

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111819\
 Data File : BF117830.D
 Acq On : 18 Nov 2019 12:54
 Operator : JU
 Sample : PB124881BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB124881BL

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-BF111319.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	2.275	22	32	36	rVB	6494801	9793986	100.00%	12.163%
2	3.110	165	174	181	rBV	104276	175873	1.80%	0.218%
3	5.145	511	520	528	rBV	734080	960274	9.80%	1.193%
4	5.539	581	587	590	rBV	5341469	5145214	52.53%	6.390%
5	6.539	751	757	761	rBV	3746256	3856580	39.38%	4.790%
6	6.692	777	783	786	rBV	7155894	7593609	77.53%	9.431%
7	6.922	818	822	825	rBV	1853036	1651460	16.86%	2.051%
8	7.081	844	849	852	rBV	6267197	5863122	59.86%	7.282%
9	7.481	911	917	920	rBV	4348118	4948678	50.53%	6.146%
10	8.204	1036	1040	1044	rBV	2248125	2123510	21.68%	2.637%
11	9.286	1218	1224	1227	rBV	8529435	8922481	91.10%	11.081%
12	9.674	1283	1290	1294	rBV	430230	386968	3.95%	0.481%
13	9.969	1332	1340	1344	rBV	2966879	2514221	25.67%	3.122%
