

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011819\
 Data File : BF112119.D
 Acq On : 18 Jan 2019 11:30
 Operator : JU/SJ
 Sample : K1157-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-04-011519

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-BF011619.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	2.163	9	13	25	rVB	188261	281322	2.98%	0.343%
2	4.463	400	404	410	rBV	80570	106705	1.13%	0.130%
3	5.087	506	510	522	rVB	399480	565024	5.98%	0.688%
4	5.498	575	580	588	rBV	7226050	7603312	80.48%	9.257%
5	6.510	746	752	768	rVB	6753805	8154709	86.32%	9.929%
6	6.633	768	773	777	rBV	7734721	8276693	87.61%	10.077%
7	6.857	807	811	818	rBV	2400133	1943755	20.58%	2.367%
8	7.016	833	838	841	rBV	7353543	6653379	70.43%	8.101%
9	7.422	901	907	910	rBV	5086372	5316283	56.27%	6.473%
10	8.139	1024	1029	1032	rBV	2864272	2481815	26.27%	3.022%
11	9.216	1206	1212	1215	rBV	9550277	9447138	100.00%	11.502%
12	9.604	1274	1278	1282	rVB	817543	664598	7.03%	0.809%
13	9.892	1323	1327	1331	rBV2	3078994	2770465	29.33%	3.373%
