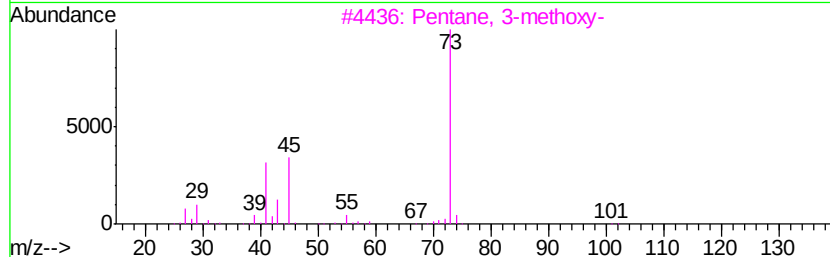
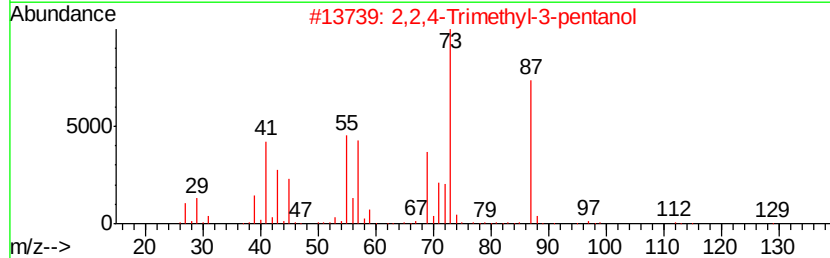
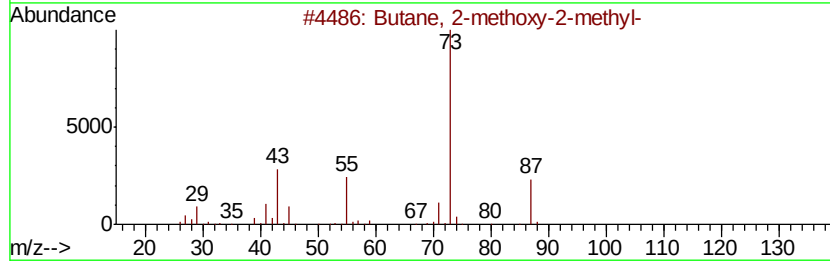
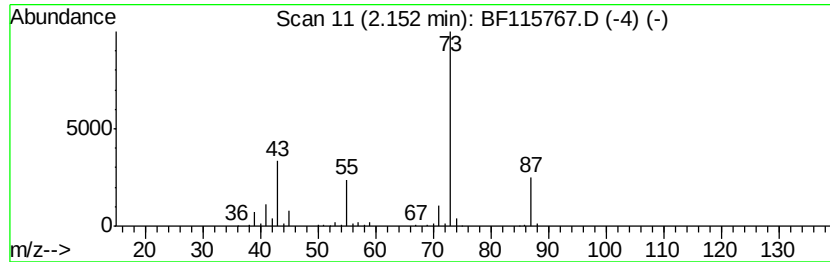
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	18.54 ng	662608	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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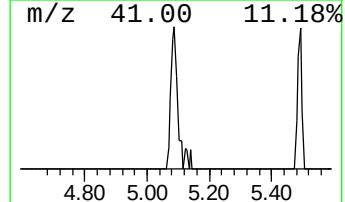
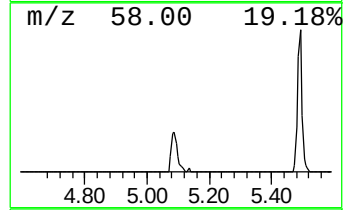
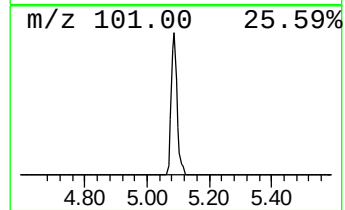
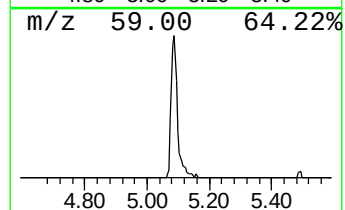
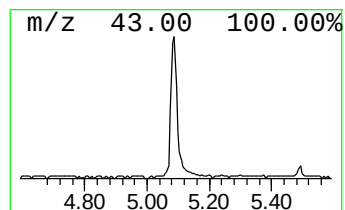
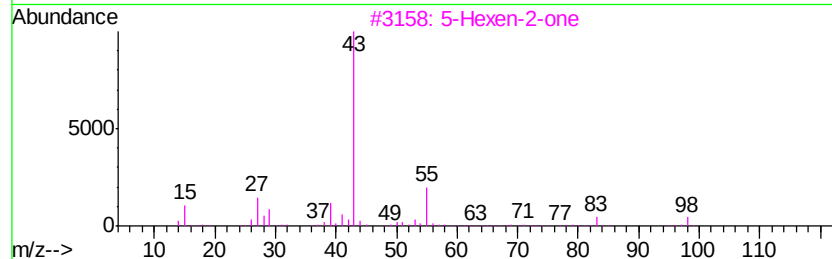
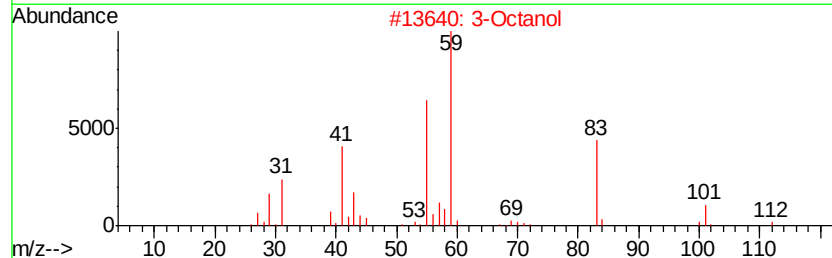
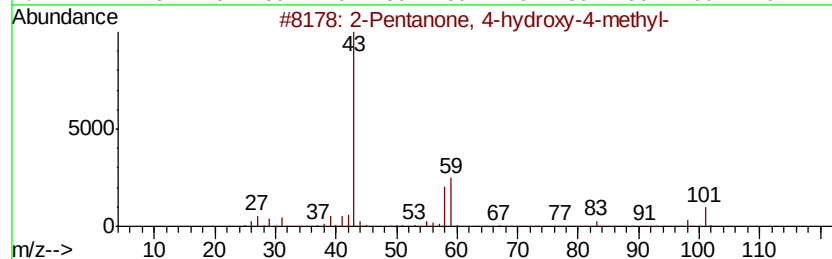
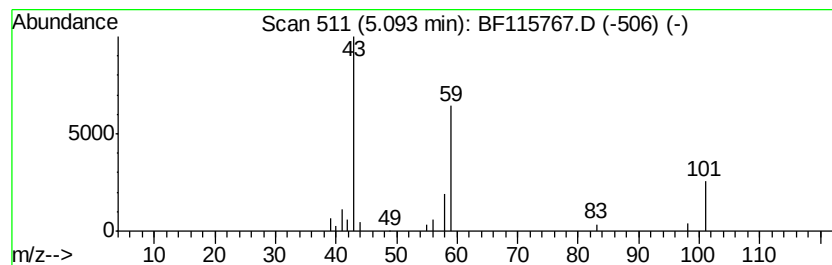
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	2.06 ng	73592	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Octanol	130	C8H18O	000589-98-0	25
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	9
5		Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9



