

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111219\
 Data File : BF117757.D
 Acq On : 12 Nov 2019 14:15
 Operator : JU
 Sample : K5785-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-12002-VNJ-221

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-BF110619.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	2.228	19	24	41	rVB	1387783	2108427	32.88%	3.287%
2	5.145	512	520	531	rBV	1021521	1218405	19.00%	1.899%
3	5.545	582	588	591	rBV	5193635	5218483	81.37%	8.135%
4	6.545	753	758	763	rBV	5188976	5657375	88.22%	8.819%
5	6.698	779	784	787	rBV	5583682	5590403	87.17%	8.715%
6	6.928	819	823	826	rBV	2172392	1715151	26.74%	2.674%
7	7.086	846	850	853	rBV	5355504	4461086	69.56%	6.954%
8	7.486	913	918	921	rBV	3817922	3483600	54.32%	5.430%
9	8.216	1038	1042	1045	rBV	2458683	2234884	34.85%	3.484%
10	9.292	1220	1225	1228	rBV	7220370	6413092	100.00%	9.997%
11	9.686	1288	1292	1295	rBV	634313	560093	8.73%	0.873%
12	9.974	1337	1341	1345	rBV	3004880	2594347	40.45%	4.044%
13	10.763	1470	1475	1479	rBV	4119443	4248433	66.25%	6.623%
14	11.468	1591	1595	1598	rBV	3066115	2652173	41.36%	4.134%
15	11.992	1678	1684	1697	rBV	866641	1066530	16.63%	1.663%
16	12.686	1798	1802	1813	rBV	259581	282937	4.41%	0.441%
17	12.774	1813	1817	1826	rBV	326262	432786	6.75%	0.675%
18	12.915	1836	1841	1846	rVB	212333	205123	3.20%	0.320%
19	13.062	1861	1866	1869	rBV	6475259	6115369	95.36%	9.533%
20	13.968	2015	2020	2036	rBV3	350846	785781	12.25%	1.225%