14	10.763	1468	1475	1478	rBV	6629328	6300999	64.34%	7.825%
15	11.463	1589	1594	1597	rBV	3052114	2665248	27.21%	3.310%
16	11.527	1600	1605	1609	rVB2	160289	144345	1.47%	0.179%
17	11.986	1676	1683	1687	rBV	842163	862130	8.80%	1.071%
18	12.774	1813	1817	1830	rBV	421440	512282	5.23%	0.636%
19	13.057	1859	1865	1868	rBV	9573003	9757725	99.63%	12.118%
20	13.951	2013	2017	2034	rBV	250729	504097	5.15%	0.626%
21	14.109	2037	2044	2047	rBV	2685409	2382737	24.33%	2.959%
22	14.268	2068	2071	2075	rBV	116710	110036	1.12%	0.137%
23	14.574	2120	2123	2129	rBV	178795	167975	1.72%	0.209%
24	14.898	2174	2178	2183	rBV	207231	207580	2.12%	0.258%
25	15.251	2234	2238	2243	rBV	204454	226189	2.31%	0.281%
26	15.615	2294	2300	2304	rBV	1614113	2139369	21.84%	2.657%
27	15.651	2304	2306	2317	rVB	188659	235950	2.41%	0.293%
28	16.115	2379	2385	2392	rBV	120252	199624	2.04%	0.248%
29	16.645	2469	2475	2482	rBV2	72446	167683	1.71%	0.208%

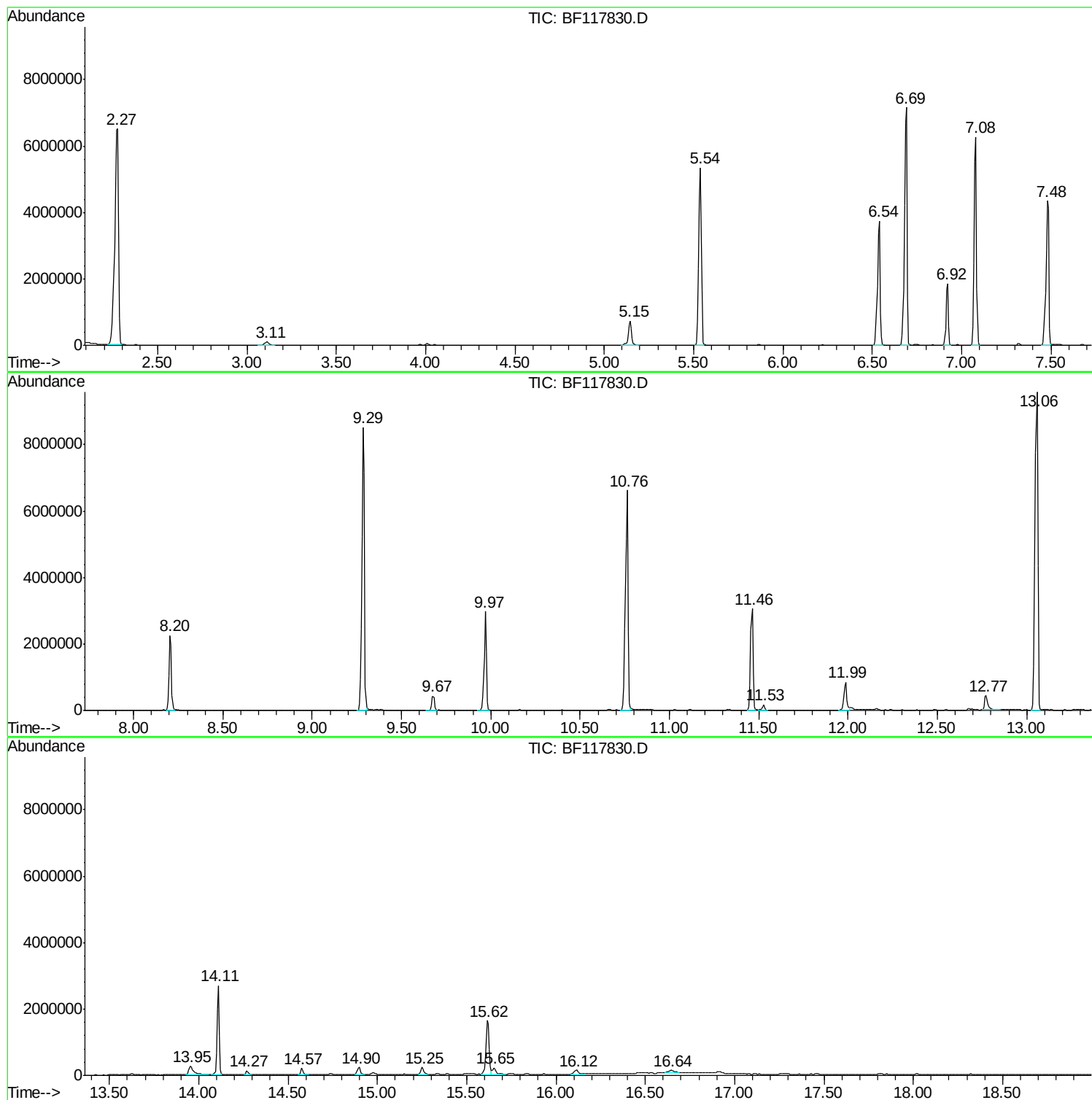
