

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102518\
 Data File : BF110165.D
 Acq On : 25 Oct 2018 17:27
 Operator : JU/SJ
 Sample : J5636-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HP-GRID-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-BF102318.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.322	35	40	46	rVB	309252	418726	16.87%	1.578%
2	3.599	255	257	274	rBV	18259	53296	2.15%	0.201%
3	5.204	526	530	537	rBV	89261	109276	4.40%	0.412%
4	5.587	590	595	598	rBV	2448475	2263785	91.22%	8.532%
5	6.587	759	765	777	rBV	2382819	2479256	99.90%	9.344%
6	6.734	785	790	793	rBV	2716215	2423469	97.66%	9.133%
7	6.963	825	829	833	rBV	1096924	896709	36.13%	3.379%
8	7.122	852	856	859	rBV	2122140	1799614	72.52%	6.782%
9	7.528	919	925	928	rBV	1541613	1499853	60.44%	5.653%
10	8.245	1043	1047	1051	rBV	1256761	1206904	48.63%	4.548%
11	9.322	1225	1230	1233	rBV	2966020	2481639	100.00%	9.353%
12	9.710	1292	1296	1304	rVB	265557	237286	9.56%	0.894%
13	10.010	1342	1347	1350	rBV	1501092	1376934	55.48%	5.189%
14	10.798	1477	1481	1494	rVB	1706176	1482541	59.74%	5.587%
15	11.498	1596	1600	1603	rBV	1510555	1345671	54.23%	5.071%
16	11.522	1603	1604	1608	rVV	106782	65489	2.64%	0.247%
17	11.575	1608	1613	1618	rVB2	27340	33666	1.36%	0.127%
18	12.004	1683	1686	1689	rBV2	57966	58463	2.36%	0.220%
19	12.716	1803	1807	1812	rBV	77694	65158	2.63%	0.246%
20	12.945	1843	1846	1848	rBV2	123533	112019	4.51%	0.422%
21	13.080	1865	1869	1873	rBV	2188673	1957749	78.89%	7.378%
22	13.298	1903	1906	1910	rVB	46369	38810	1.56%	0.146%
23	13.639	1960	1964	1967	rBV2	64150	61214	2.47%	0.231%
24	13.969	2014	2020	2024	rBV2	167073	195184	7.87%	0.736%
25	14.004	2024	2026	2031	rVB	64264	59262	2.39%	0.223%
26	14.145	2046	2050	2053	rBV	1031610	878913	35.42%	3.312%
27	14.286	2070	2074	2082	rVB	113411	112258	4.52%	0.423%
28	14.592	2122	2126	2129	rBV	170134	157253	6.34%	0.593%
29	14.910	2176	2180	2186	rBV	263557	273911	11.04%	1.032%
30	15.268	2235	2241	2249	rVB	310730	410074	16.52%	1.545%
31	15.539	2284	2287	2292	rVB4	19278	28594	1.15%	0.108%
32	15.668	2303	2309	2316	rBV2	873190	1193304	48.09%	4.497%
33	16.127	2381	2387	2394	rBV	238239	396344	15.97%	1.494%
34	16.662	2473	2478	2485	rVB	123774	223324	9.00%	0.842%

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

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.304	2580	2587	2592	rvB4	39453	87889	3.54%	0.331%
36	18.045	2710	2713	2722	rvB8	21681	50471	2.03%	0.190%