21	14.115	2040	2045	2048	rVV	2273781	2188634	34.13%	3.412%
22	14.139	2048	2049	2056	rVB	100868	93336	1.46%	0.145%
23	14.280	2069	2073	2076	rBV	138900	140174	2.19%	0.219%
24	14.586	2121	2125	2128	rBV	239379	239197	3.73%	0.373%
25	14.909	2176	2180	2184	rVB	302163	309566	4.83%	0.483%
26	14.992	2190	2194	2200	rBV	191795	211668	3.30%	0.330%
27	15.180	2222	2226	2235	rVB	87702	188921	2.95%	0.294%
28	15.262	2236	2240	2249	rBV	303120	405214	6.32%	0.632%
29	15.498	2277	2280	2284	rVB	61184	77789	1.21%	0.121%
30	15.556	2288	2290	2296	rVB	75629	87985	1.37%	0.137%
31	15.627	2297	2302	2306	rBV	1629350	2136515	33.31%	3.330%
32	15.668	2306	2309	2315	rVB	302954	399988	6.24%	0.624%
33	16.133	2383	2388	2394	rBV	215710	342132	5.33%	0.533%
34	16.668	2474	2479	2491	rVB	131994	284813	4.44%	0.444%

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Instrument :
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ClientSampleId :
72-12002-VNJ-221

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-BF110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

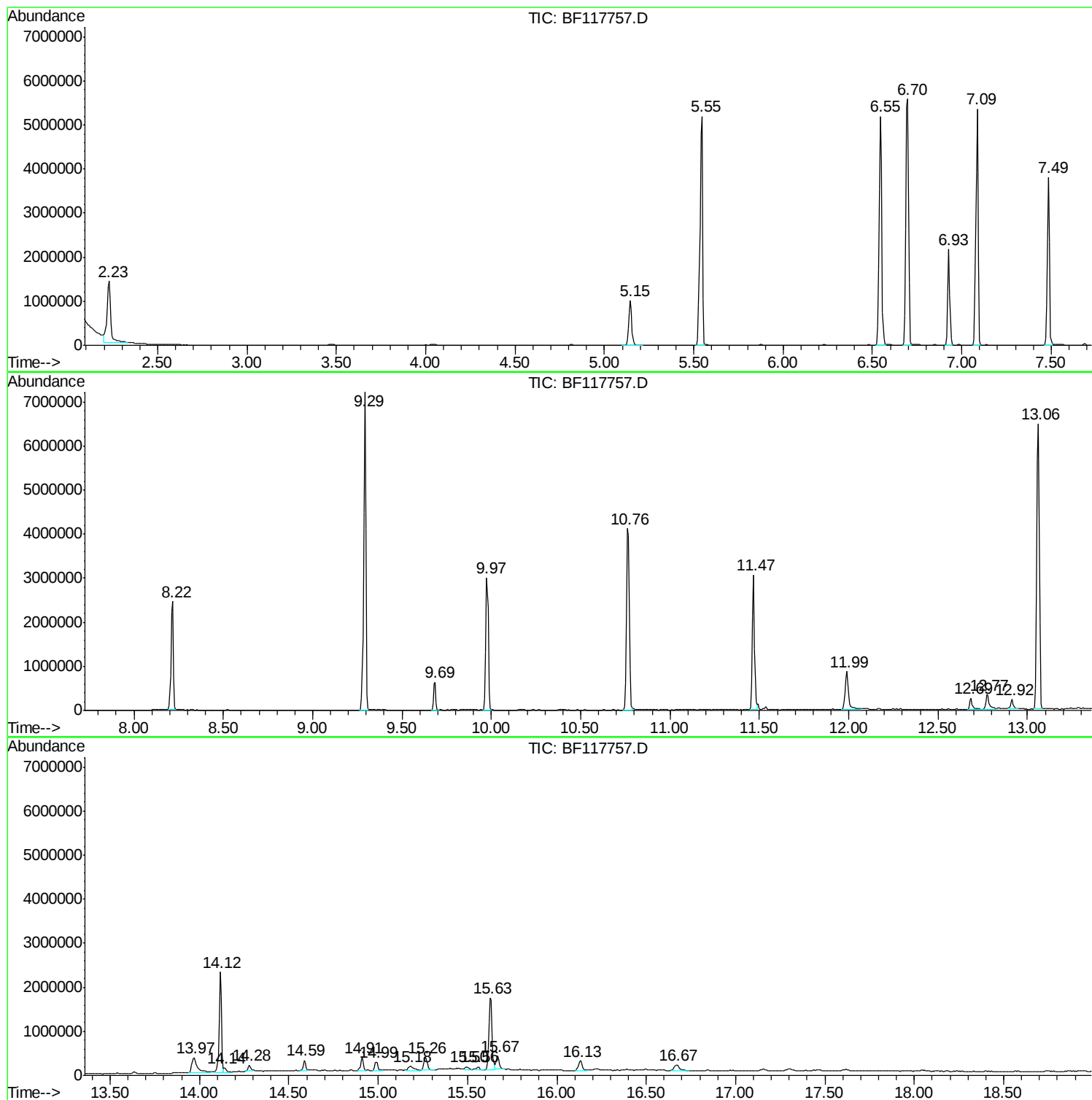
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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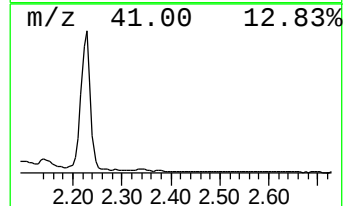
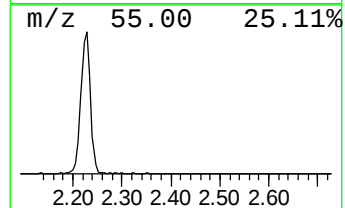
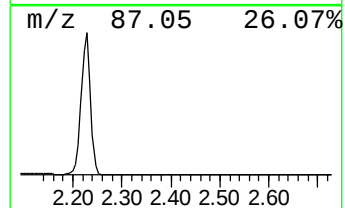
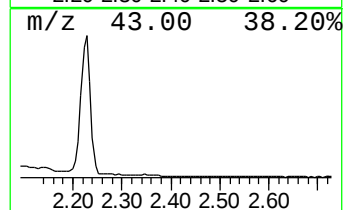
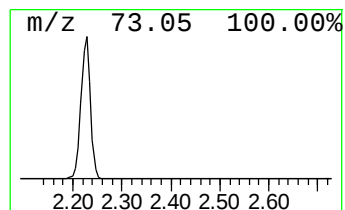
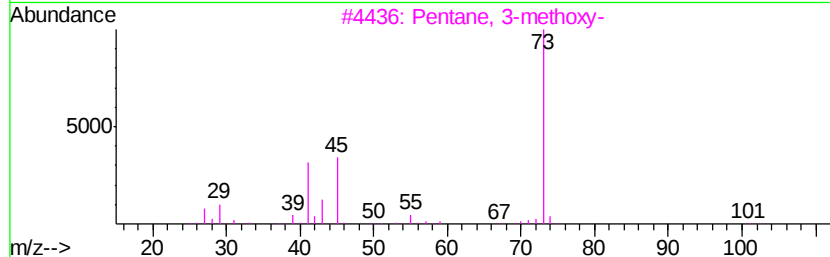