14	10.686	1457	1462	1465	rBV	5791851	5632762	59.62%	6.858%
15	11.380	1576	1580	1582	rBV	2990037	2494867	26.41%	3.038%
16	11.404	1582	1584	1587	rVB	375862	298823	3.16%	0.364%
17	11.904	1667	1669	1676	rVB3	403199	369434	3.91%	0.450%
18	12.433	1753	1759	1762	rBV2	67901	112816	1.19%	0.137%
19	12.592	1783	1786	1791	rVB	533451	432165	4.57%	0.526%
20	12.686	1799	1802	1806	rBV	111718	121722	1.29%	0.148%
21	12.821	1819	1825	1830	rVB	440840	439316	4.65%	0.535%
22	12.962	1845	1849	1853	rBV	7071208	7035616	74.47%	8.566%
23	13.851	1997	2000	2013	rVB2	973939	1110936	11.76%	1.353%
24	14.021	2021	2029	2032	rBV	2227147	2289499	24.23%	2.788%
25	14.045	2032	2033	2042	rVB	242326	166416	1.76%	0.203%
26	14.174	2052	2055	2063	rVB3	156393	194885	2.06%	0.237%
27	14.486	2104	2108	2113	rBV	514646	579410	6.13%	0.705%
28	14.786	2156	2159	2165	rBV	236234	278829	2.95%	0.339%
29	14.933	2181	2184	2187	rVB	138554	125646	1.33%	0.153%
30	15.062	2202	2206	2209	rBV	212303	319344	3.38%	0.389%