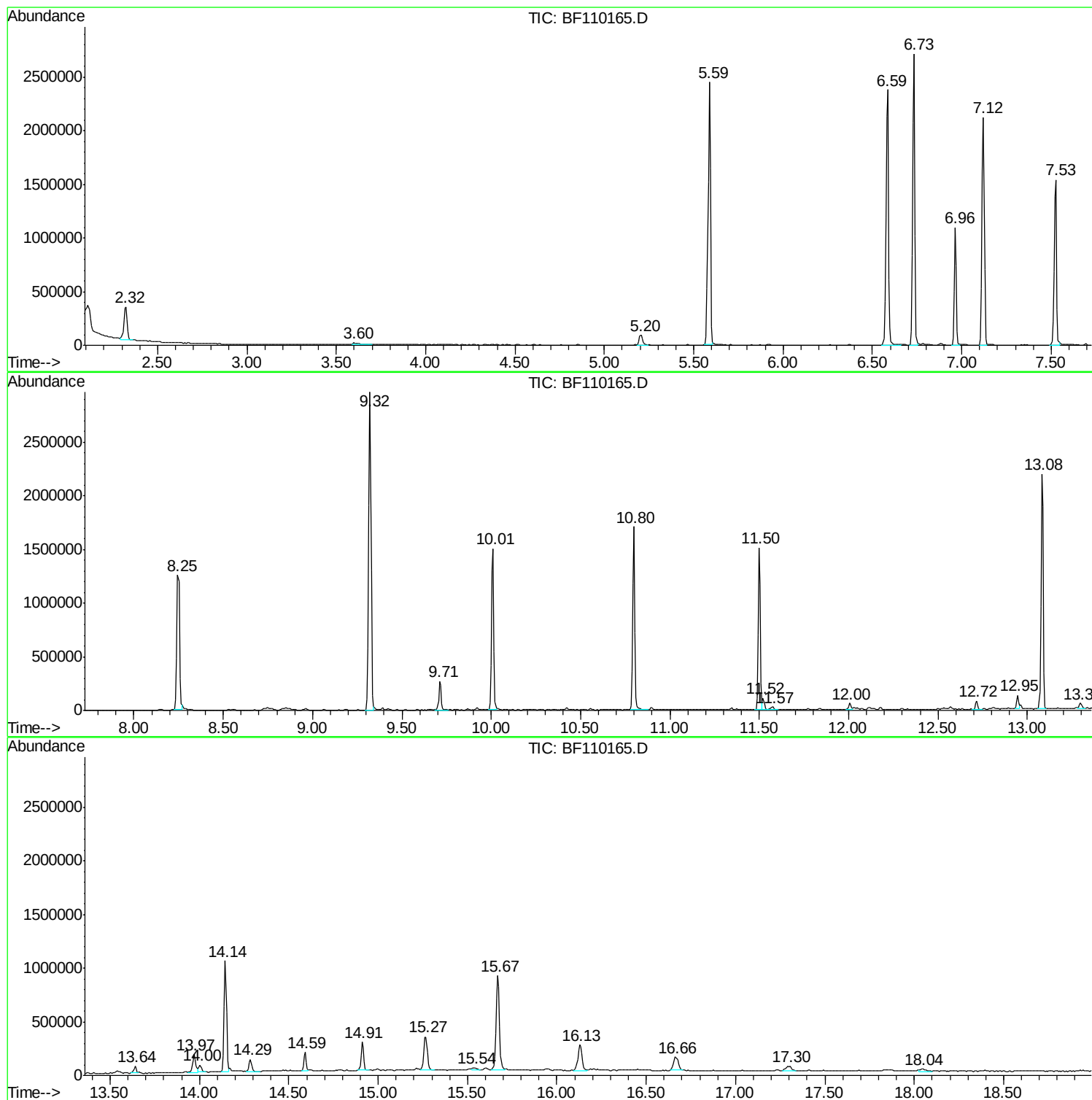
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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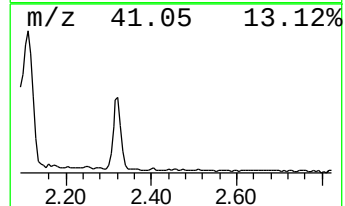
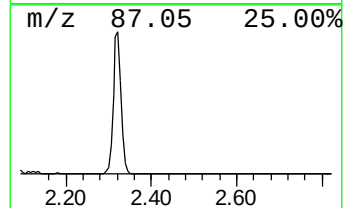
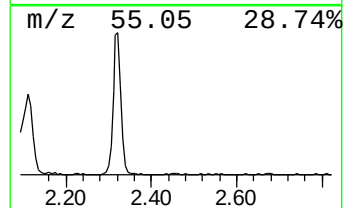
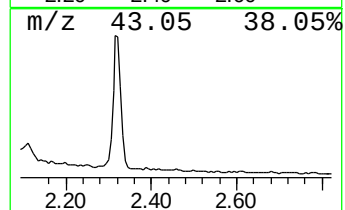
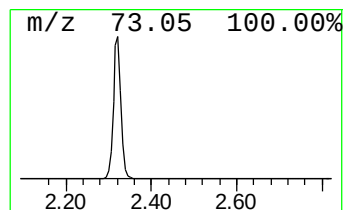
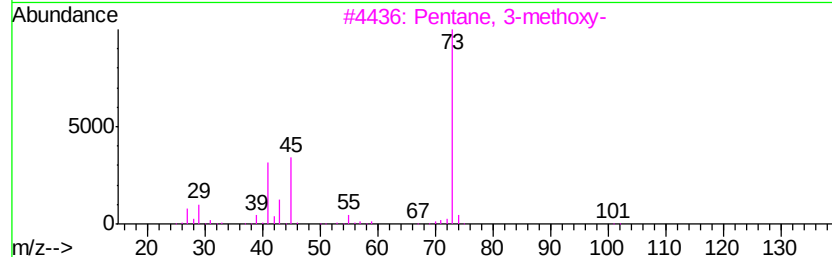
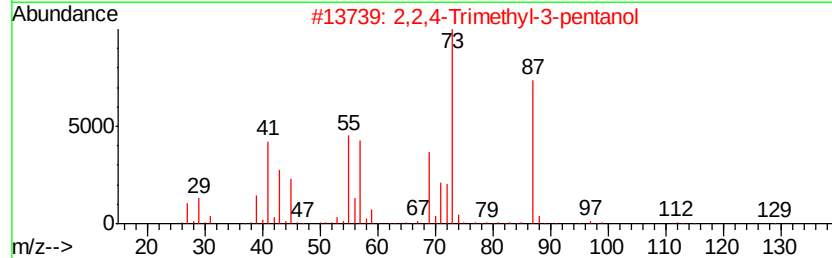
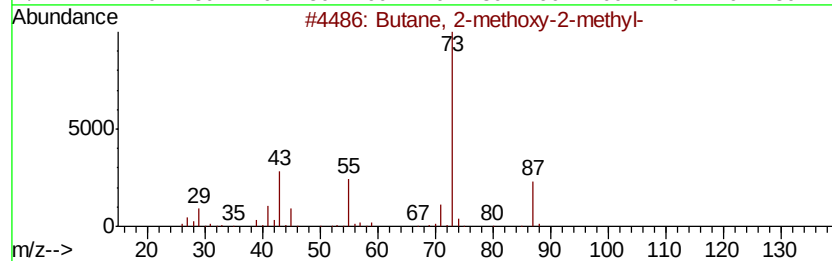
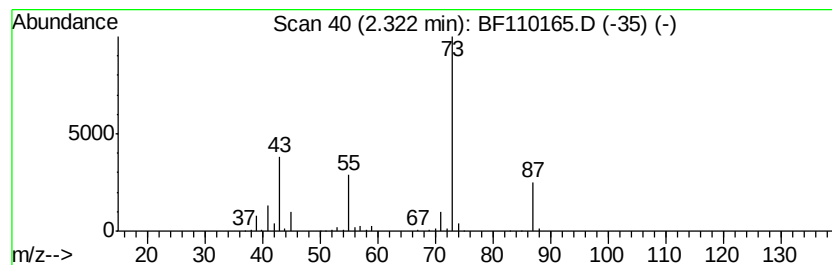
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.32	9.34 ng	418726	1,4-Dichlorobenzene-d4	6.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	12
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9