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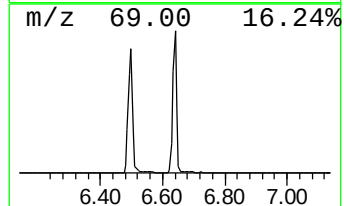
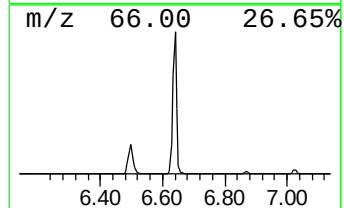
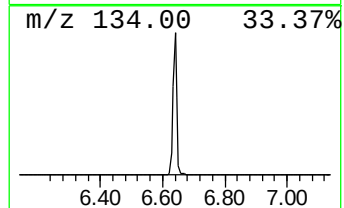
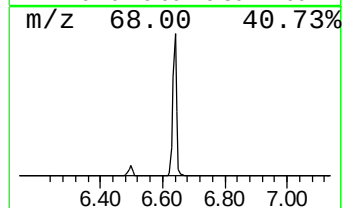
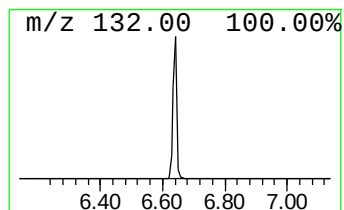
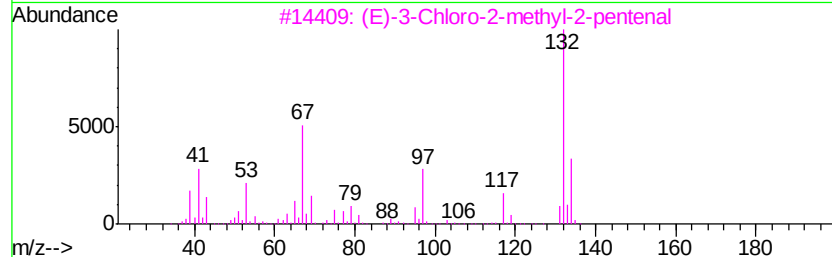
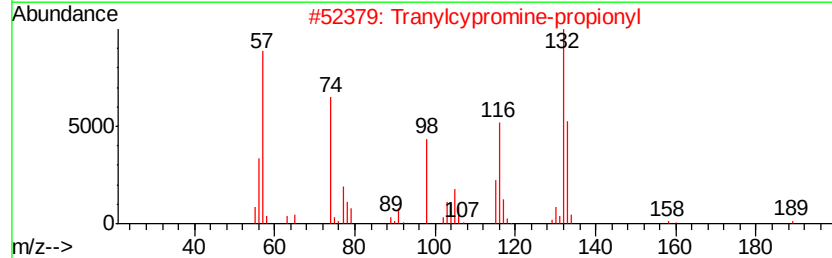
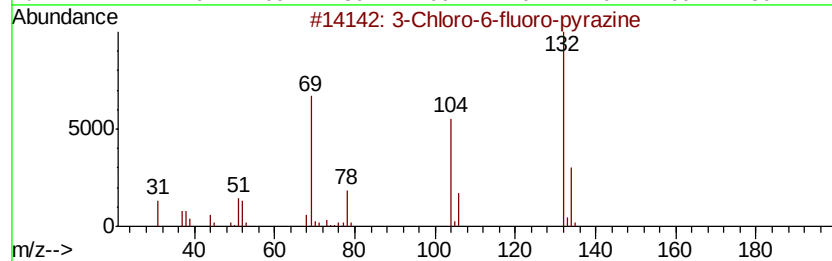
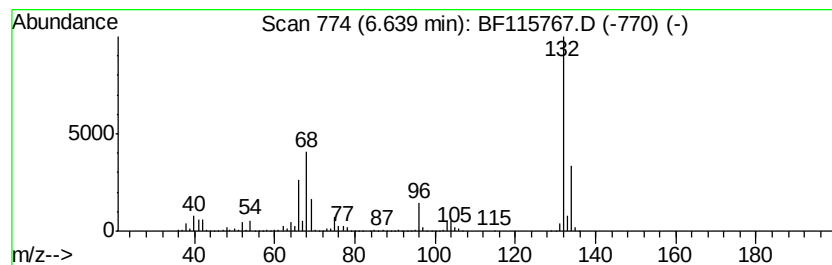
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	65.44 ng	2338690	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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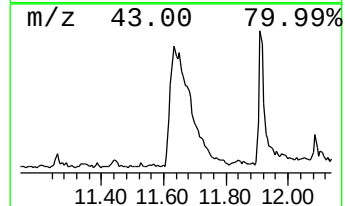
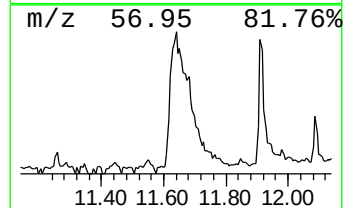
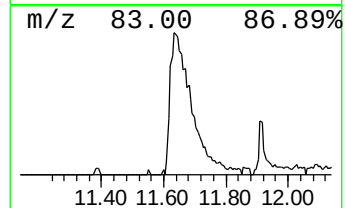
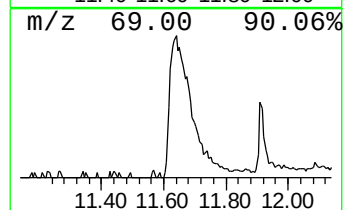
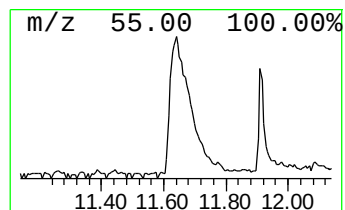
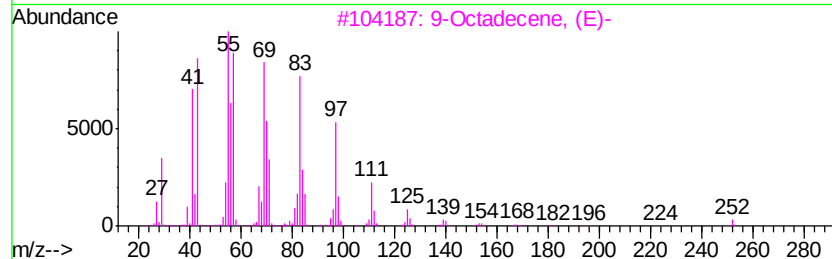
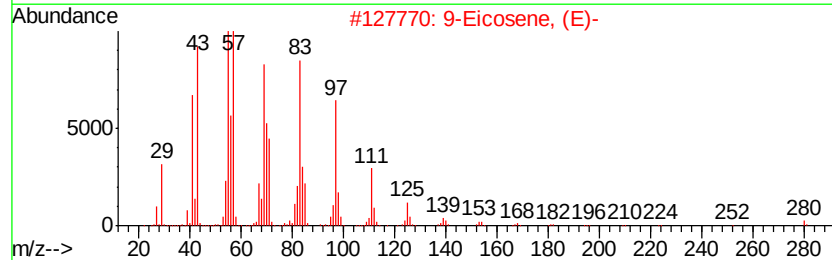
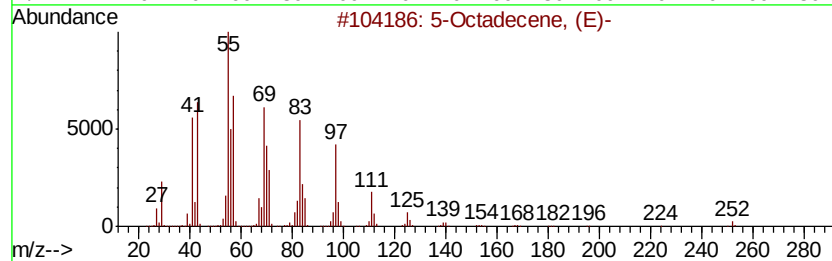
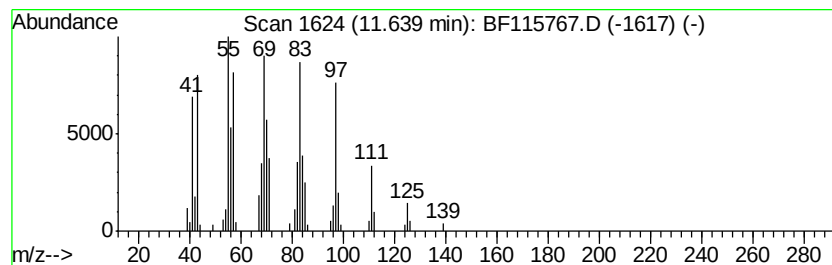