31	15.127	2213	2217	2220	rBV	438854	558763	5.91%	0.680%
32	15.368	2254	2258	2263	rVB	128386	192763	2.04%	0.235%
33	15.427	2265	2268	2273	rVB	161797	194923	2.06%	0.237%
34	15.492	2274	2279	2292	rBV	1666021	2455062	25.99%	2.989%

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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 >
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35	15.709	2312	2316	2321	rBV3	95404	137845	1.46%	0.168%
36	15.945	2351	2356	2361	rBV	492208	742430	7.86%	0.904%
37	15.992	2361	2364	2372	rVB3	104303	192188	2.03%	0.234%
38	16.450	2437	2442	2446	rBV	162056	262278	2.78%	0.319%
39	16.739	2487	2491	2500	rVB4	140802	240518	2.55%	0.293%
40	17.045	2538	2543	2551	rVB2	163508	339218	3.59%	0.413%
41	18.168	2728	2734	2746	rVB4	201148	548017	5.80%	0.667%

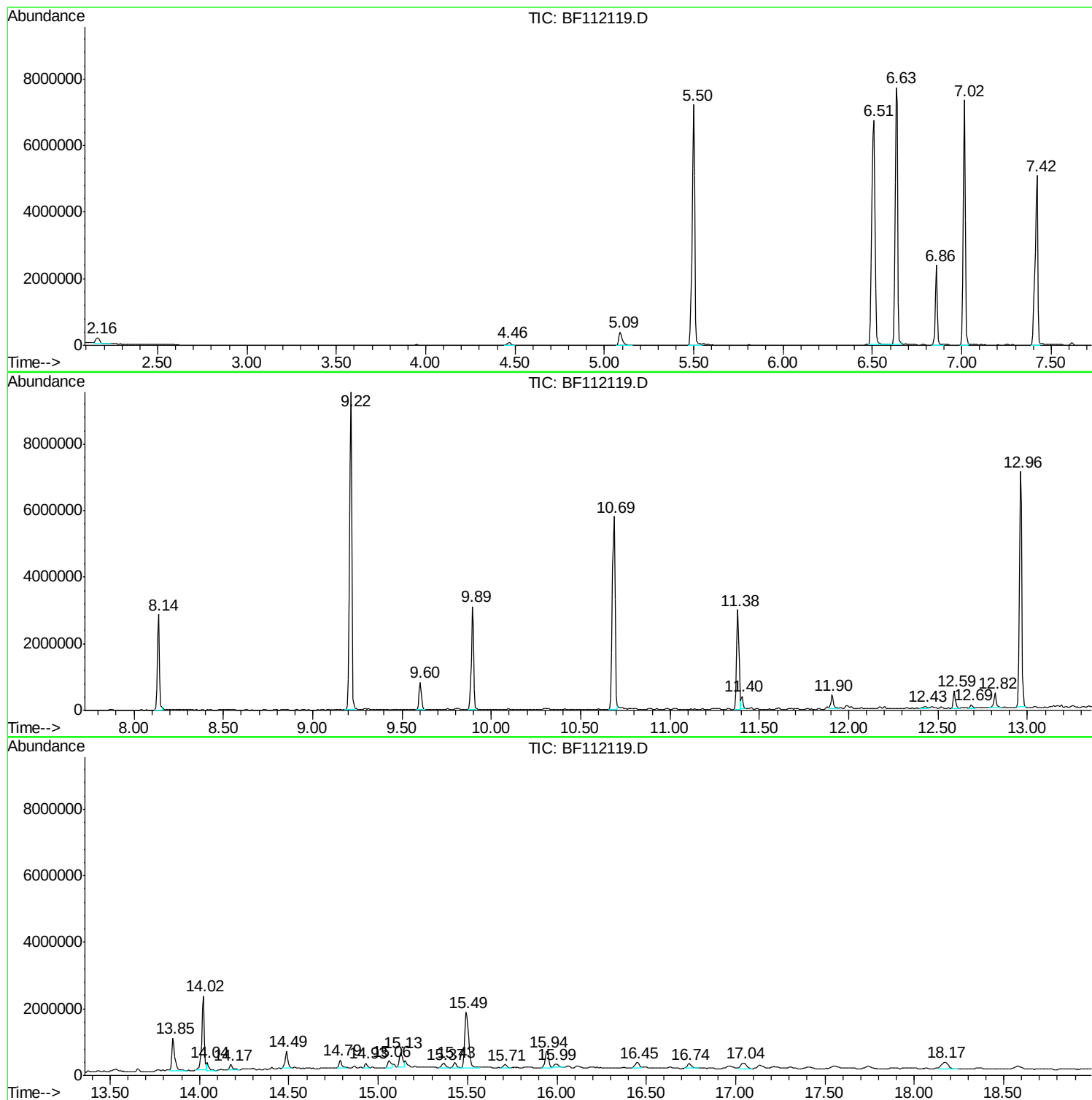
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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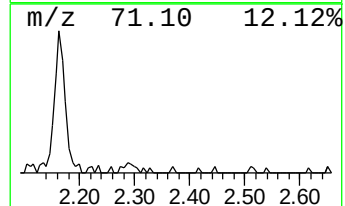
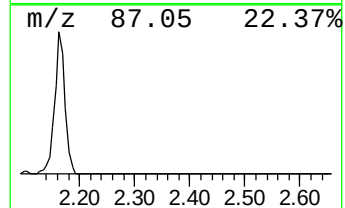