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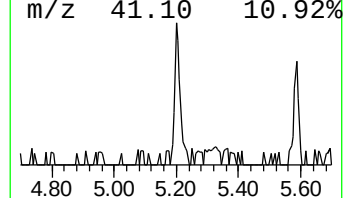
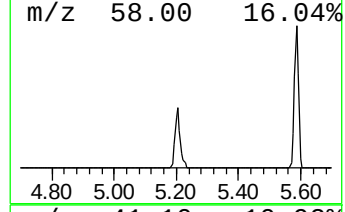
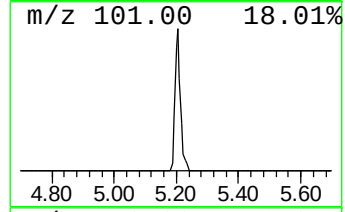
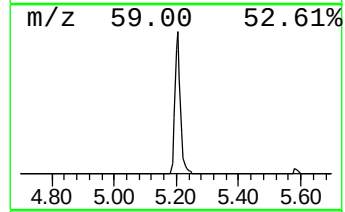
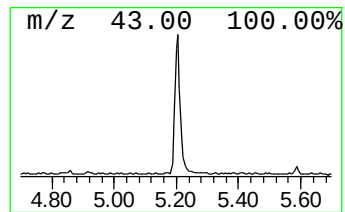
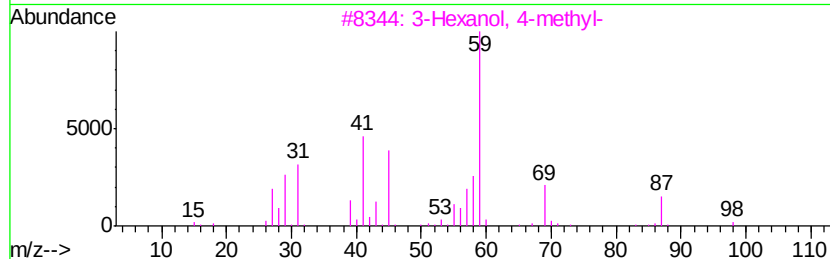
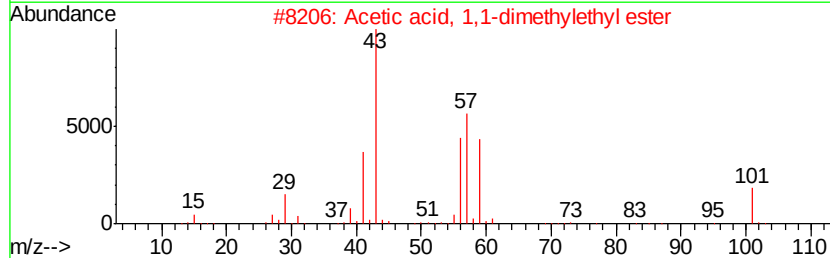
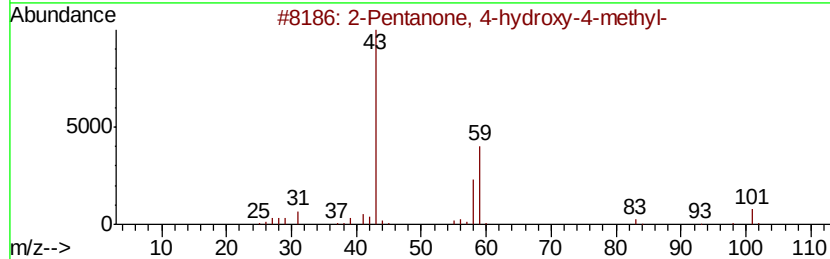
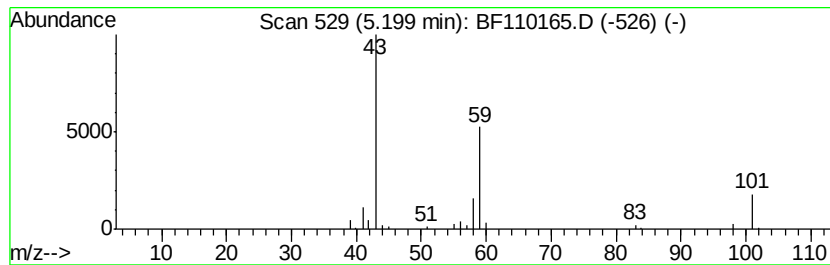
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.44 ng	109276	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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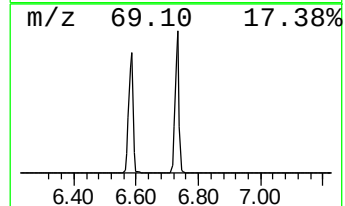
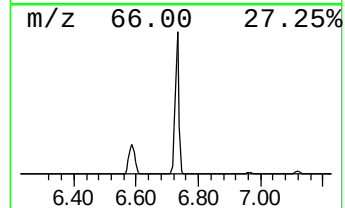
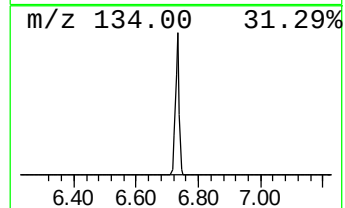
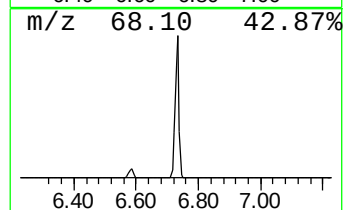
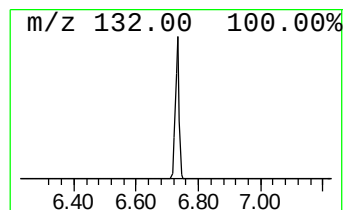
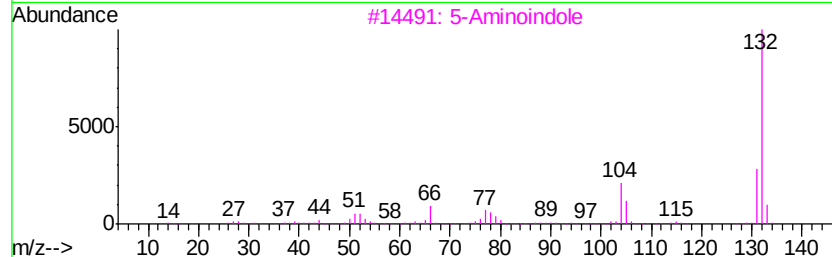
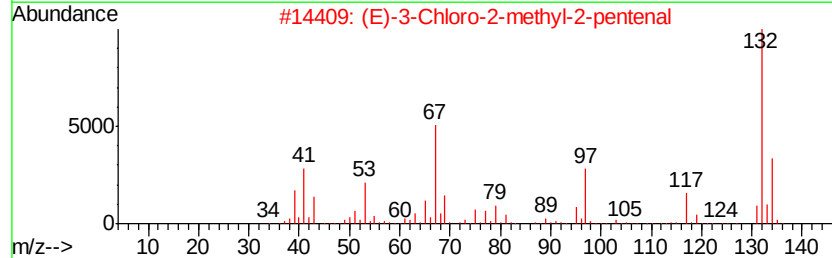
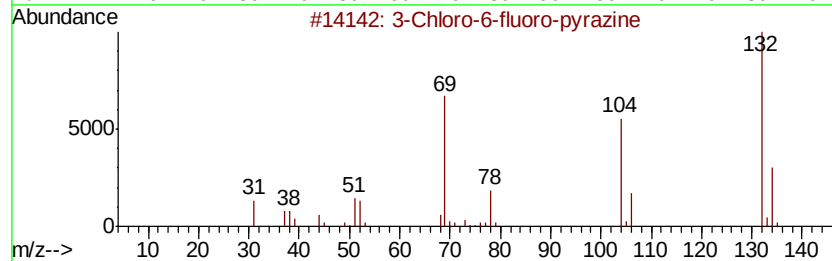
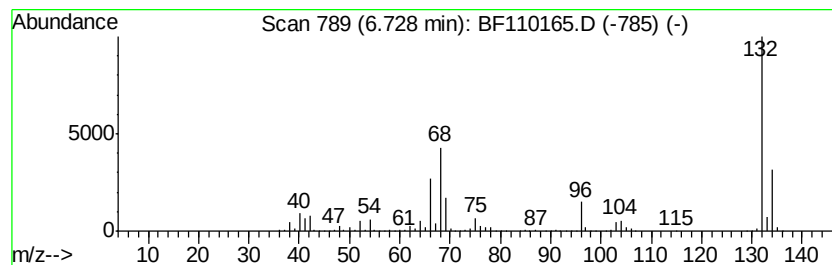
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	54.05 ng	2423470	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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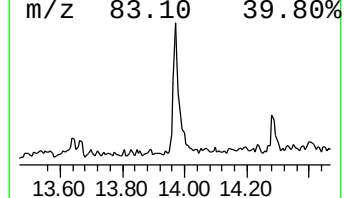
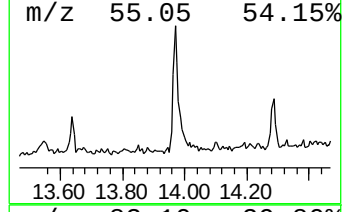
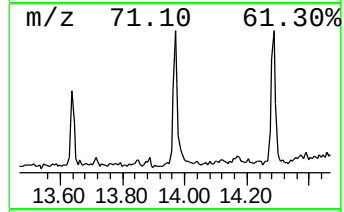
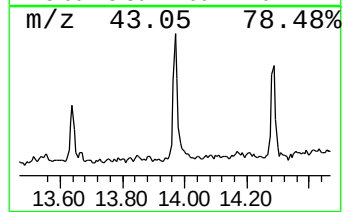
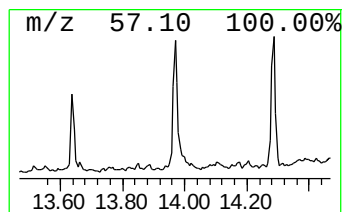
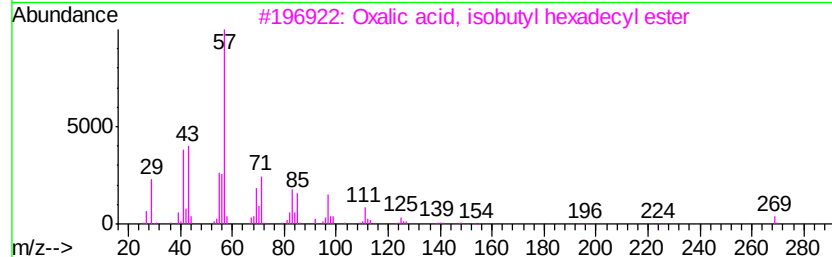
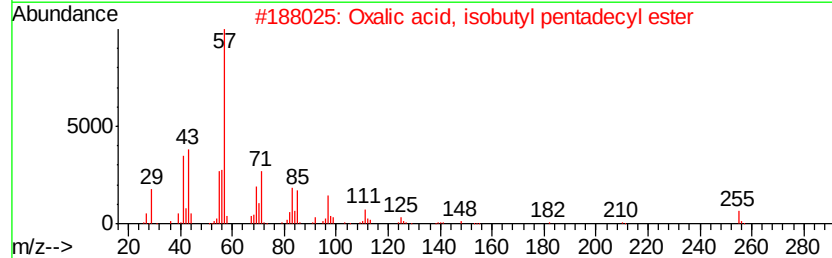
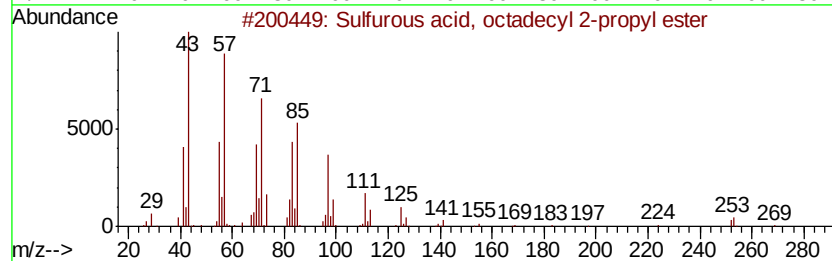
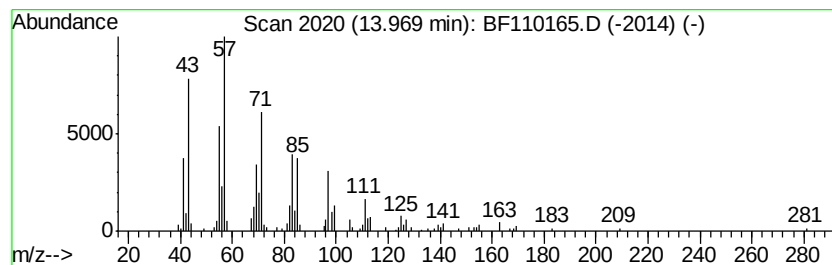
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Sulfurous acid, octadecyl 2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	4.44 ng	195184	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
2		Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87
3		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
4		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87
5		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87