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 5-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.64	7.62 ng	469642	Phenanthrene-d10		11.39
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
4	4-Heptafluorobutylxyloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	81



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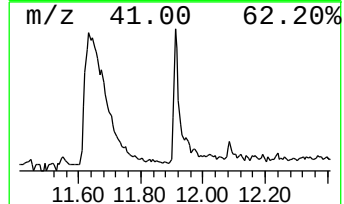
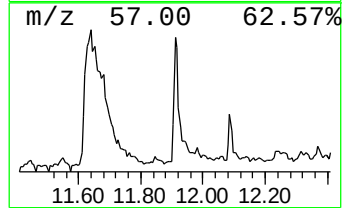
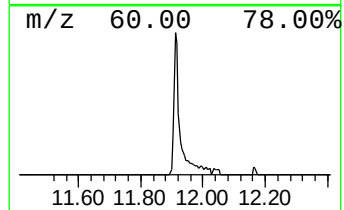
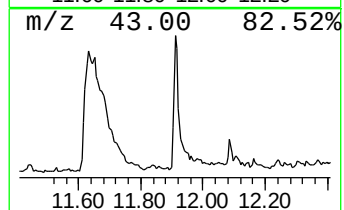
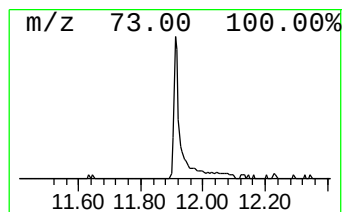
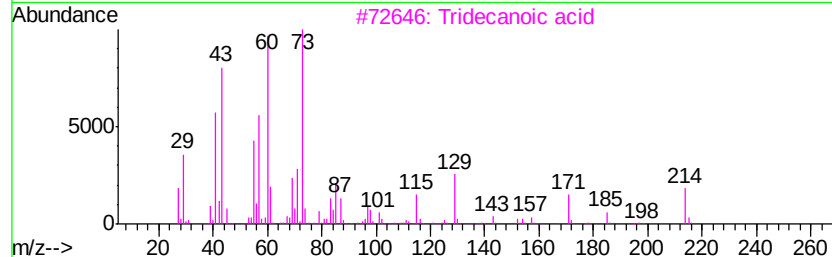
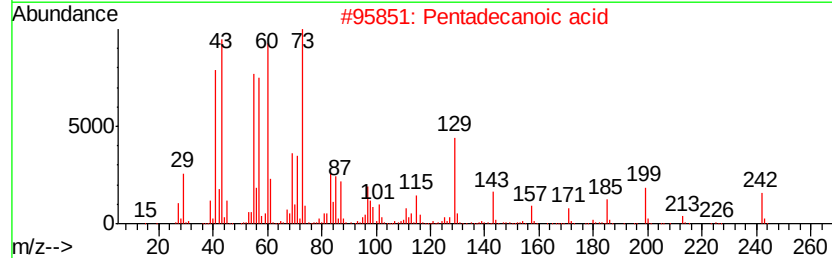
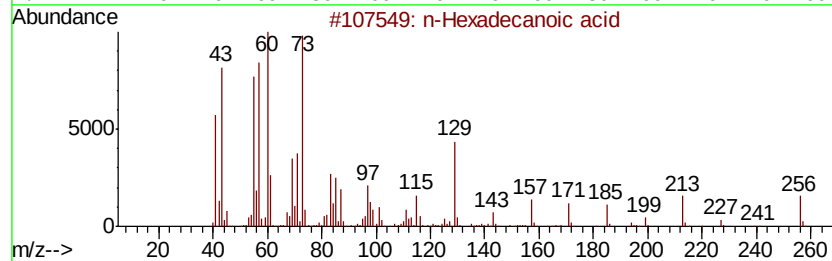
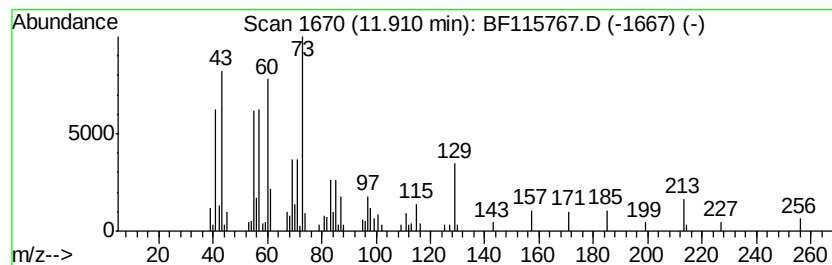
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.14 ng	131934	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



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Misc :
ALS Vial : 10 Sample Multiplier: 1

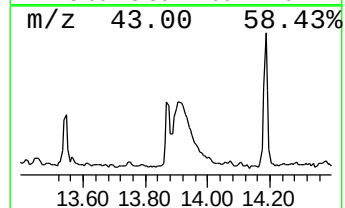
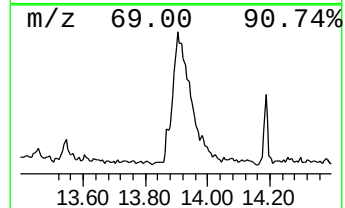
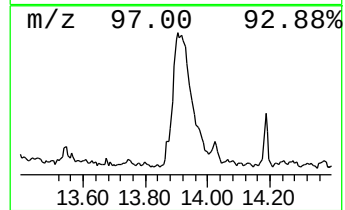