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.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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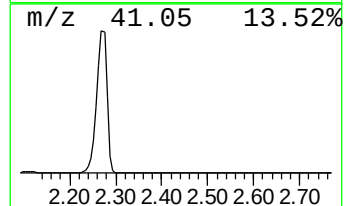
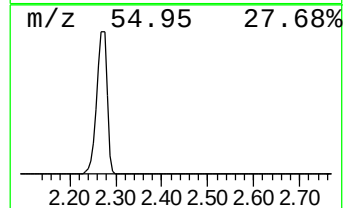
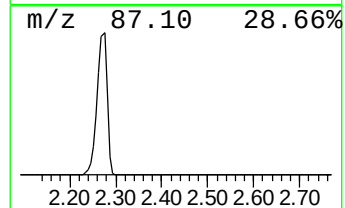
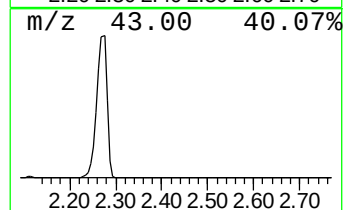
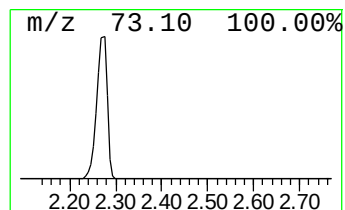
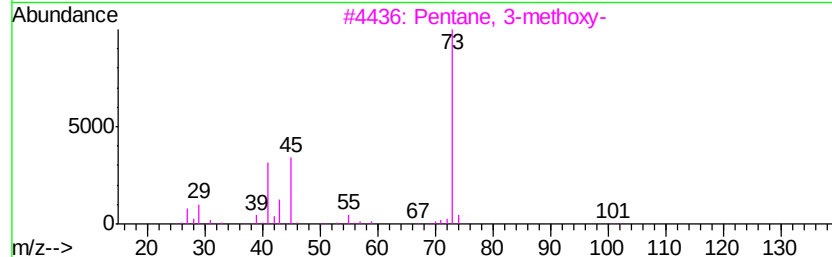
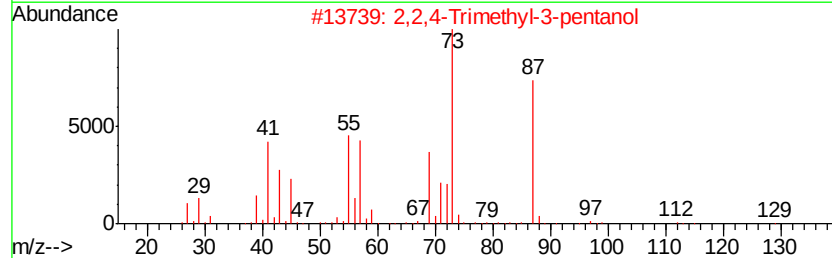
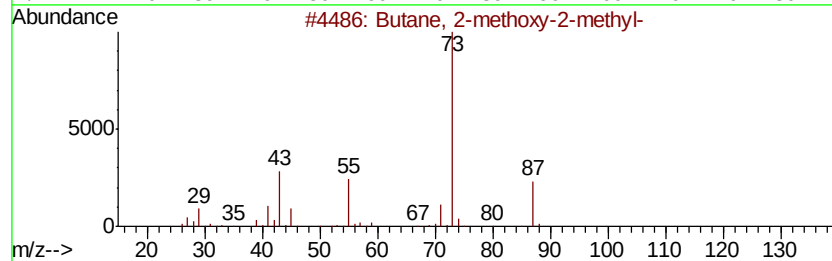
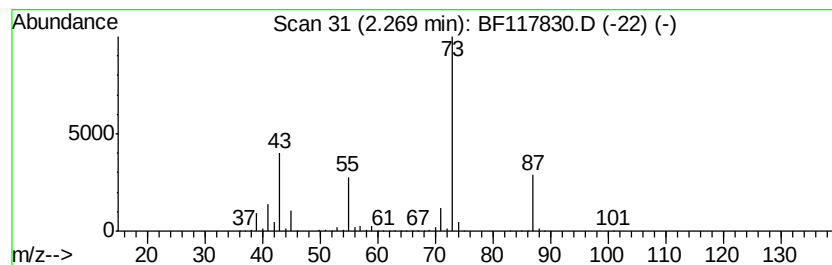
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	118.61 ng	9793990	1,4-Dichlorobenzene-d4	6.92

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		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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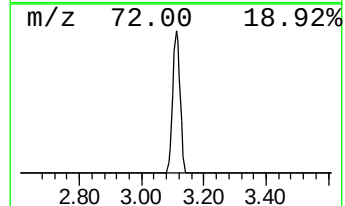
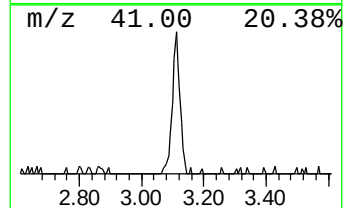
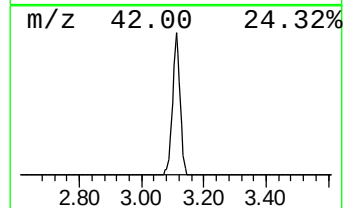
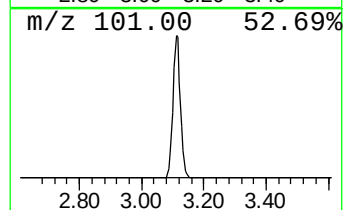
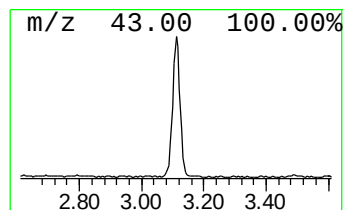
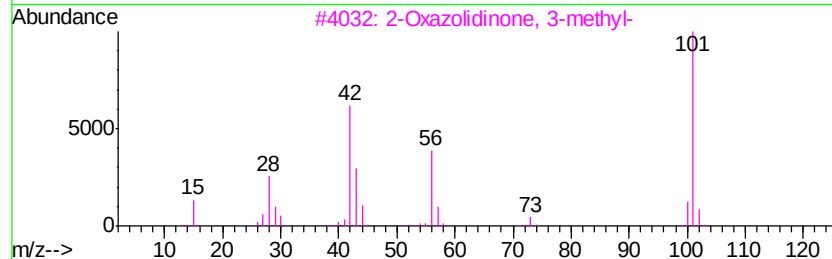
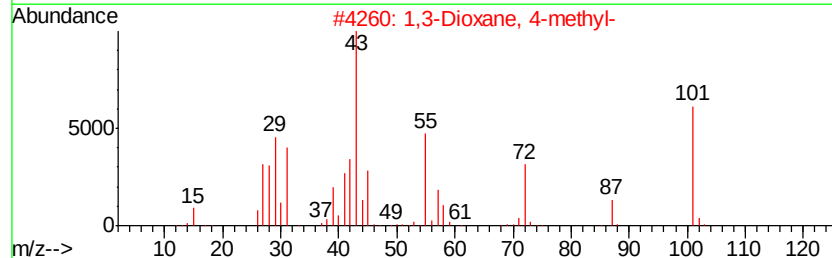