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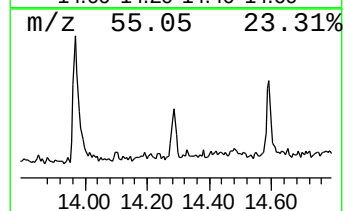
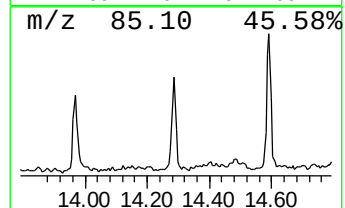
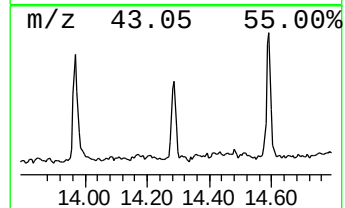
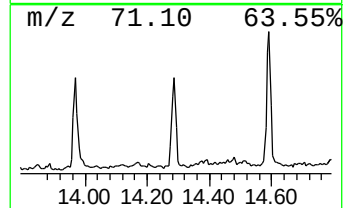
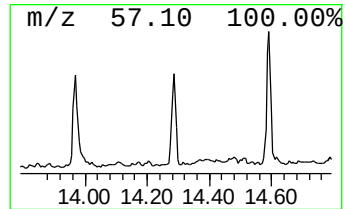
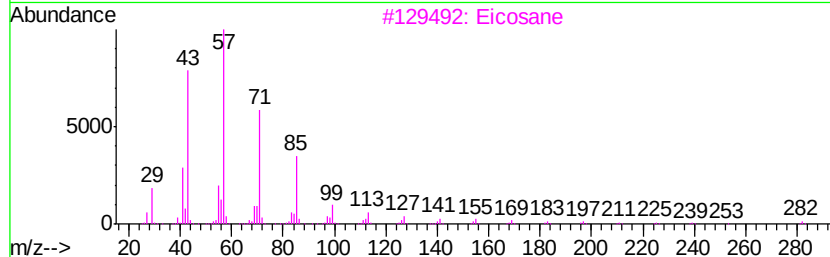
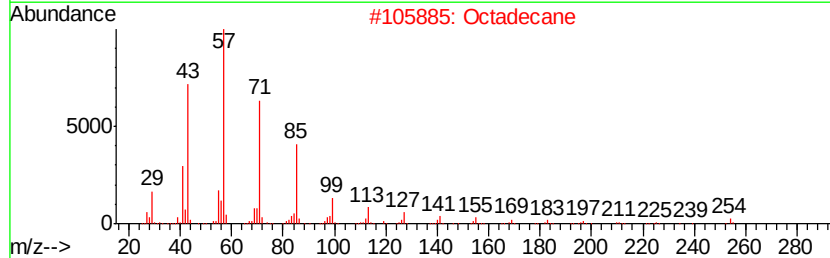
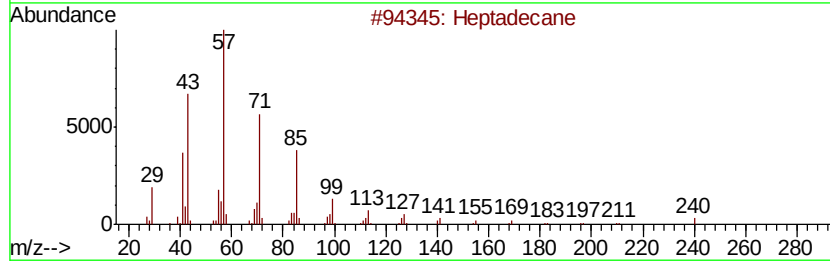
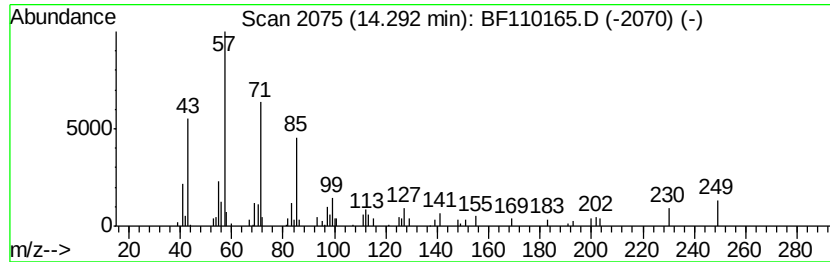
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.29	2.55 ng	112258	Chrysene-d12	14.15	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Octadecane	254	C18H38	000593-45-3	87
3	Eicosane	282	C20H42	000112-95-8	87
4	Docosane	310	C22H46	000629-97-0	87
5	Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110165.D
Acq On : 25 Oct 2018 17:27
Operator : JU/SJ
Sample : J5636-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