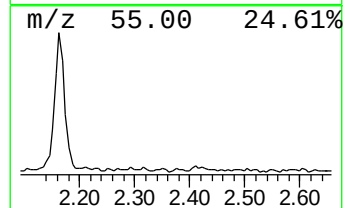
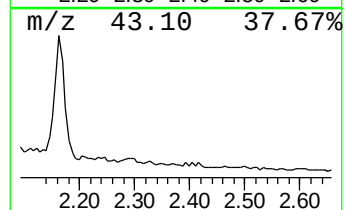
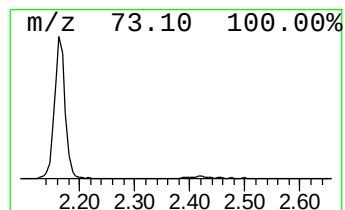
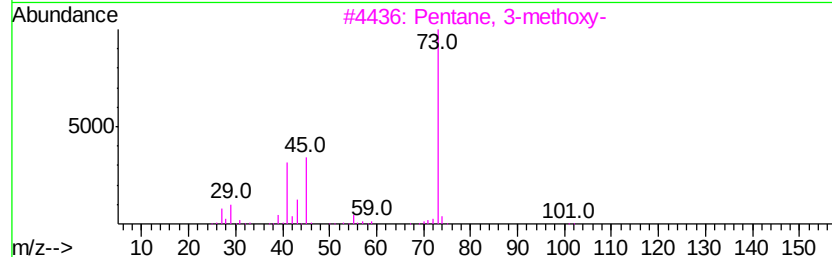
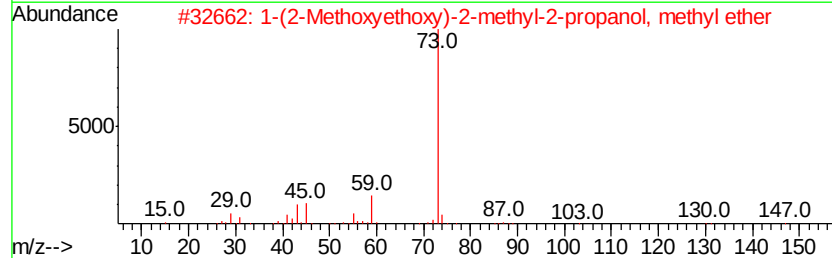
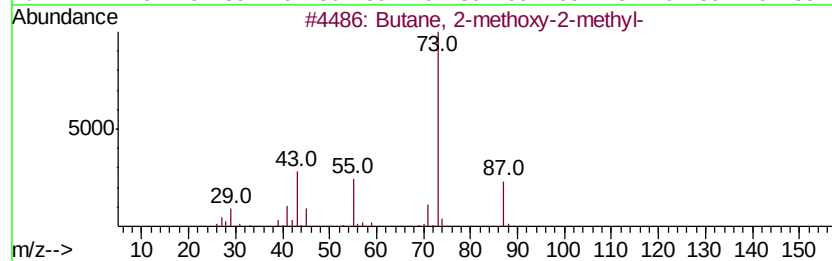
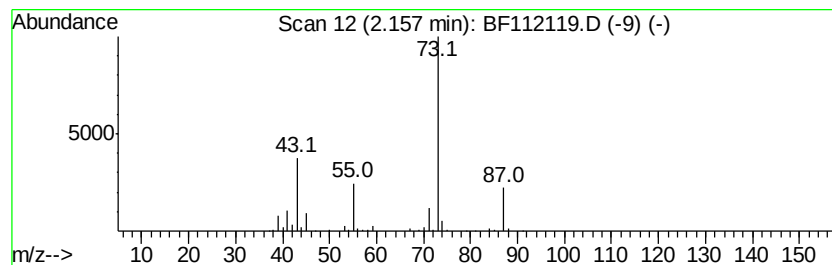
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	2.89 ng	281322	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			1-(2-Methoxyethoxy)-2-methyl-2-propanol, methyl ether	162	C8H18O3	1000364-24-4	25
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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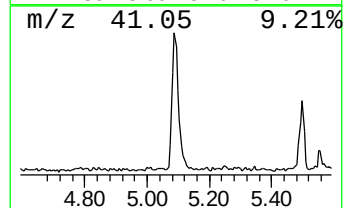
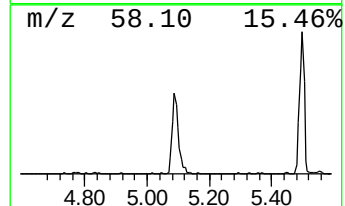
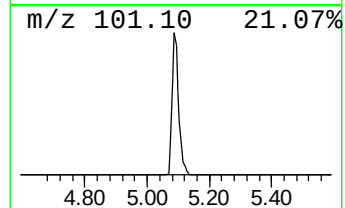
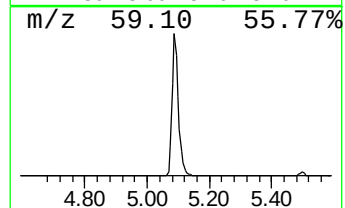
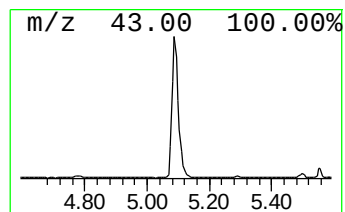
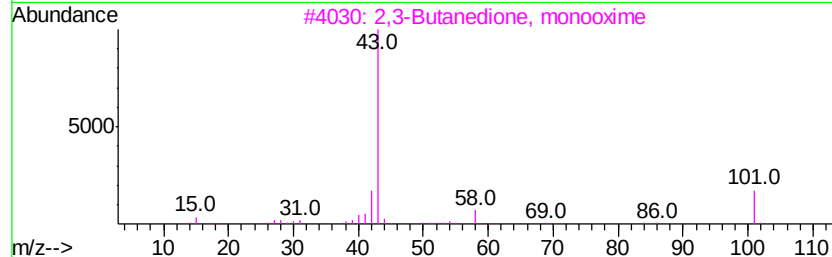
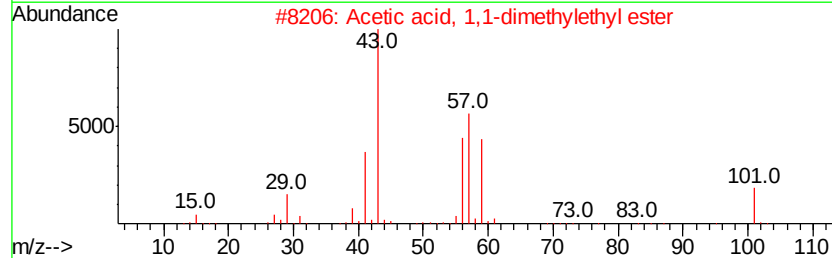
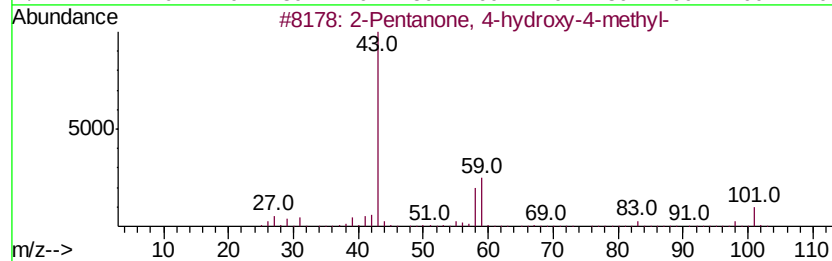
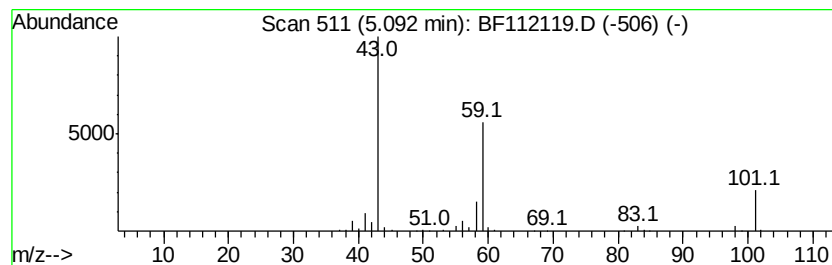