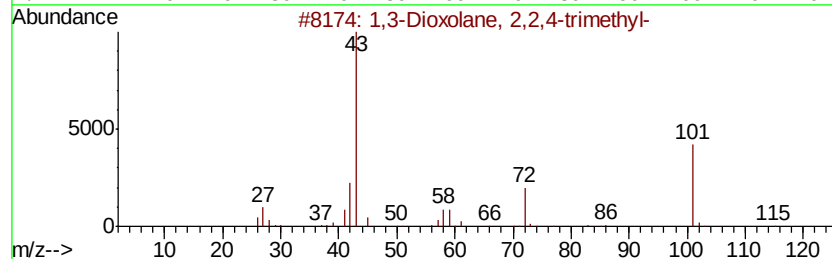
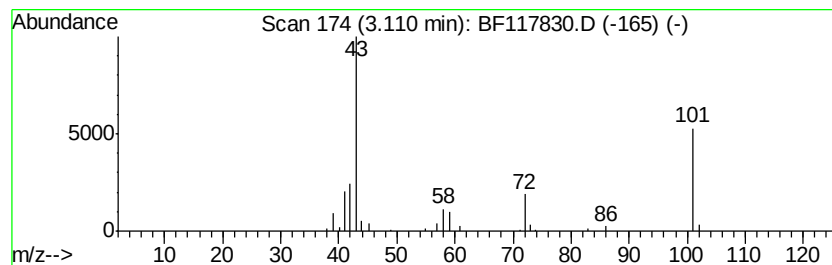
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Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.11	2.13 ng	175873	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	64
3			2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	43
4			Butane	58	C4H10	000106-97-8	10
5			1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	10



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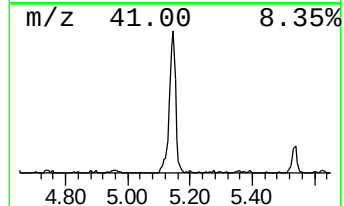
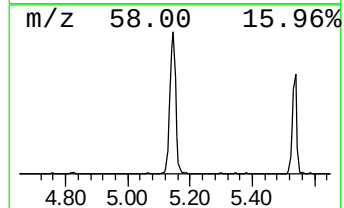
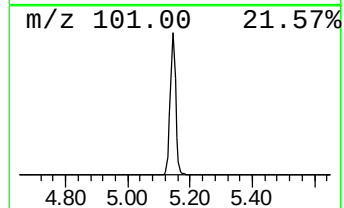
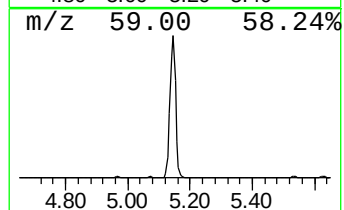
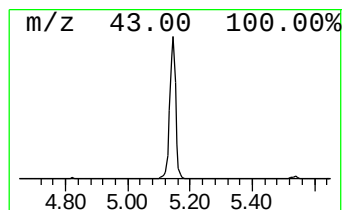
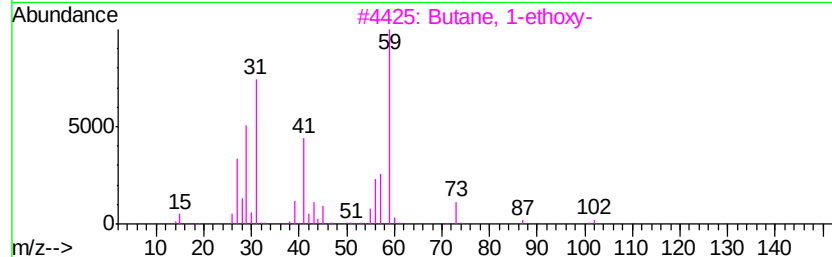
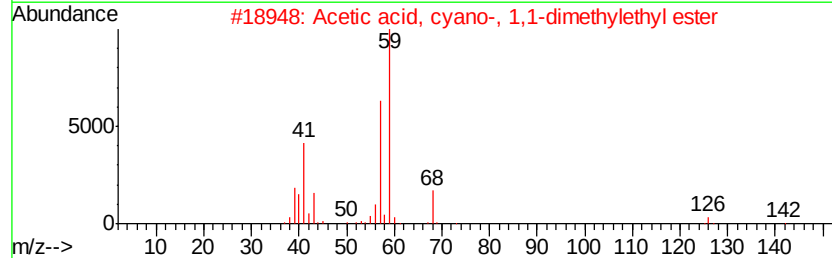
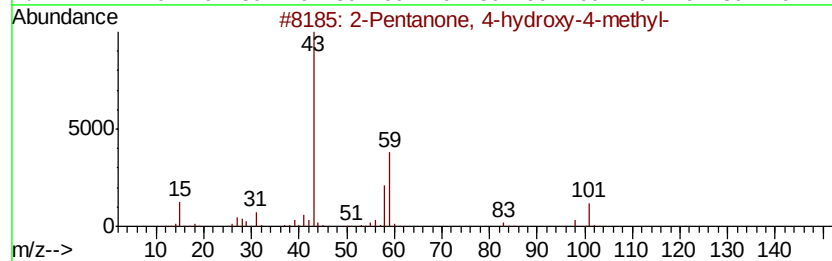
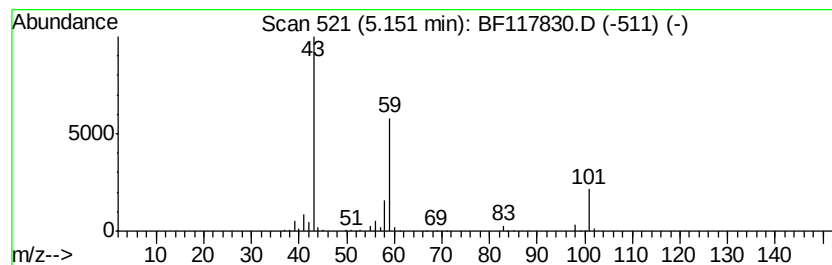
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	11.63 ng	960274	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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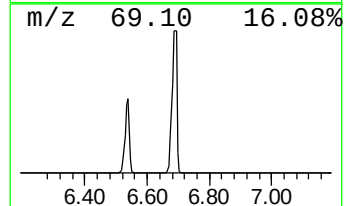