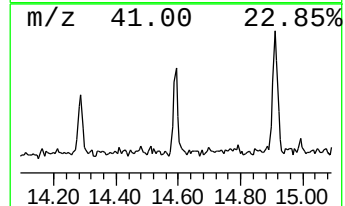
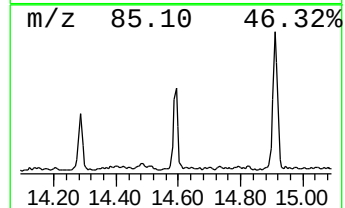
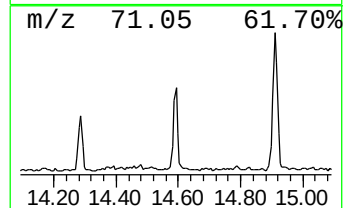
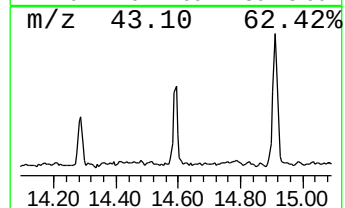
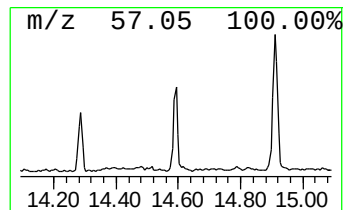
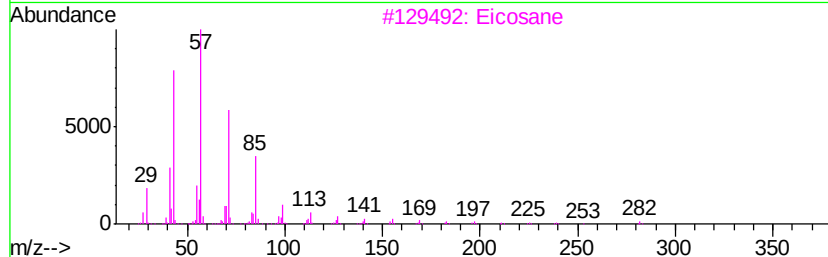
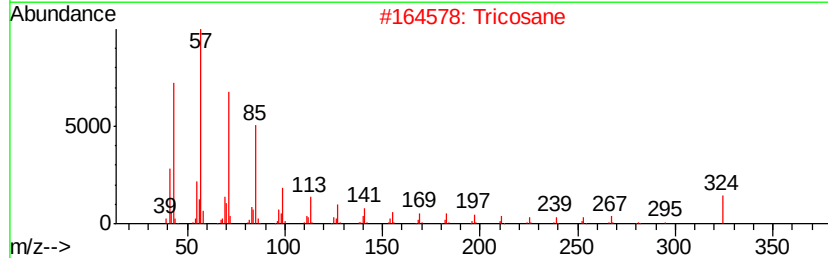
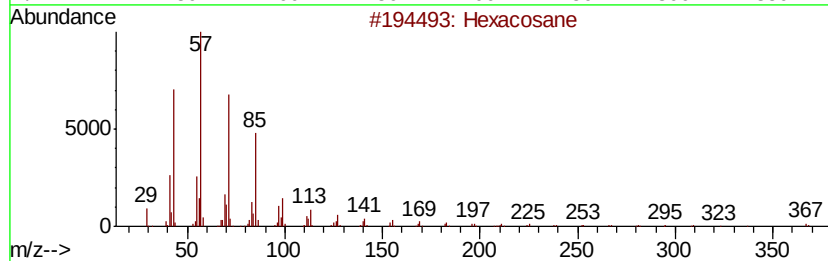
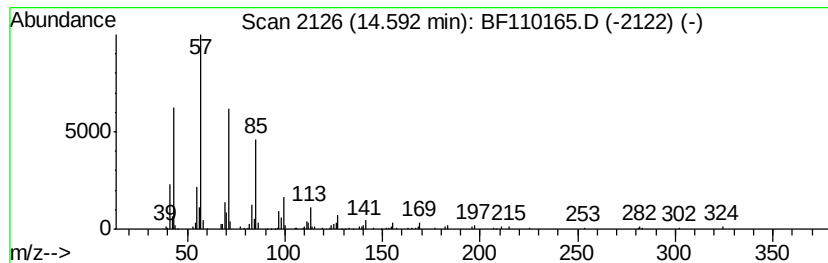
Instrument :
BNA_F
ClientSampleId :
HP-GRID-B