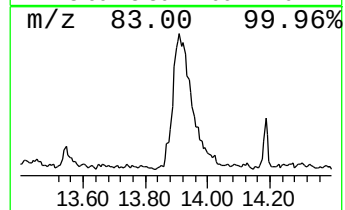
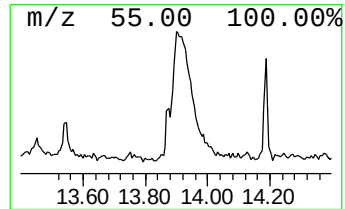
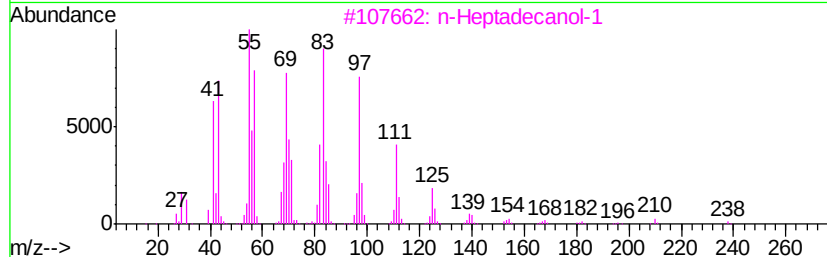
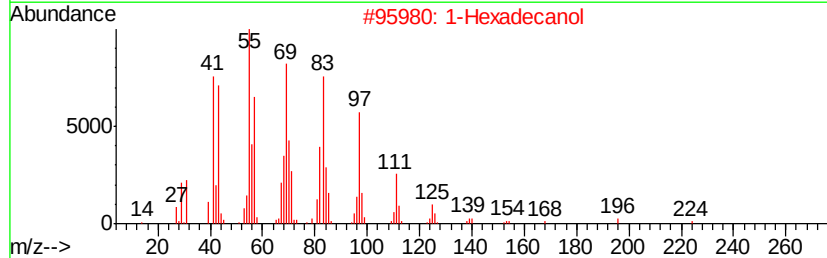
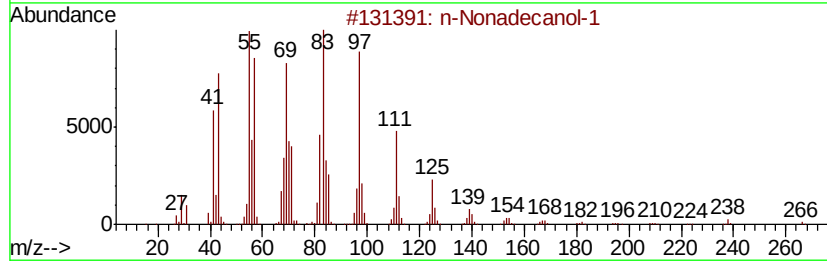
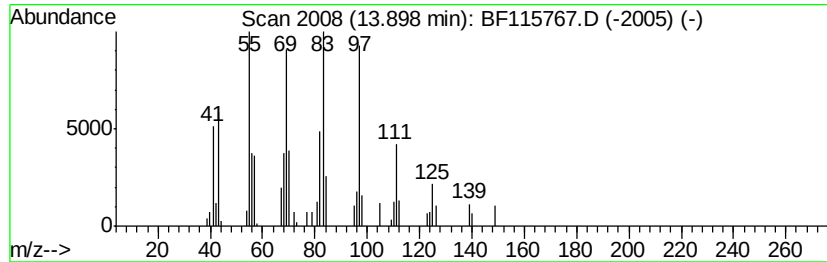
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	6.21 ng	372615	Chrysene-d12	14.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
4	Behenic alcohol	326	C22H46O	000661-19-8	87
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
 Data File : BF115767.D
 Acq On : 25 Jul 2019 19:34
 Operator : HP/JU
 Sample : K3990-10
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

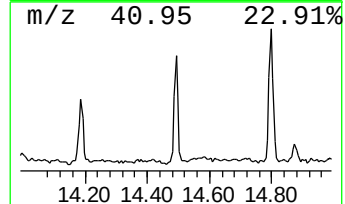
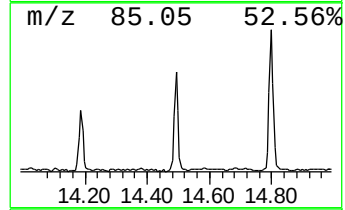
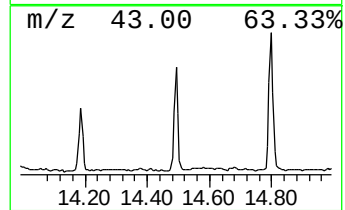
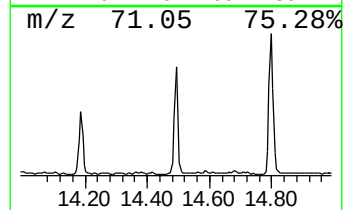
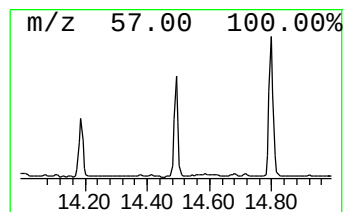
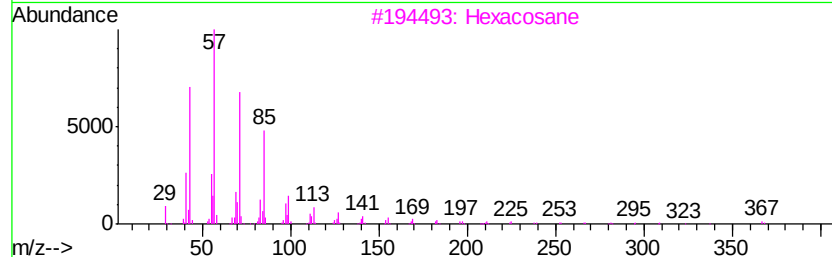
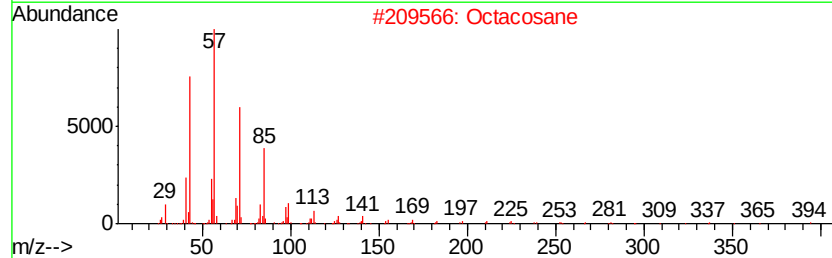
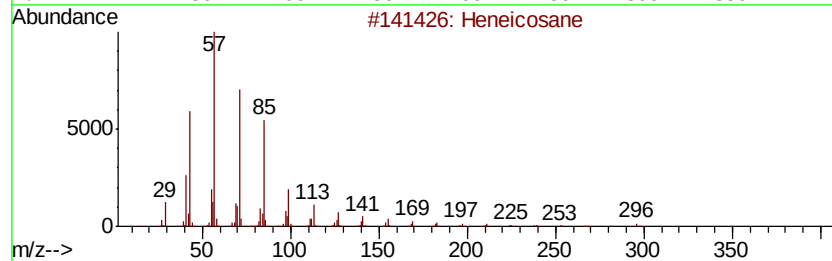
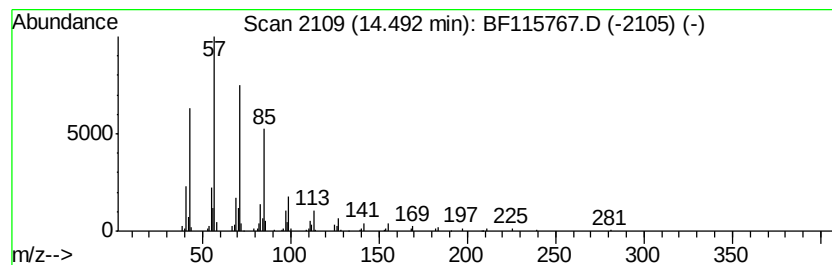