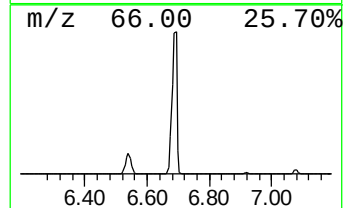
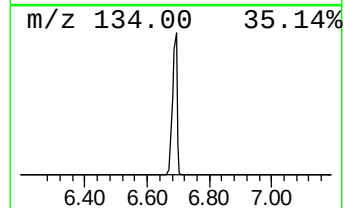
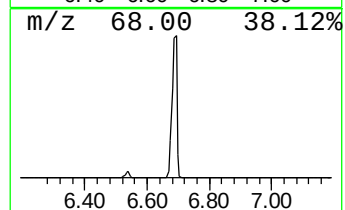
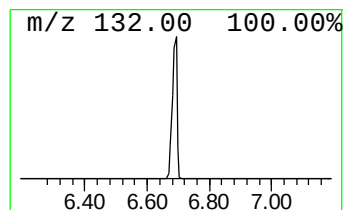
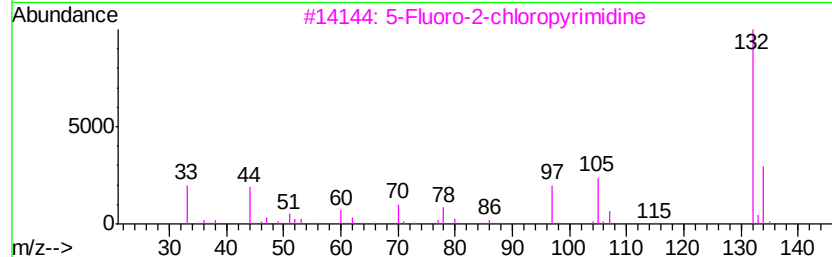
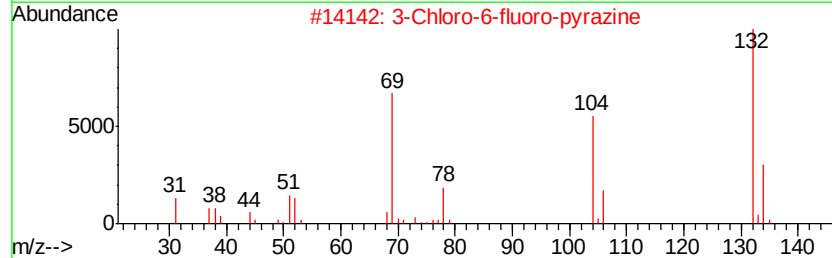
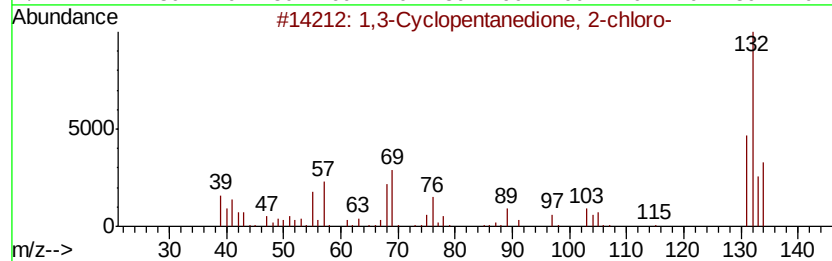
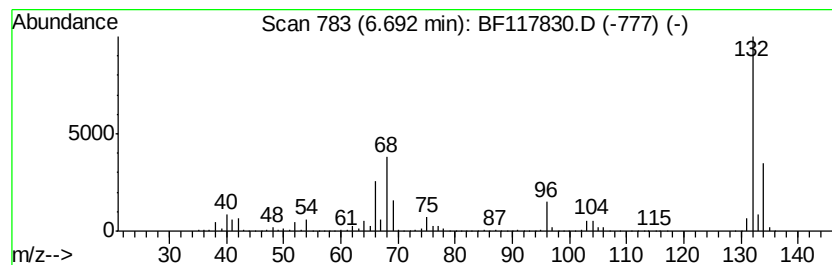
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	91.96 ng	7593610	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	37
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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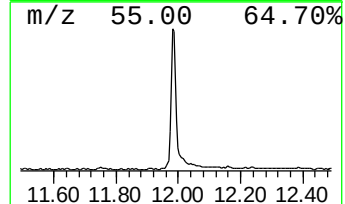
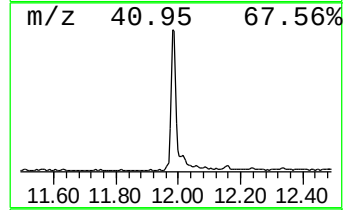
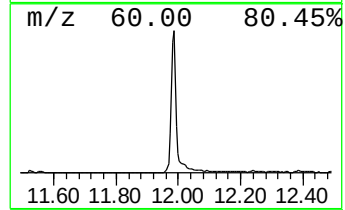
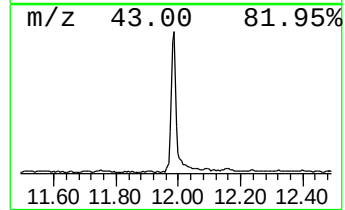
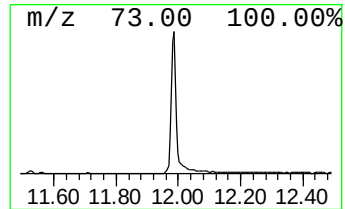
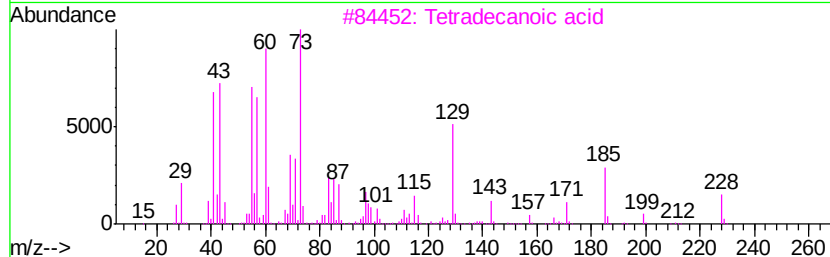
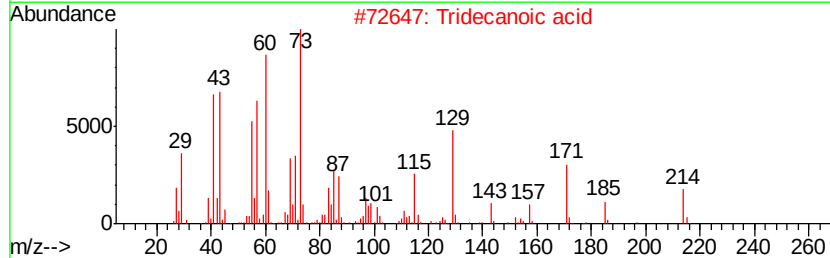
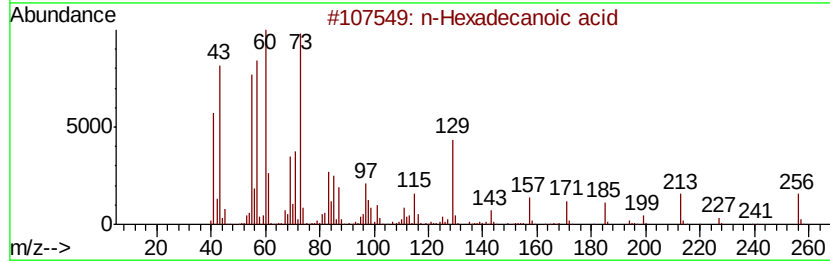
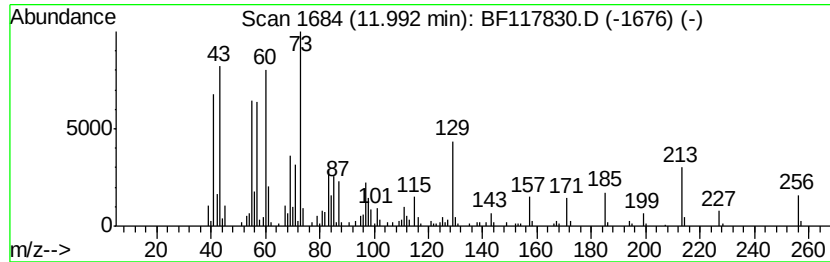