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

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

Peak Number 8 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	3.58 ng	157253	Chrysene-d12	14.15
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	93
2	Tricosane	324 C23H48	000638-67-5	93
3	Eicosane	282 C20H42	000112-95-8	92
4	Docosane	310 C22H46	000629-97-0	91
5	Tetracosane	338 C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110165.D
Acq On : 25 Oct 2018 17:27
Operator : JU/SJ
Sample : J5636-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HP-GRID-B

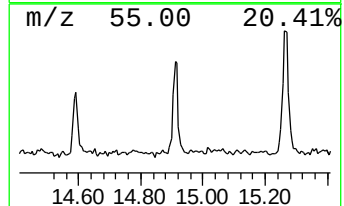
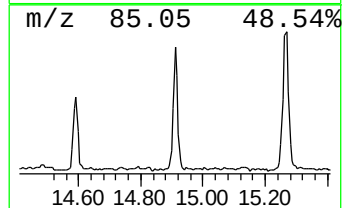
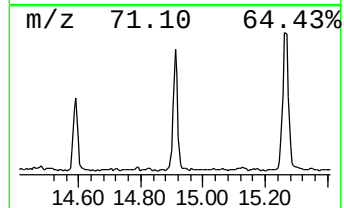
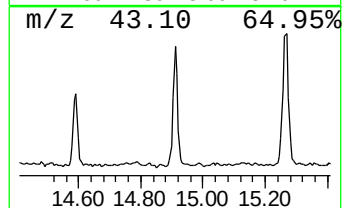
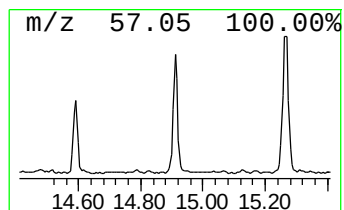
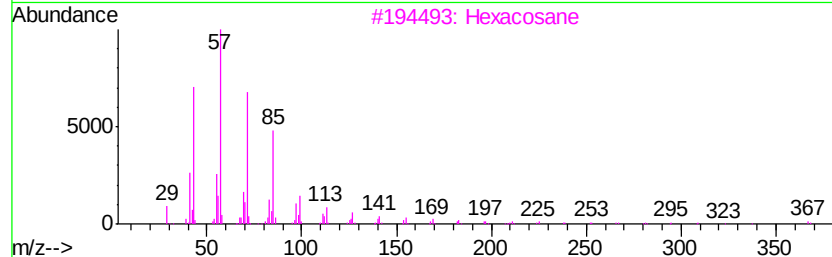
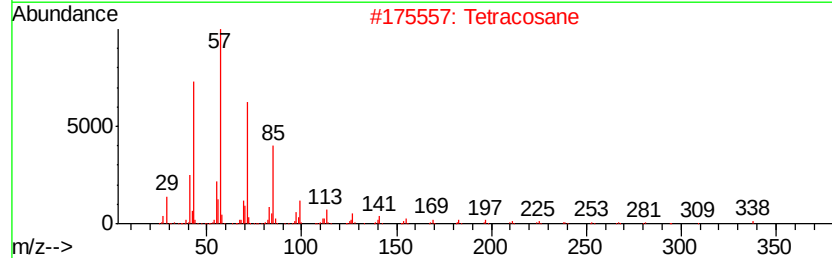
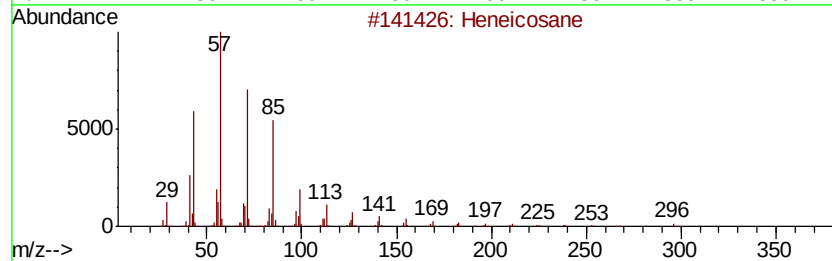
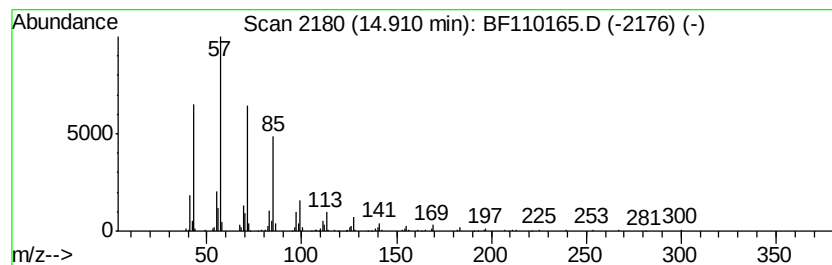
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	4.59 ng	273911	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110165.D
Acq On : 25 Oct 2018 17:27
Operator : JU/SJ
Sample : J5636-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HP-GRID-B