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.49	3.15 ng	188621	Chrysene-d12		14.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
 Data File : BF115767.D
 Acq On : 25 Jul 2019 19:34
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 Sample : K3990-10
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

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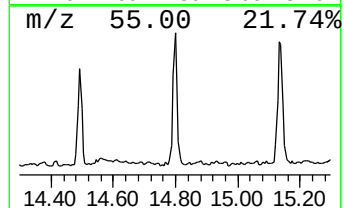
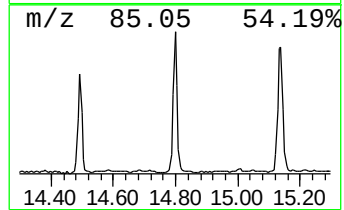
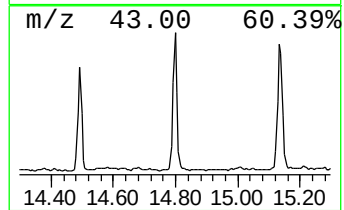
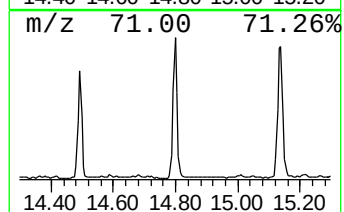
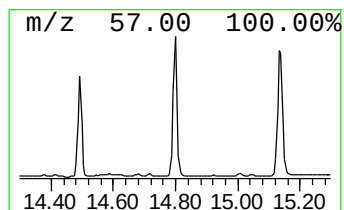
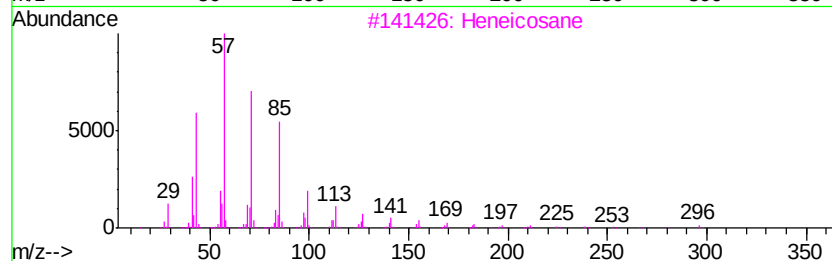
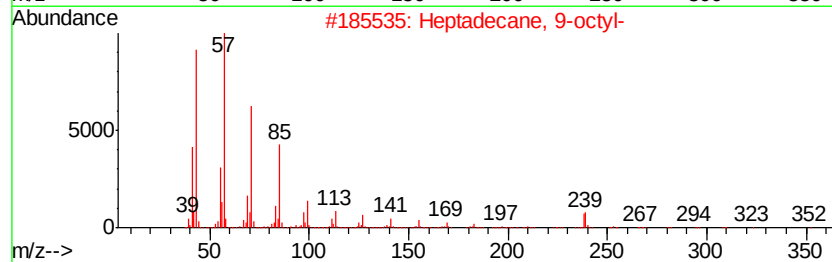
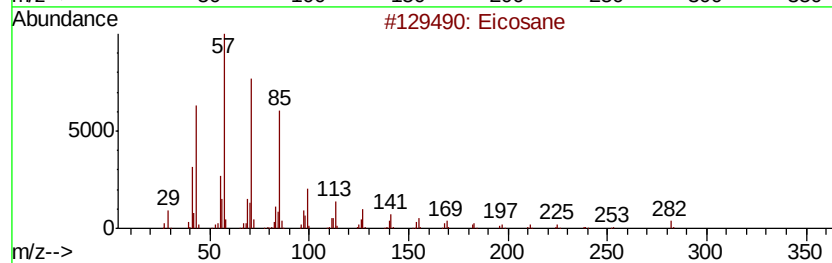
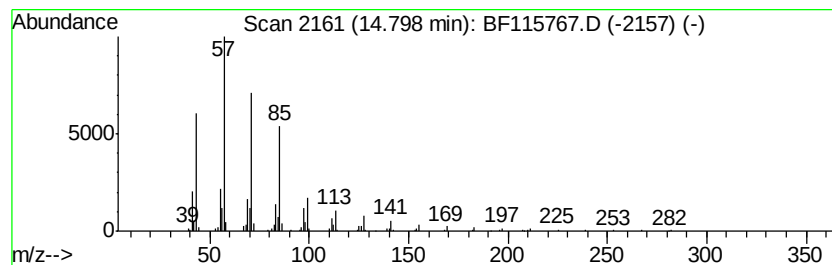
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	3.95 ng	272182	Perylene-d12	15.50

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
Data File : BF115767.D
Acq On : 25 Jul 2019 19:34
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-5-B