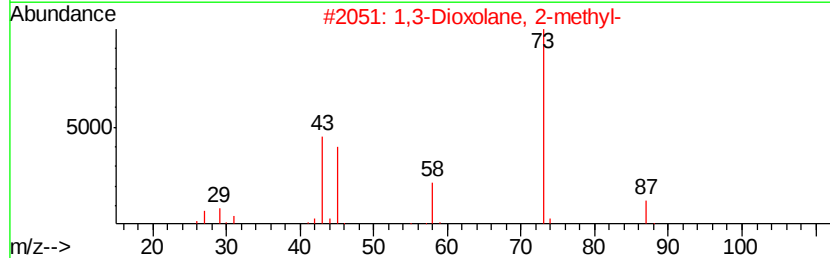
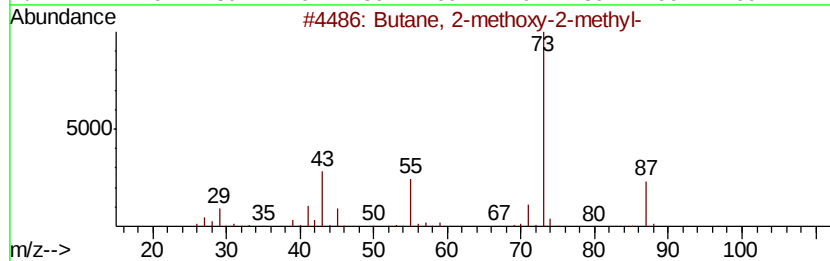
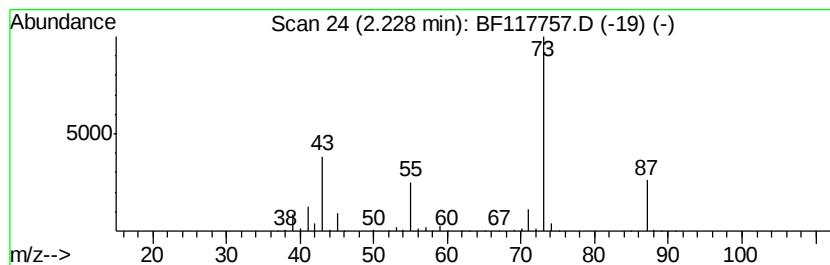
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	24.59 ng	2108430	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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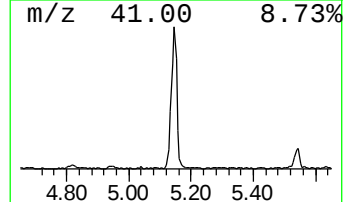
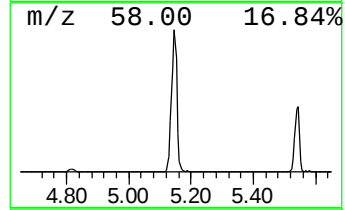
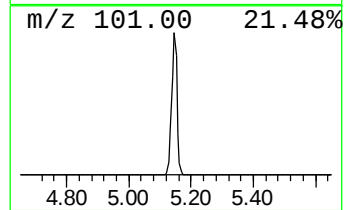
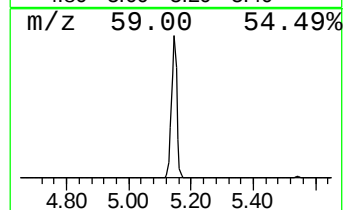
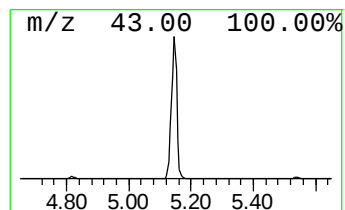
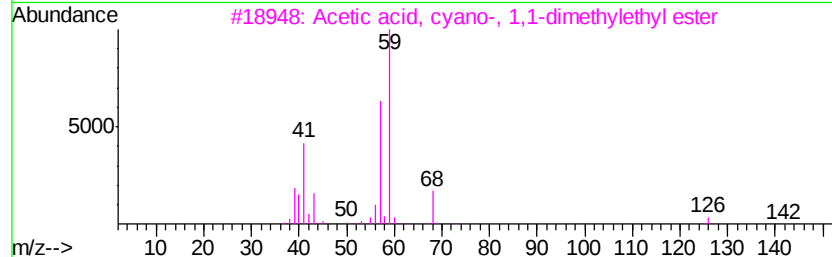
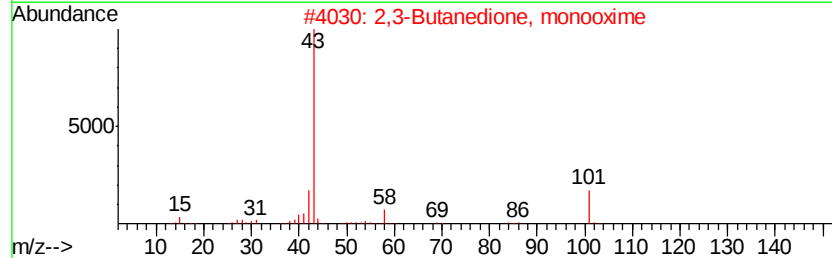
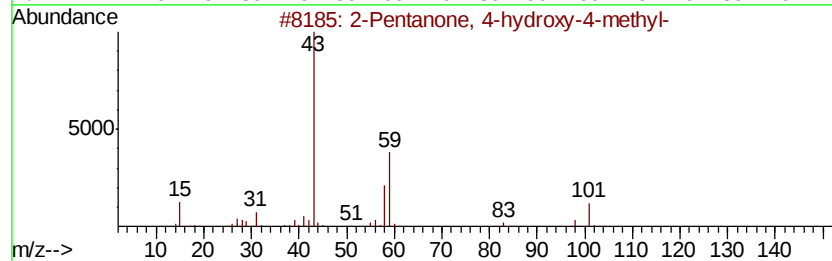
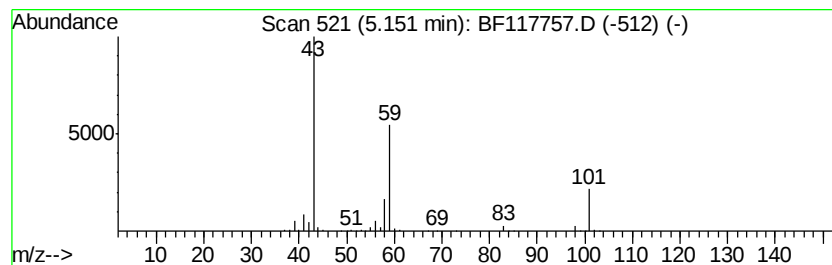
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	14.21 ng	1218410	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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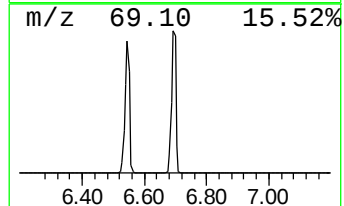
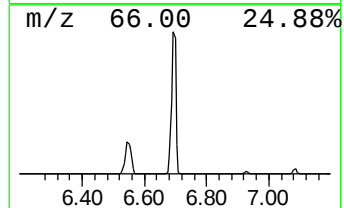
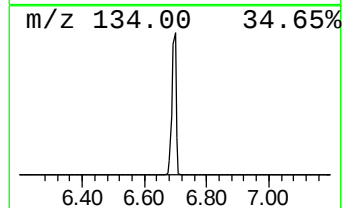
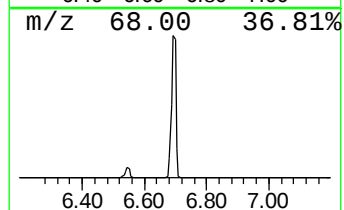
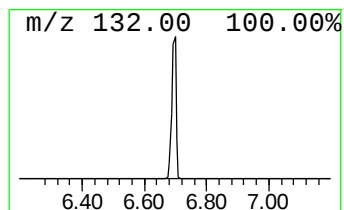
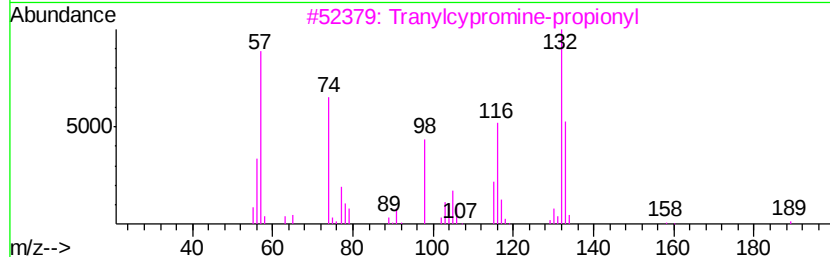
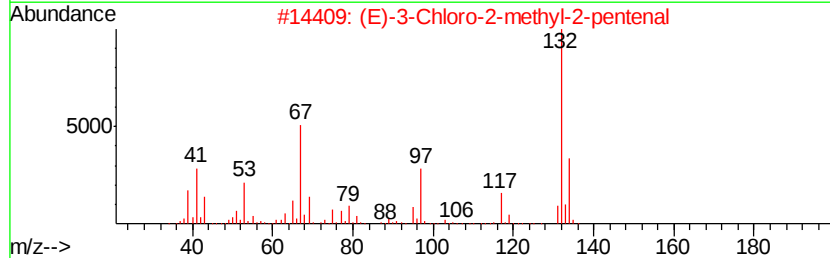
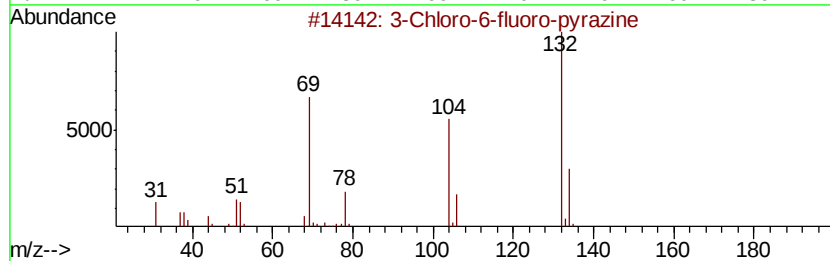
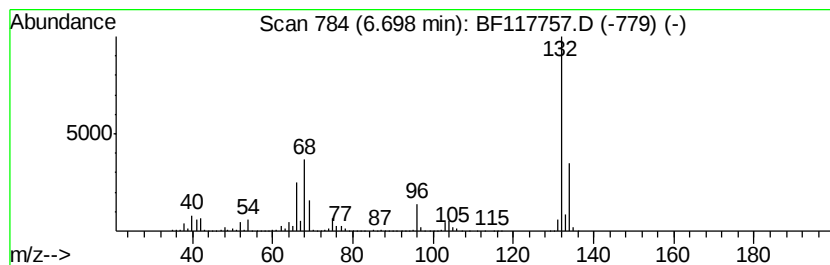
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	65.19 ng	5590400	1,4-Dichlorobenzene-d4	6.93

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	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9