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.99	6.47 ng	862130	Phenanthrene-d10	11.46	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	93



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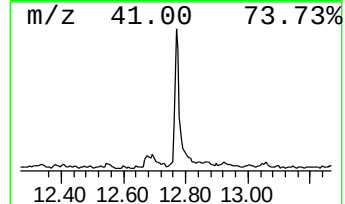
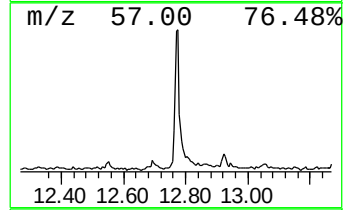
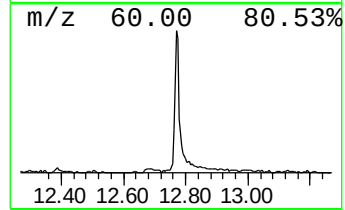
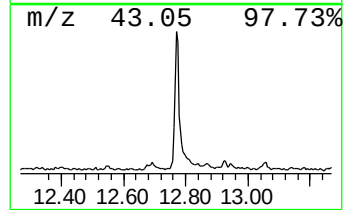
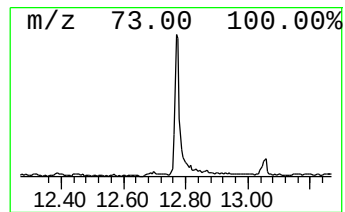
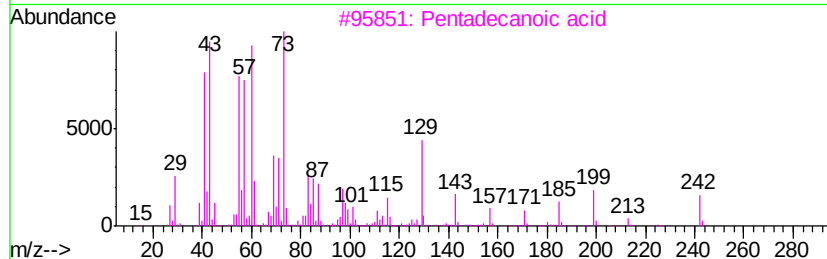
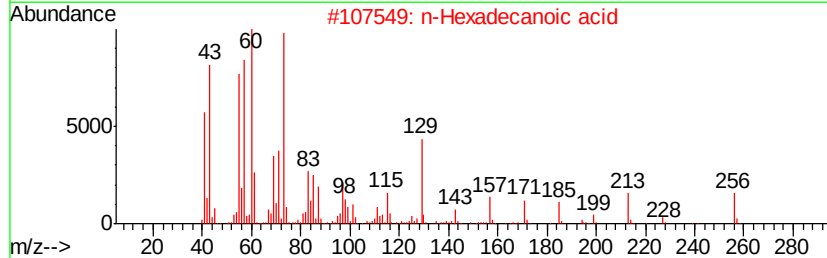
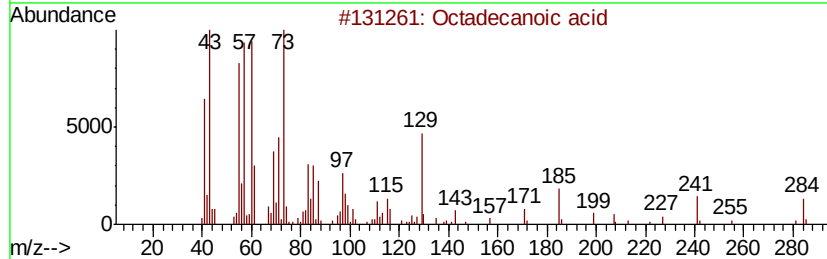
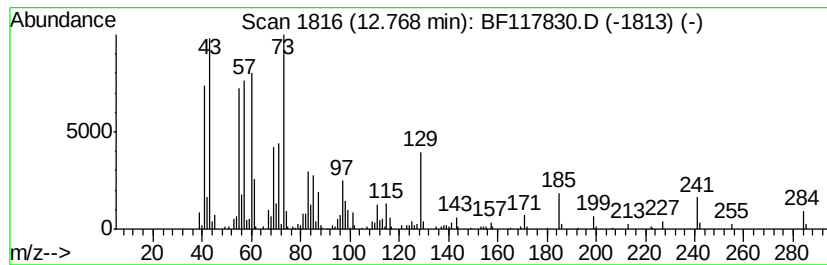
Instrument :
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ClientSampleId :
PB124881BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.77	3.84 ng	512282	Phenanthrene-d10		11.46
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	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111819\
Data File : BF117830.D
Acq On : 18 Nov 2019 12:54
Operator : JU
Sample : PB124881BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

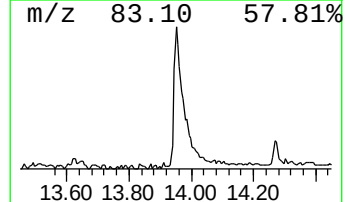
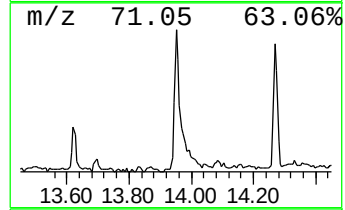