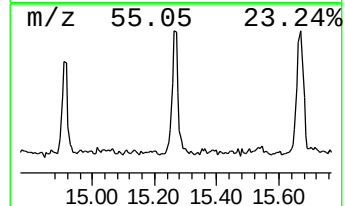
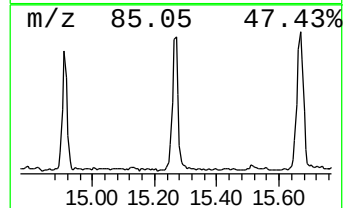
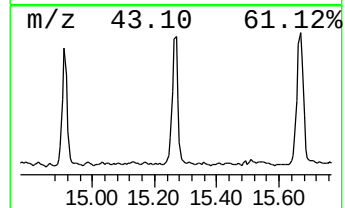
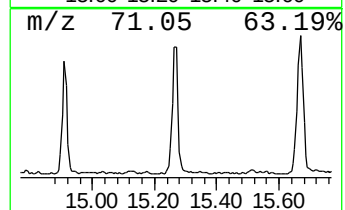
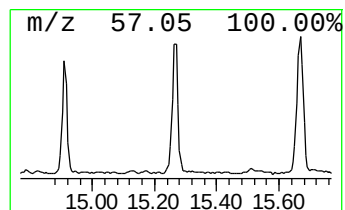
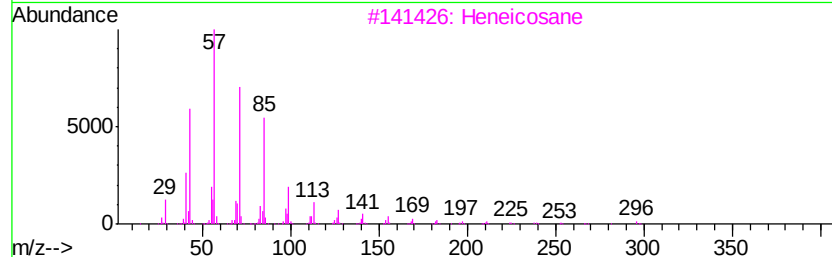
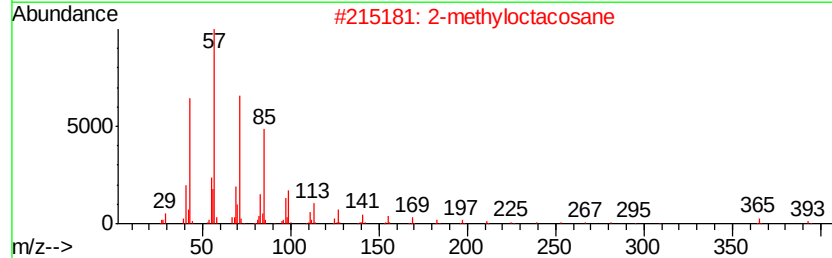
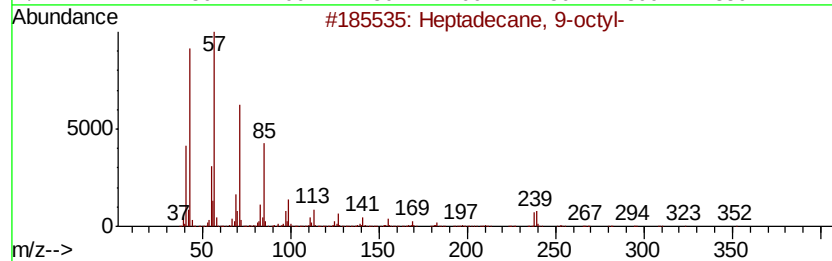
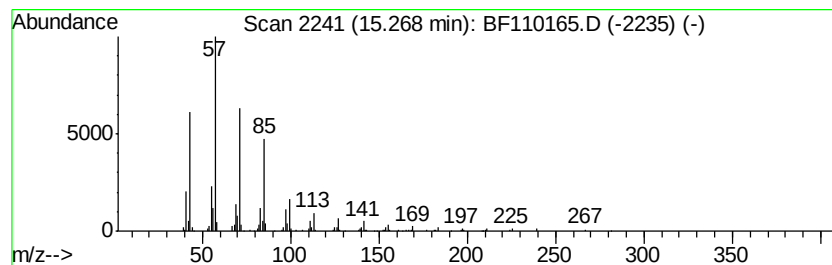
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	6.87 ng	410074	Perylene-d12	15.67

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	90
4			Triacontane	422	C30H62	000638-68-6	90
5			Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110165.D
Acq On : 25 Oct 2018 17:27
Operator : JU/SJ
Sample : J5636-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HP-GRID-B

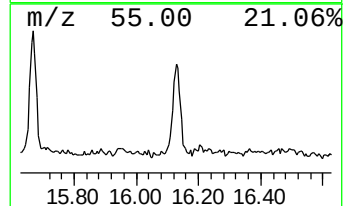
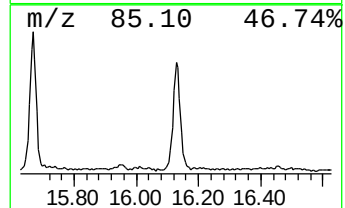
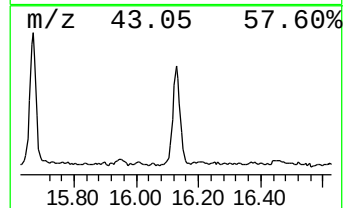
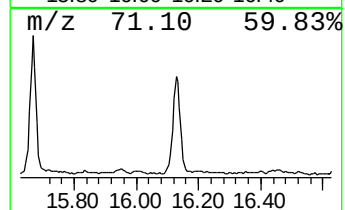
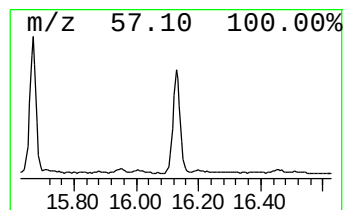
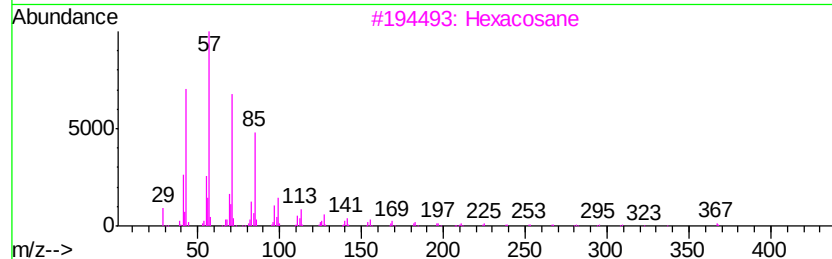
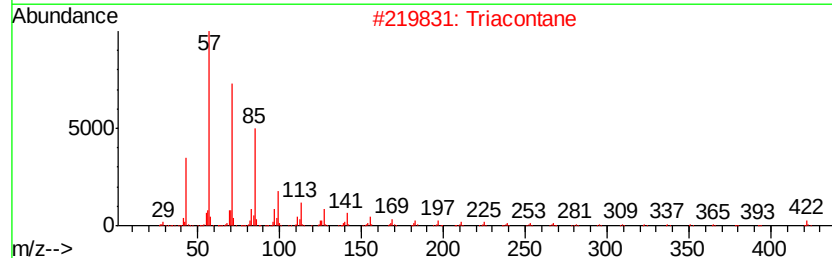
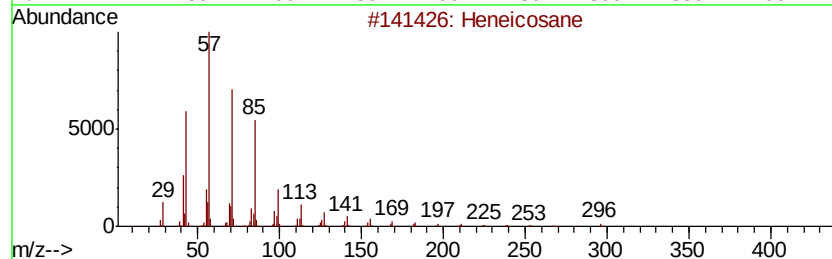
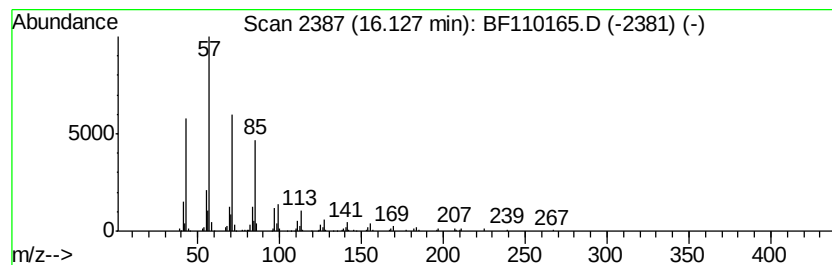
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	6.64 ng	396344	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Triacontane	422	C30H62	000638-68-6	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Tetracosane	338	C24H50	000646-31-1	90
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110165.D
Acq On : 25 Oct 2018 17:27
Operator : JU/SJ
Sample : J5636-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HP-GRID-B