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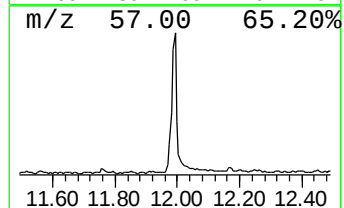
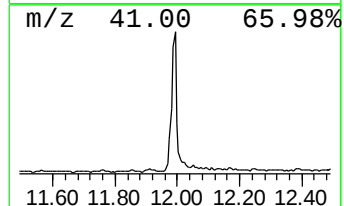
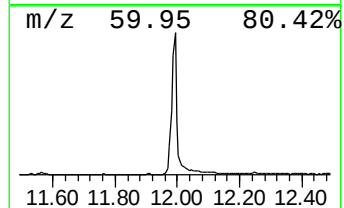
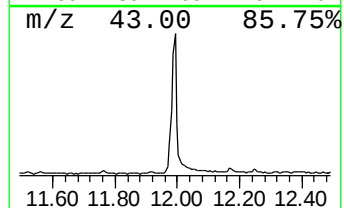
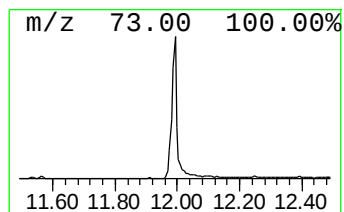
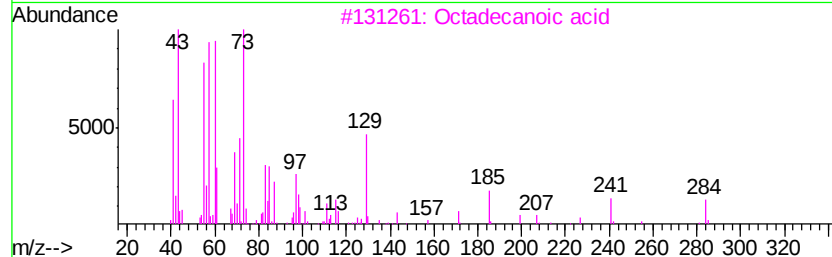
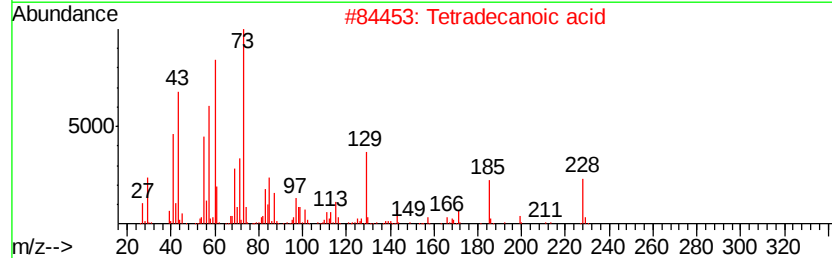
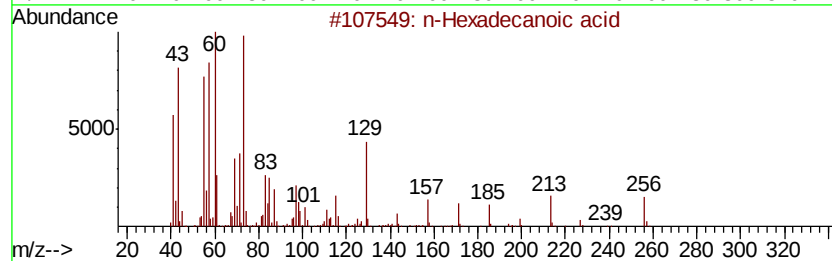
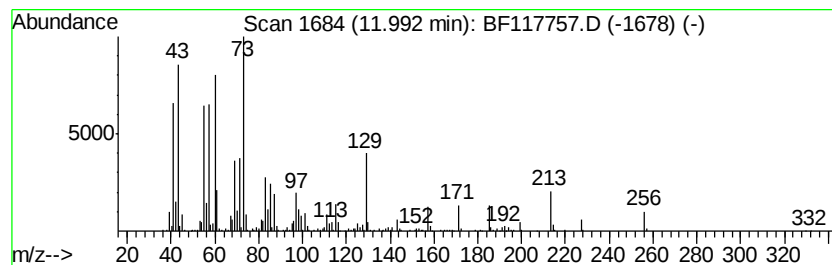
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.99	8.04 ng	1066530	Phenanthrene-d10		11.47
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Tridecanoic acid	214	C13H26O2	000638-53-9	90



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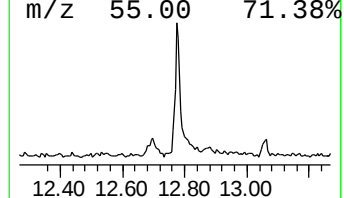
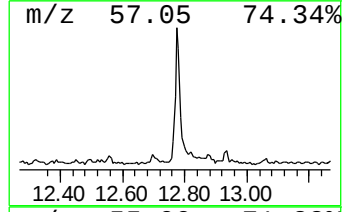
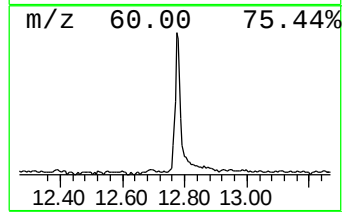
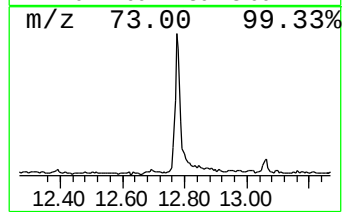
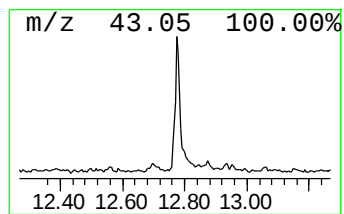
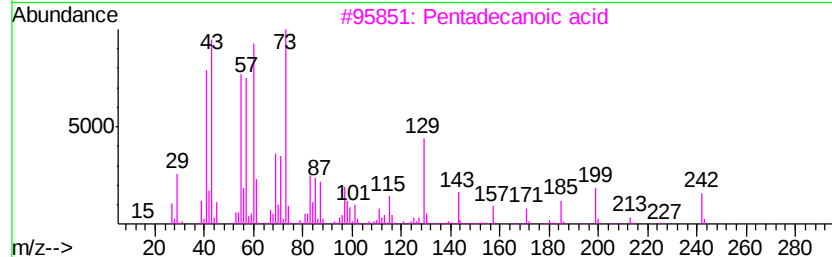
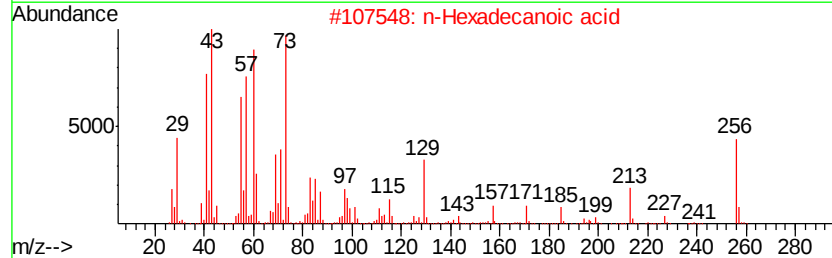
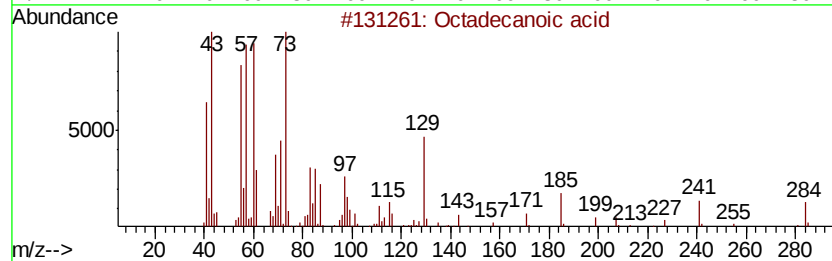
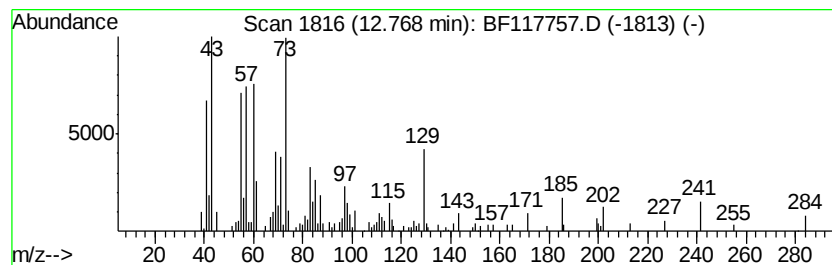
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	3.26 ng	432786	Phenanthrene-d10	11.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111219\
Data File : BF117757.D
Acq On : 12 Nov 2019 14:15
Operator : JU
Sample : K5785-01
Misc :
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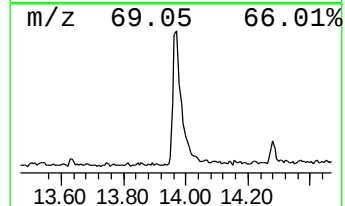
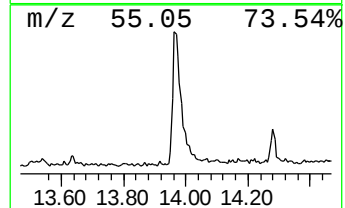