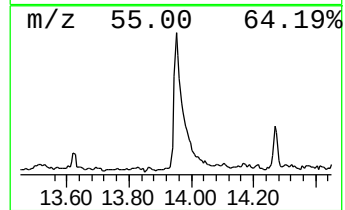
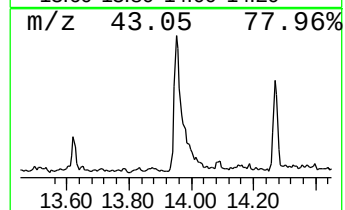
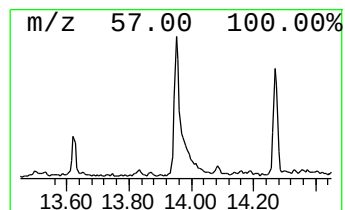
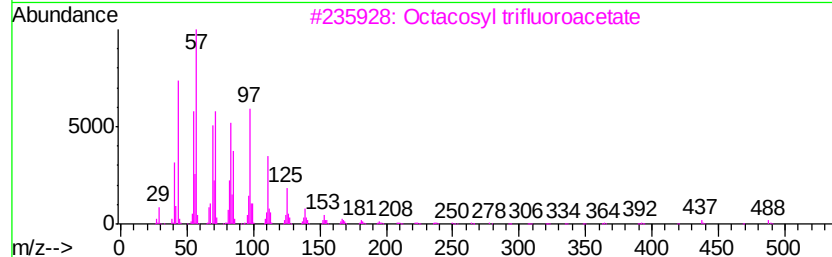
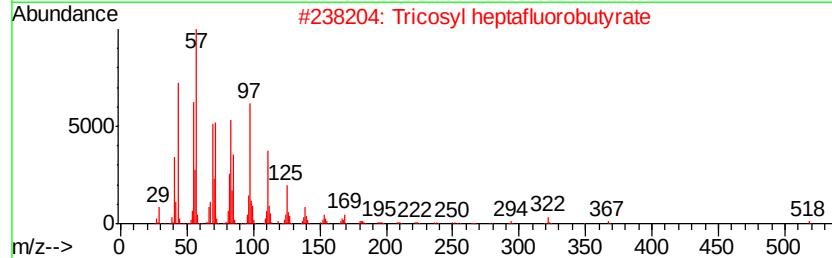
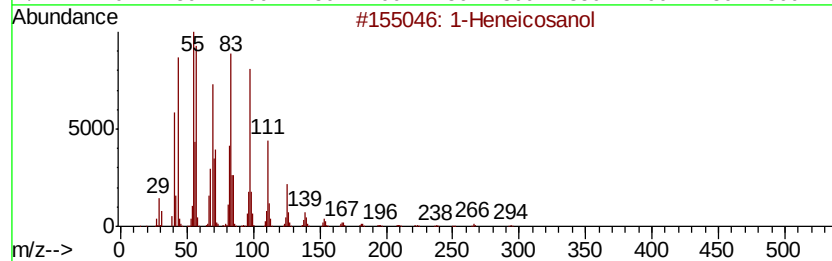
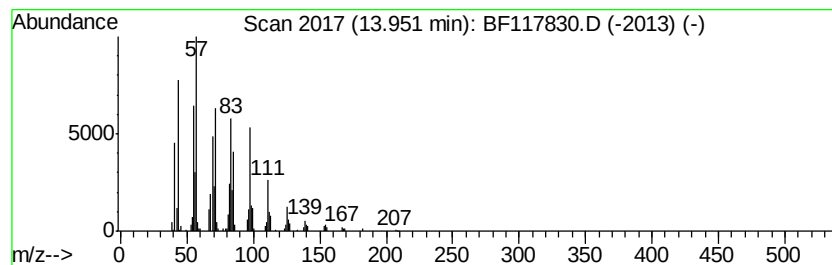
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.23 ng	504097	Chrysene-d12	14.11
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	93
2	Tricosyl heptafluorobutyrate	536 C27H47F7O2	1000351-83-4	87
3	Octacosyl trifluoroacetate	506 C30H57F3O2	1000351-74-9	87
4	1-Dodecanol, 2-hexyl-	270 C18H38O	110225-00-8	81
5	1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111819\
Data File : BF117830.D
Acq On : 18 Nov 2019 12:54
Operator : JU
Sample : PB124881BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB124881BL

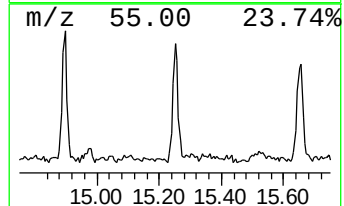
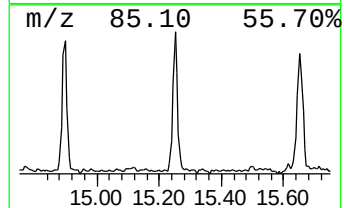
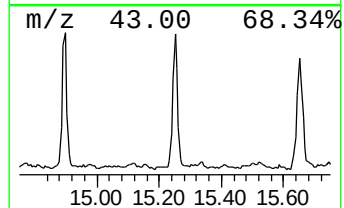
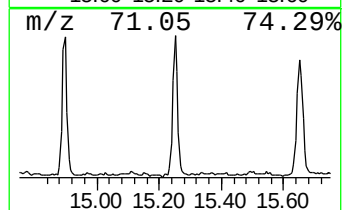
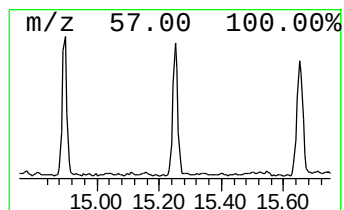