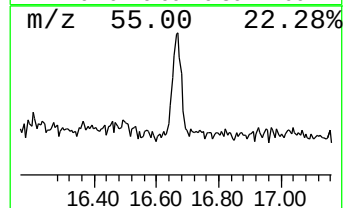
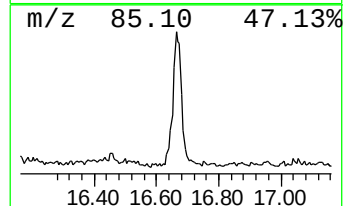
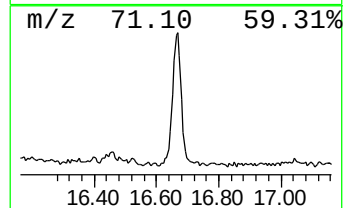
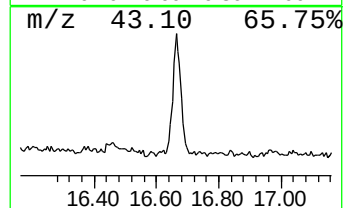
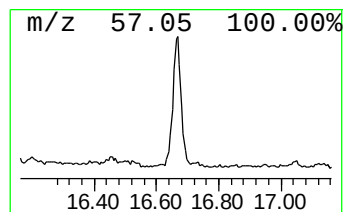
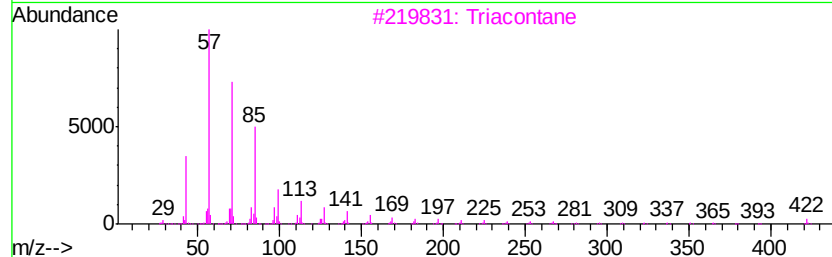
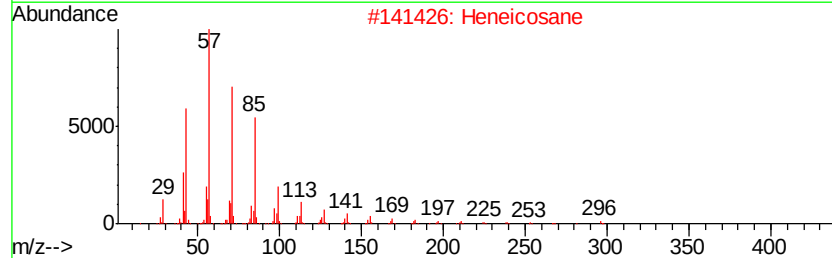
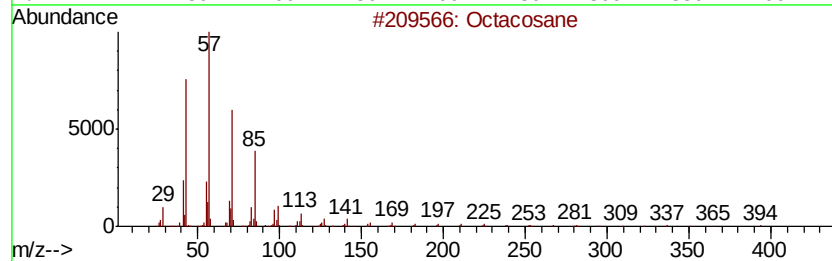
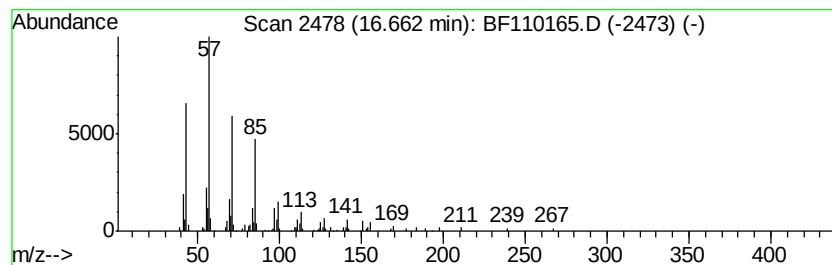
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	3.74 ng	223324	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102518\
Data File : BF110165.D
Acq On : 25 Oct 2018 17:27
Operator : JU/SJ
Sample : J5636-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HP-GRID-B

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.32	9.3	ng	418726	1	6.96	896709	20.0
2-Pentanone, 4-hy...	5.20	2.4	ng	109276	1	6.96	896709	20.0
unknown6.73	6.73	54.0	ng	2423470	1	6.96	896709	20.0
Sulfurous acid, o...	13.97	4.4	ng	195184	5	14.15	878913	20.0
Heptadecane	14.29	2.5	ng	112258	5	14.15	878913	20.0
Hexacosane	14.59	3.6	ng	157253	5	14.15	878913	20.0
Heneicosane	14.91	4.6	ng	273911	6	15.67	1193300	20.0
Heptadecane, 9-oc...	15.27	6.9	ng	410074	6	15.67	1193300	20.0
triacontane	16.13	6.6	ng	396344	6	15.67	1193300	20.0
Octacosane	16.66	3.7	ng	223324	6	15.67	1193300	20.0