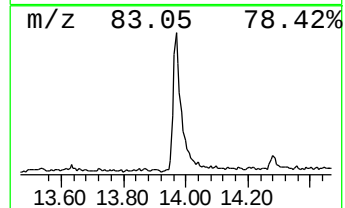
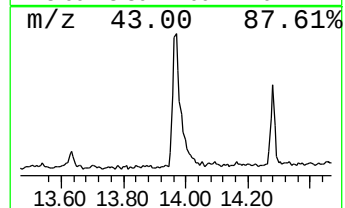
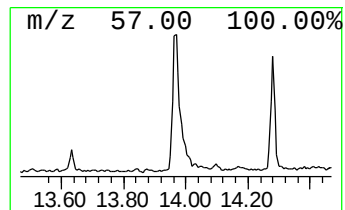
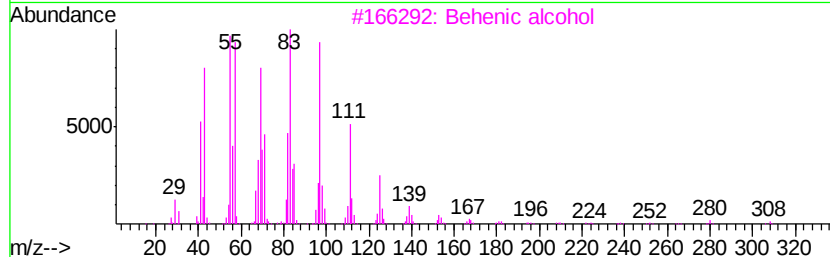
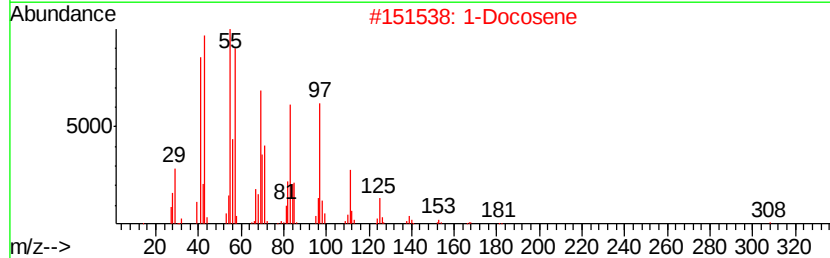
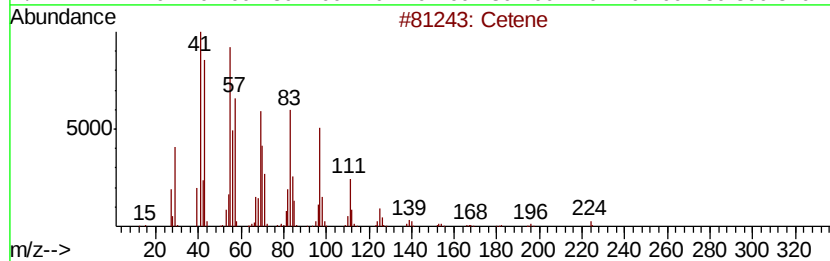
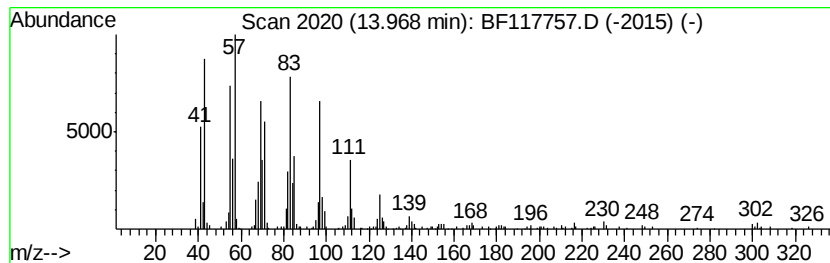
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ClientSampleId :
72-12002-VNJ-221

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cetene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	7.18 ng	785781	Chrysene-d12	14.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cetene	224 C16H32	000629-73-2	95
2	1-Docosene	308 C22H44	001599-67-3	95
3	Behenic alcohol	326 C22H46O	000661-19-8	93
4	Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2	93
5	n-Tetracosanol-1	354 C24H50O	000506-51-4	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111219\
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Acq On : 12 Nov 2019 14:15
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Sample : K5785-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

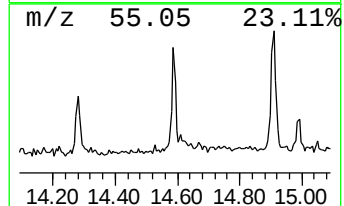
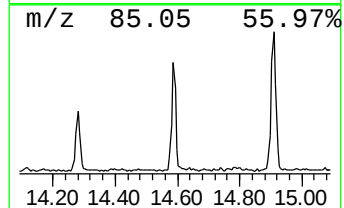
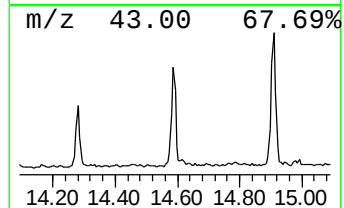
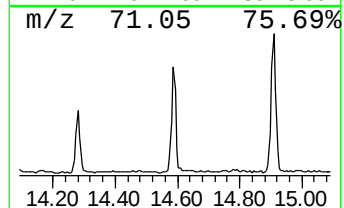
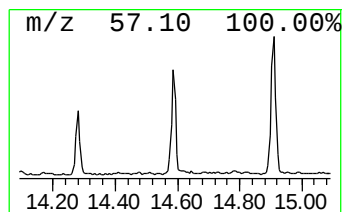
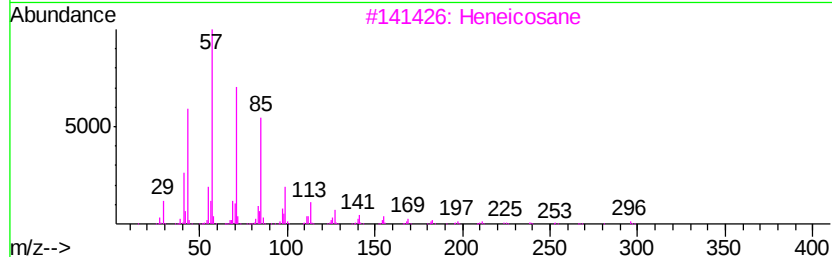
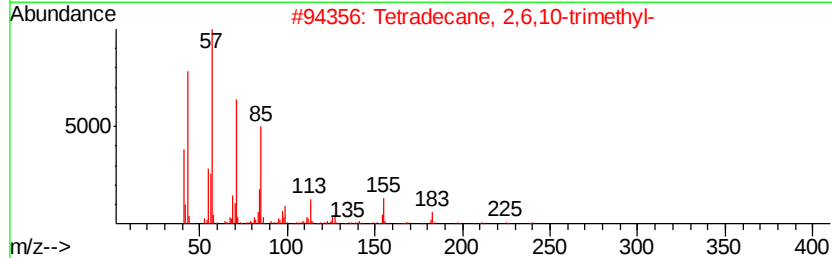
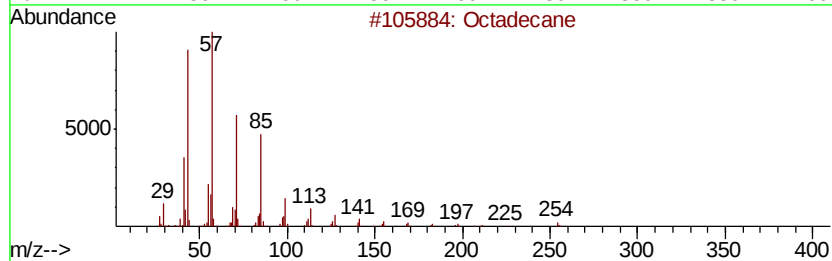
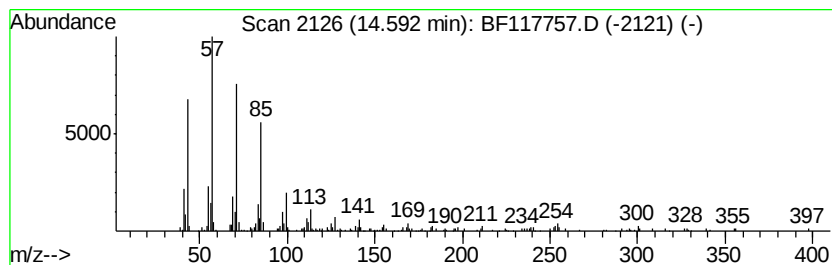