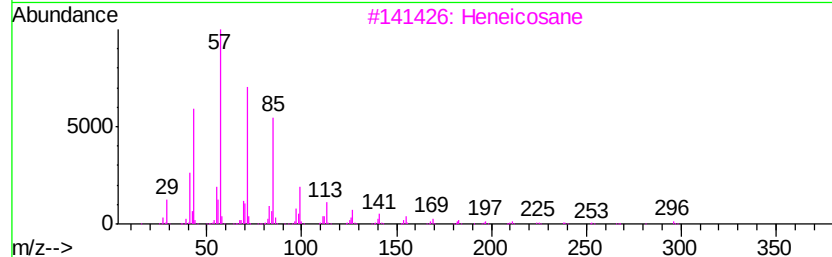
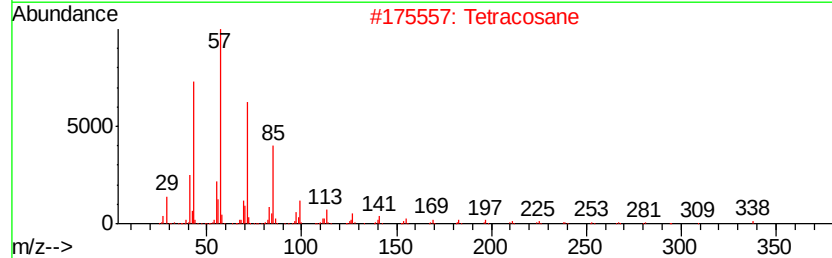
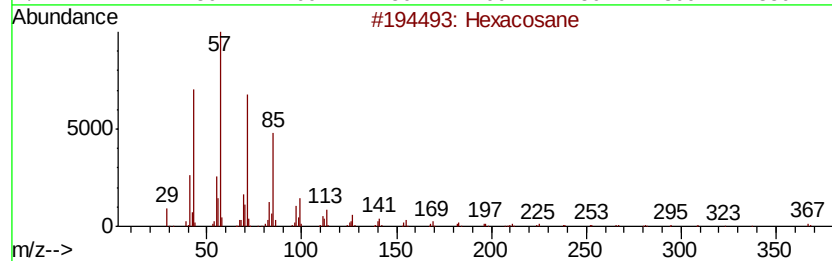
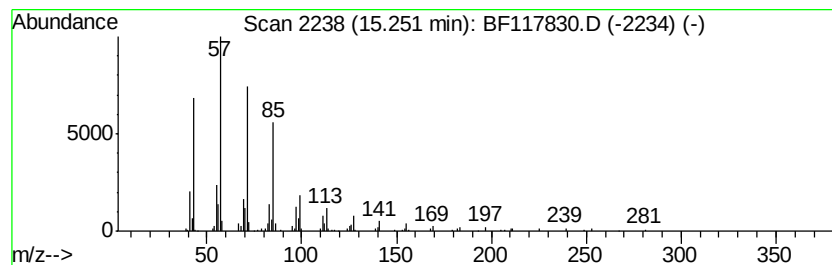
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	2.11 ng	226189	Perylene-d12	15.62

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111819\
Data File : BF117830.D
Acq On : 18 Nov 2019 12:54
Operator : JU
Sample : PB124881BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB124881BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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...	2.27	118.6	ng	9793990	1	6.92	1651460	20.0
1,3-Dioxolane, 2,...	3.11	2.1	ng	175873	1	6.92	1651460	20.0
2-Pentanone, 4-hy...	5.15	11.6	ng	960274	1	6.92	1651460	20.0
unknown6.69	6.69	92.0	ng	7593610	1	6.92	1651460	20.0
n-Hexadecanoic acid	11.99	6.5	ng	862130	4	11.46	2665250	20.0
Octadecanoic acid	12.77	3.8	ng	512282	4	11.46	2665250	20.0
1-Heneicosanol	13.95	4.2	ng	504097	5	14.11	2382740	20.0
Hexacosane	15.25	2.1	ng	226189	6	15.62	2139370	20.0