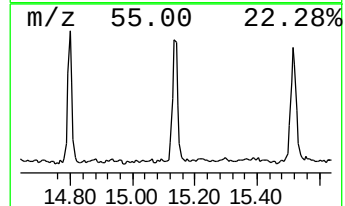
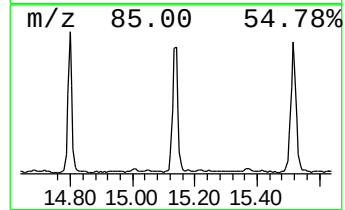
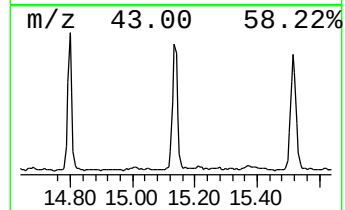
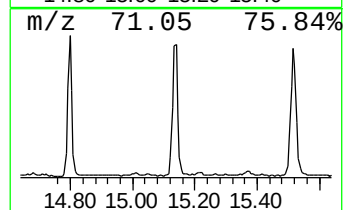
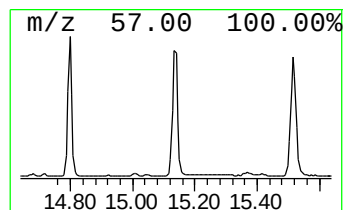
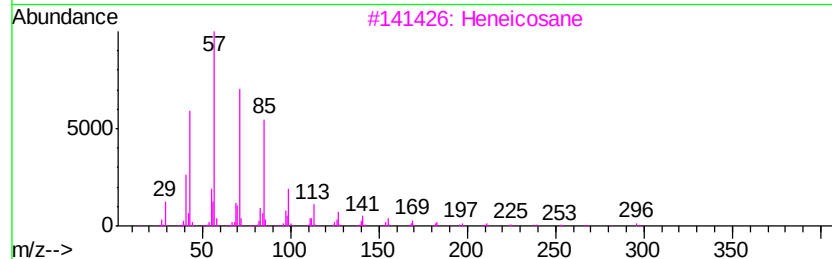
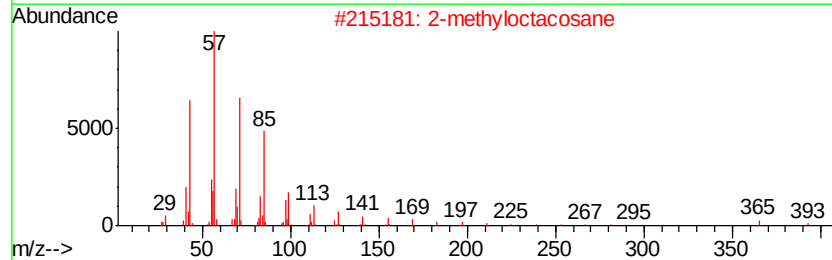
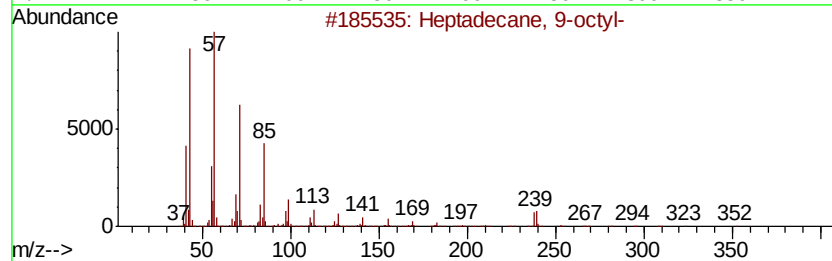
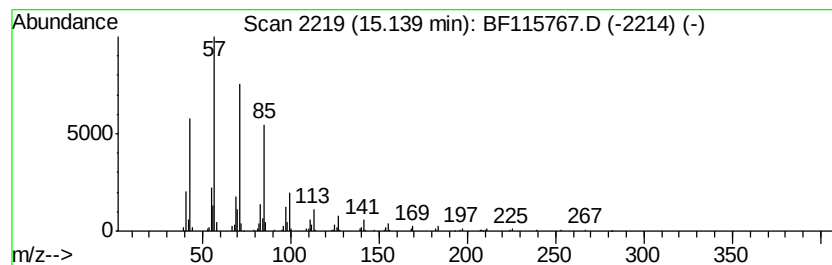
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	4.68 ng	322758	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
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Operator : HP/JU
Sample : K3990-10
Misc :
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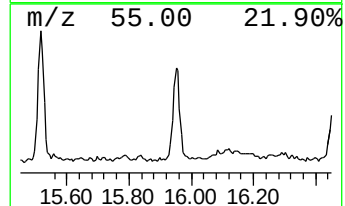
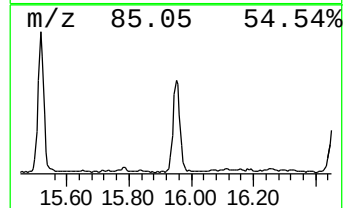
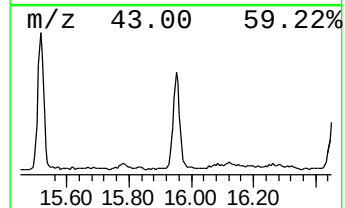
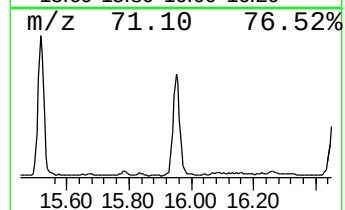
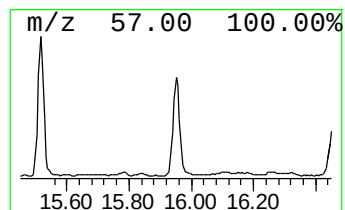
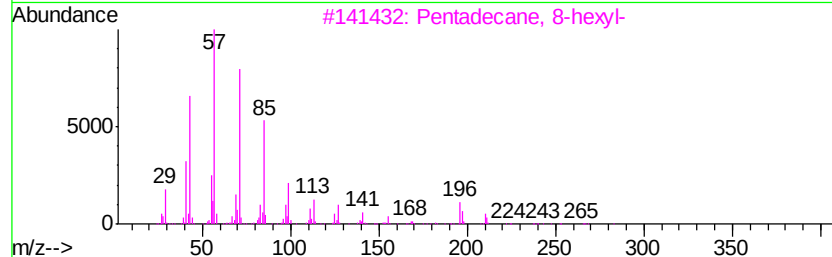
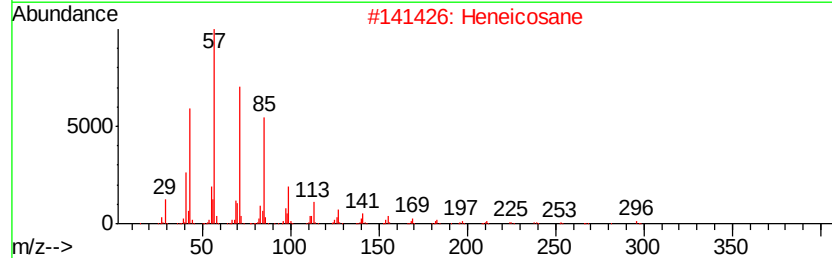
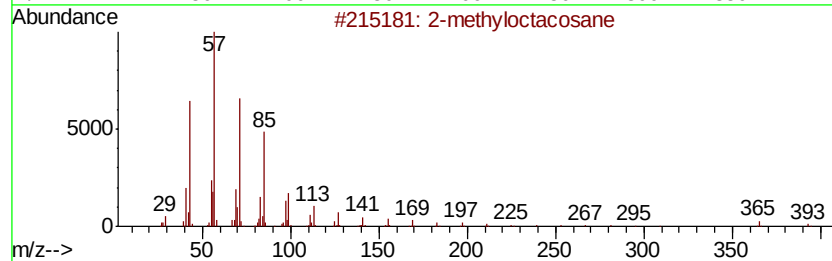
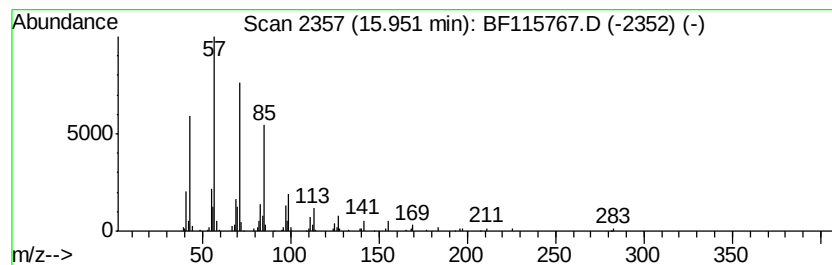