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.19 ng	239197	Chrysene-d12	14.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	94
2	Tetradecane, 2,6,10-trimethyl-	240 C17H36	014905-56-7	93
3	Heneicosane	296 C21H44	000629-94-7	90
4	Heptadecane	240 C17H36	000629-78-7	87
5	Hexacosane	366 C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111219\
Data File : BF117757.D
Acq On : 12 Nov 2019 14:15
Operator : JU
Sample : K5785-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12002-VNJ-221

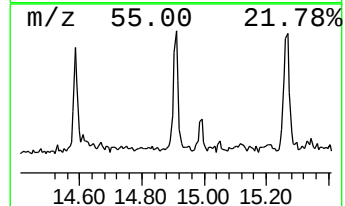
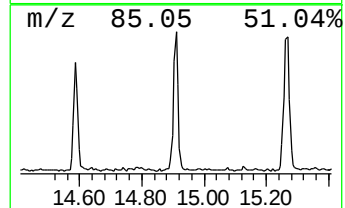
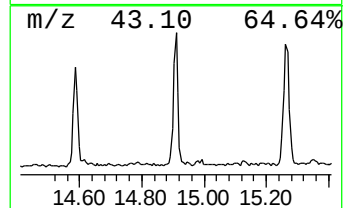
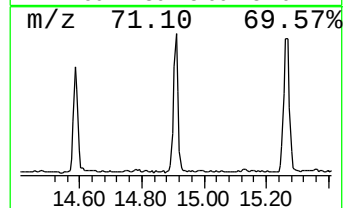
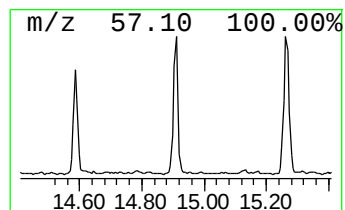
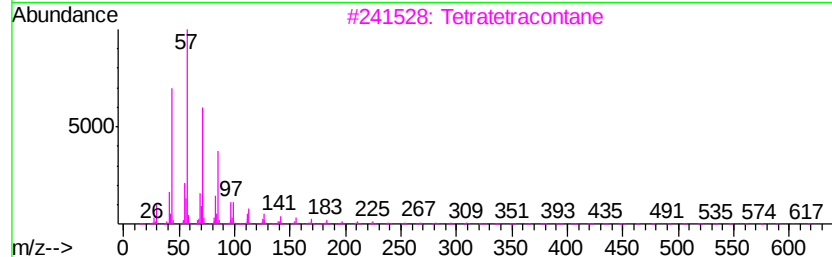
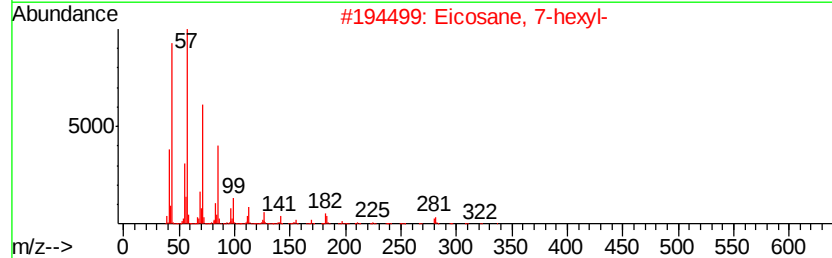
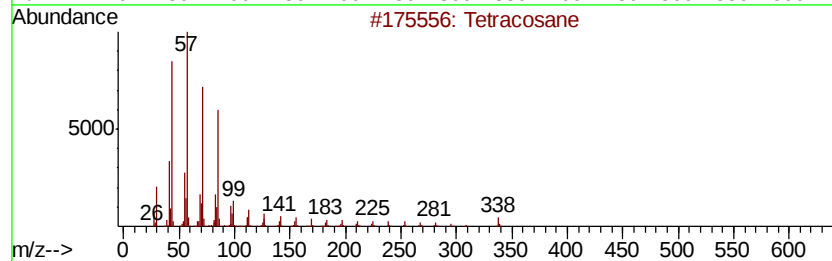
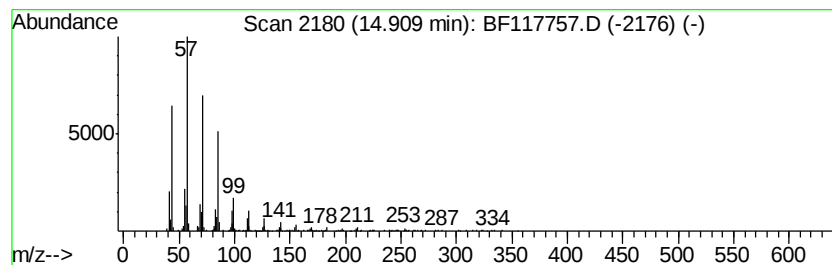
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	2.90 ng	309566	Perylene-d12	15.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3			Tetratetracontane	619	C44H90	007098-22-8	87
4			Heneicosane	296	C21H44	000629-94-7	87
5			Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111219\
Data File : BF117757.D
Acq On : 12 Nov 2019 14:15
Operator : JU
Sample : K5785-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

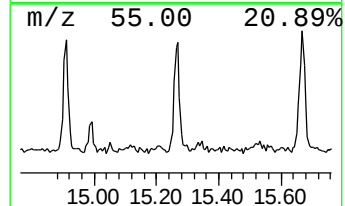
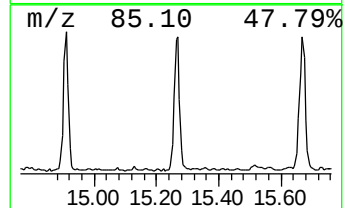
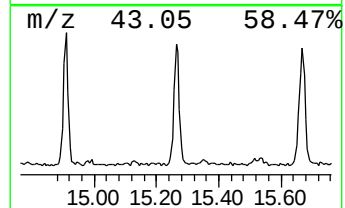
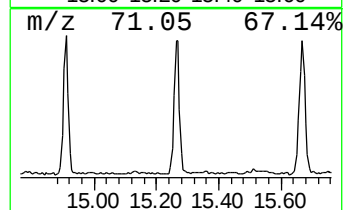
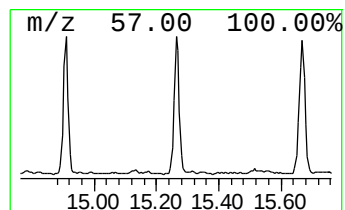
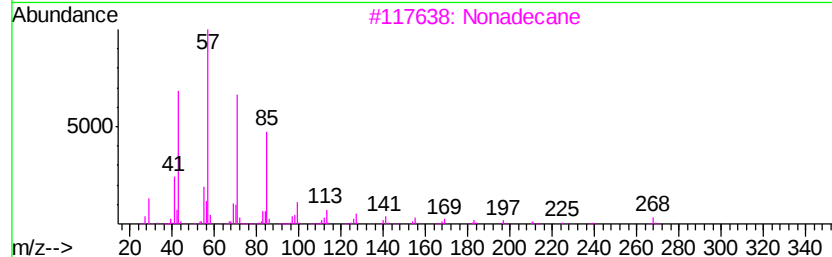
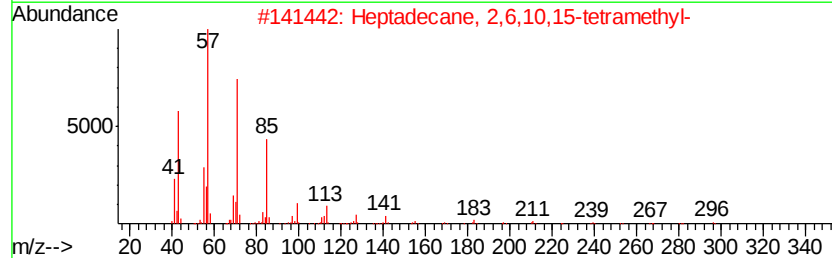
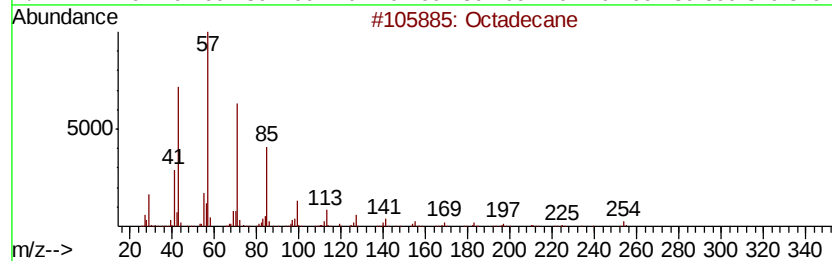
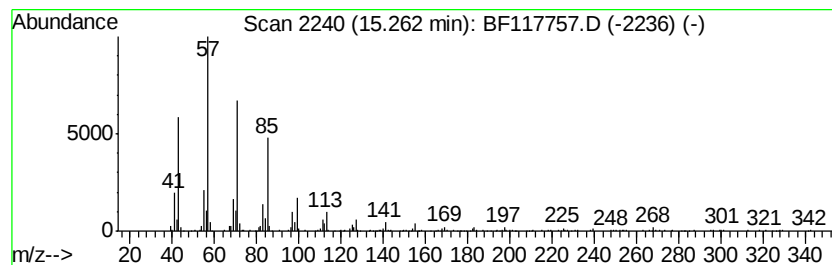
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.26	3.79 ng	405214	Perylene-d12	15.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	94
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Nonadecane	268	C19H40	000629-92-5	93
4	Hexacosane	366	C26H54	000630-01-3	91
5	Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111219\
Data File : BF117757.D
Acq On : 12 Nov 2019 14:15
Operator : JU
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ClientSampleId :
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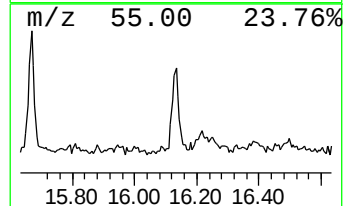
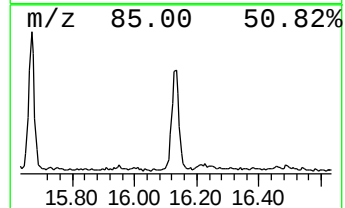
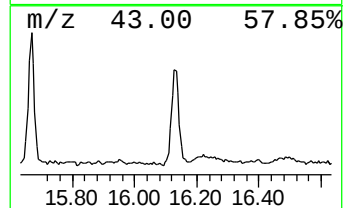
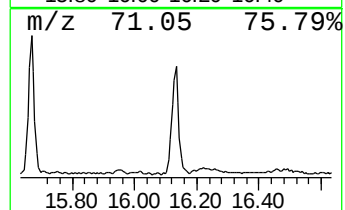
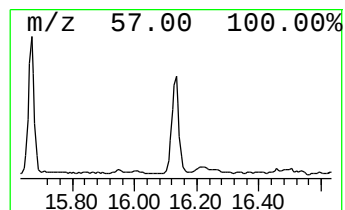
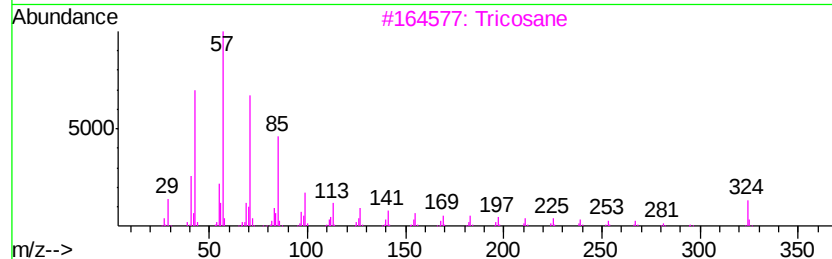
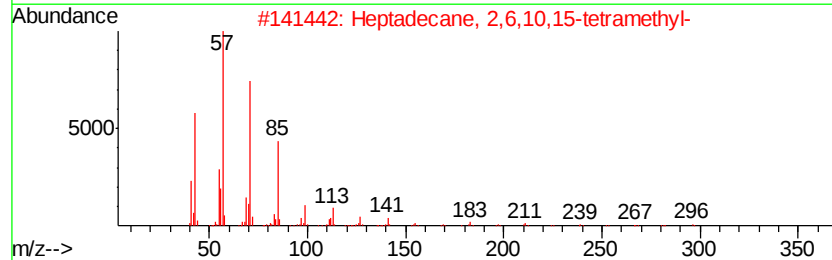
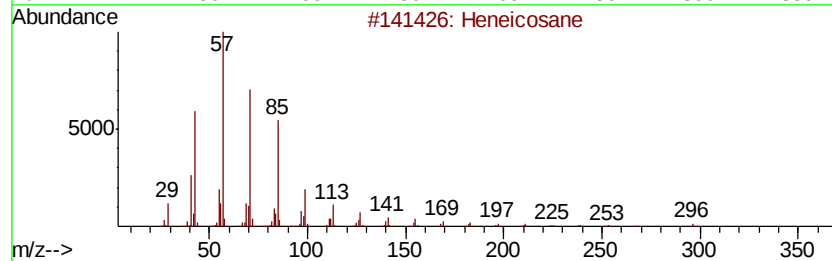
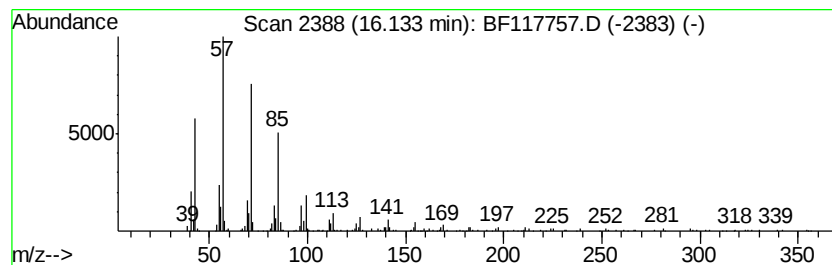
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	3.20 ng	342132	Perylene-d12	15.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	97
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3		Tricosane	324	C23H48	000638-67-5	93
4		Heptacosane	380	C27H56	000593-49-7	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111219\
Data File : BF117757.D