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	4.30 ng	296568	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-methyloctacosane	408 C29H60	1000376-72-8	91
2	Heneicosane	296 C21H44	000629-94-7	91
3	Pentadecane, 8-hexyl-	296 C21H44	013475-75-7	91
4	Octadecane, 1-iodo-	380 C18H37I	000629-93-6	91
5	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
Data File : BF115767.D
Acq On : 25 Jul 2019 19:34
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Sample : K3990-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

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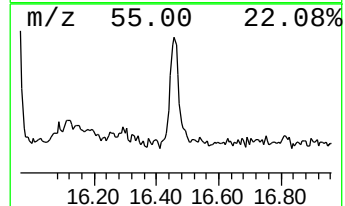
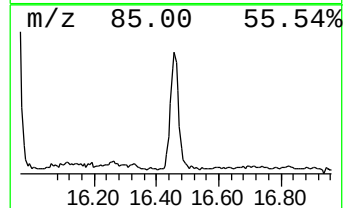
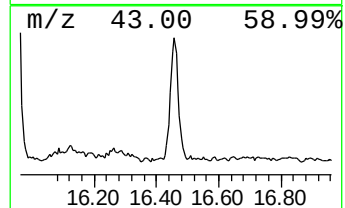
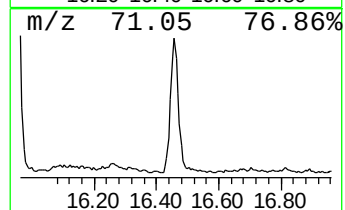
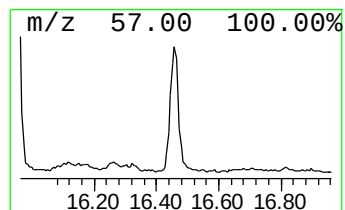
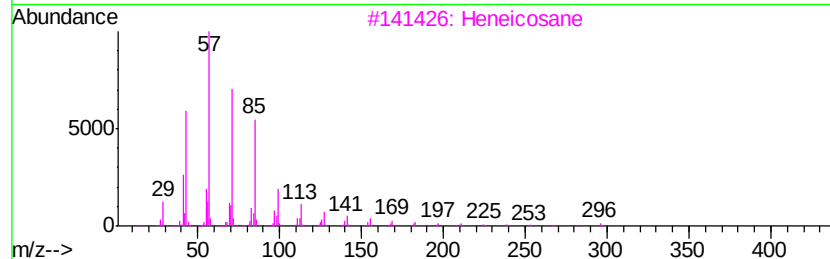
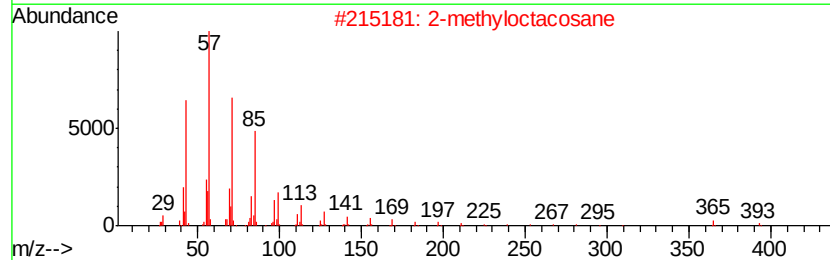
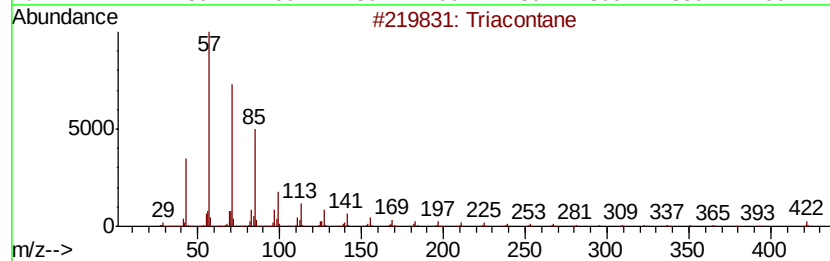
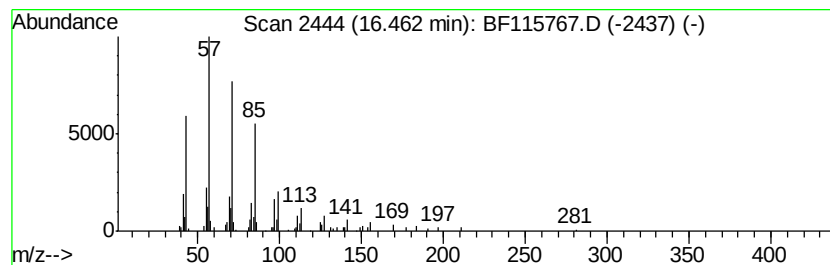
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Triacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.68 ng	184431	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
5		Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072519\
Data File : BF115767.D
Acq On : 25 Jul 2019 19:34
Operator : HP/JU
Sample : K3990-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-5-B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.15	18.5	ng	662608	1	6.87	714719	20.0
2-Pentanone, 4-hy...	5.09	2.1	ng	73592	1	6.87	714719	20.0
unknown6.64	6.64	65.4	ng	2338690	1	6.87	714719	20.0
5-Octadecene, (E)-	11.64	7.6	ng	469642	4	11.39	1232450	20.0
n-Hexadecanoic acid	11.91	2.1	ng	131934	4	11.39	1232450	20.0
n-Nonadecanol-1	13.90	6.2	ng	372615	5	14.03	1199300	20.0
Heneicosane	14.49	3.1	ng	188621	5	14.03	1199300	20.0
Eicosane	14.80	4.0	ng	272182	6	15.50	1378000	20.0
Heptadecane, 9-oc...	15.14	4.7	ng	322758	6	15.50	1378000	20.0
2-methyloctacosane	15.95	4.3	ng	296568	6	15.50	1378000	20.0
Triacontane	16.46	2.7	ng	184431	6	15.50	1378000	20.0