Acq On : 12 Nov 2019 14:15
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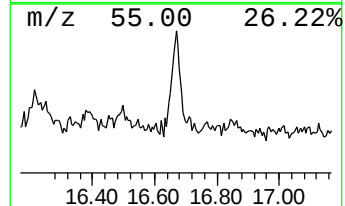
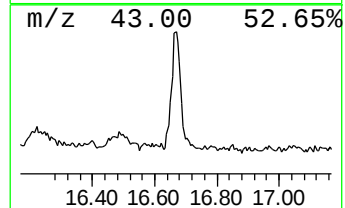
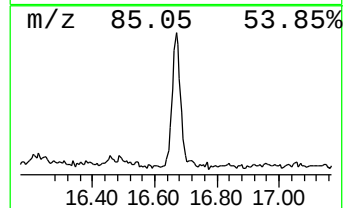
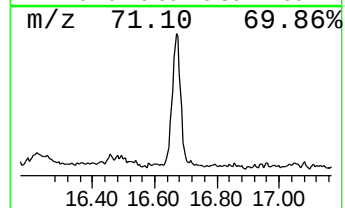
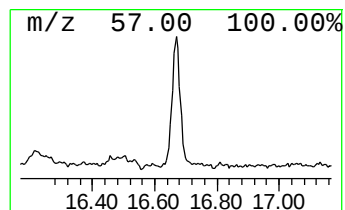
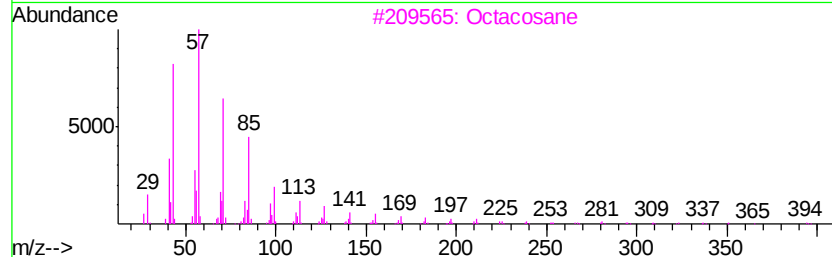
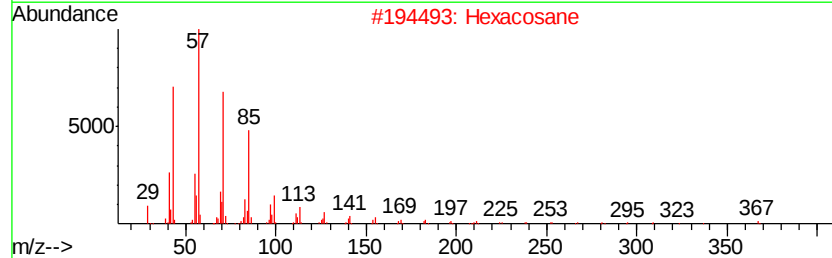
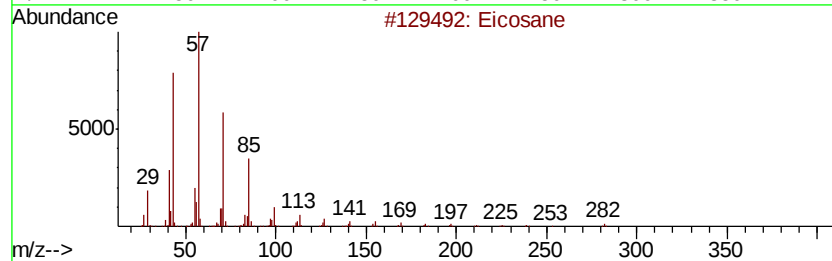
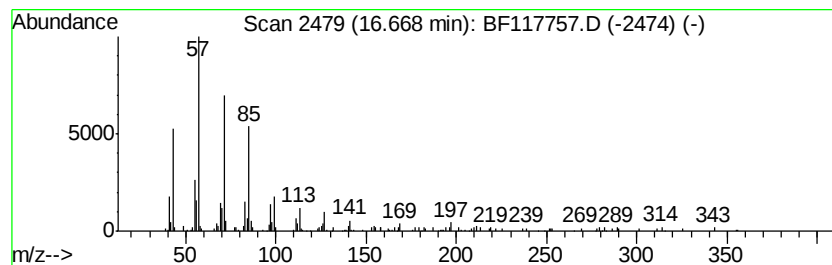
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	2.67 ng	284813	Perylene-d12	15.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hentriacontane	437	C31H64	000630-04-6	91
5		Docosane, 7-hexyl-	394	C28H58	055373-86-9	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111219\
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 Acq On : 12 Nov 2019 14:15
 Operator : JU
 Sample : K5785-01
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.15	14.2	ng	1218410	1	6.93	1715150	20.0
unknown6.70	6.70	65.2	ng	5590400	1	6.93	1715150	20.0
n-Hexadecanoic acid	11.99	8.0	ng	1066530	4	11.47	2652170	20.0
Octadecanoic acid	12.77	3.3	ng	432786	4	11.47	2652170	20.0
Cetene	13.97	7.2	ng	785781	5	14.12	2188630	20.0
Octadecane	14.59	2.2	ng	239197	5	14.12	2188630	20.0
Tetracosane	14.91	2.9	ng	309566	6	15.63	2136520	20.0
Heptadecane, 2,6,...	15.26	3.8	ng	405214	6	15.63	2136520	20.0
Heneicosane	16.13	3.2	ng	342132	6	15.63	2136520	20.0
Eicosane	16.67	2.7	ng	284813	6	15.63	2136520	20.0