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	5.81 ng	565024	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		3-Hexanol	102	C6H14O	000623-37-0	28
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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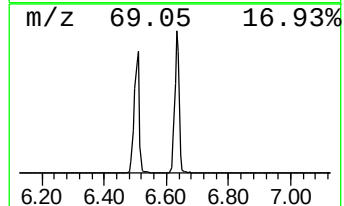
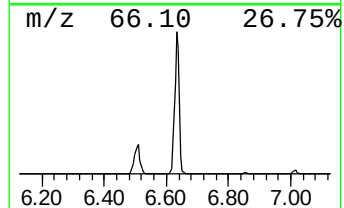
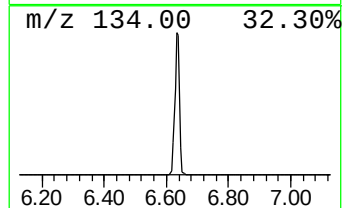
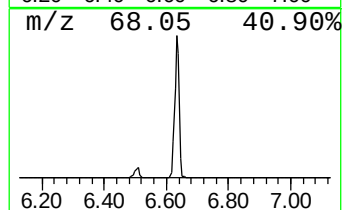
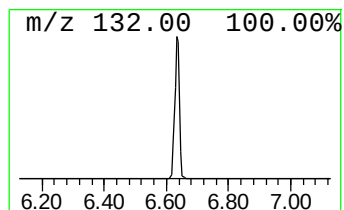
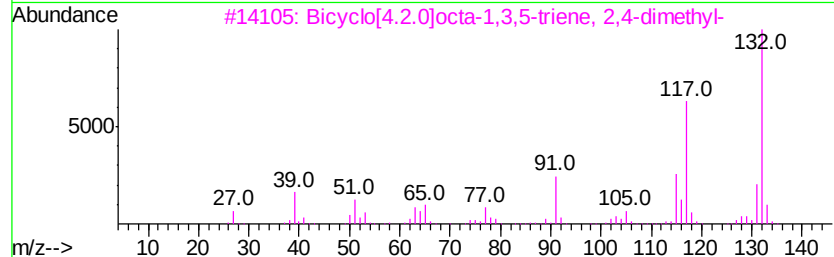
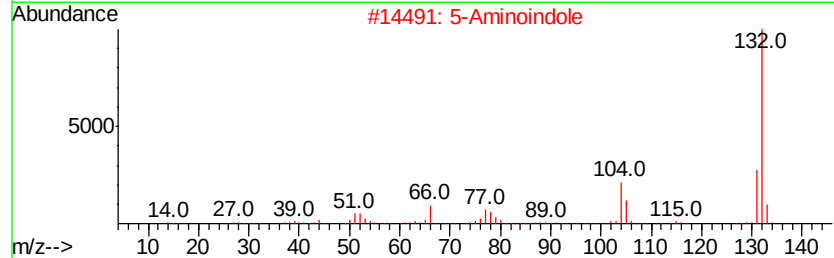
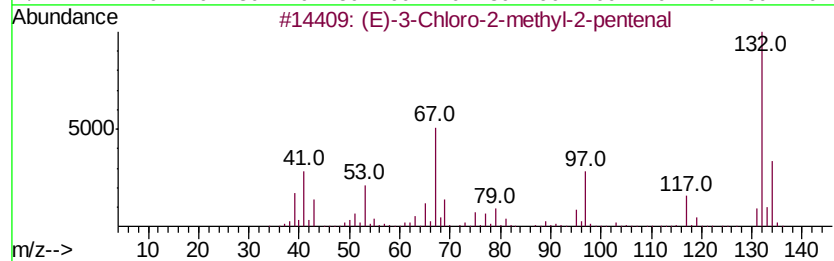
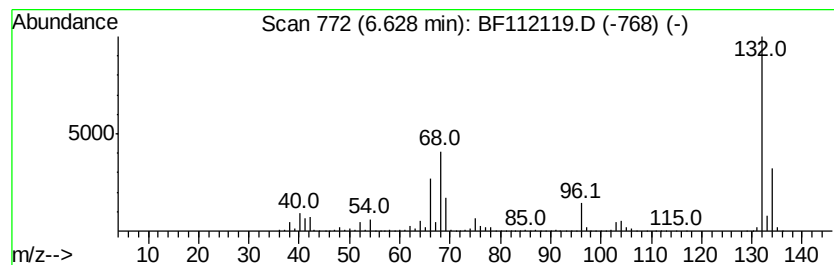
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	85.16 ng	8276690	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		Xenon	132	Xe	007440-63-3	9



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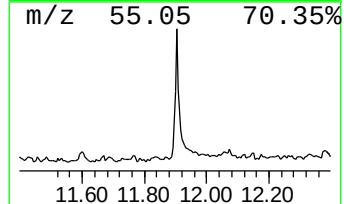
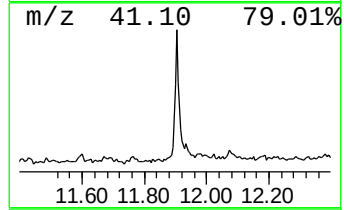
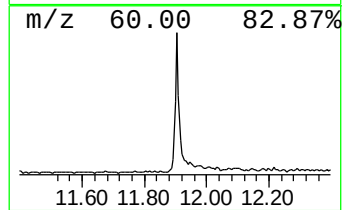
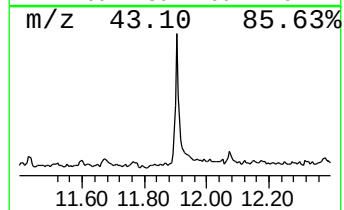
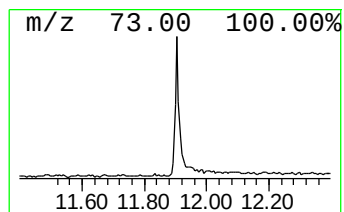
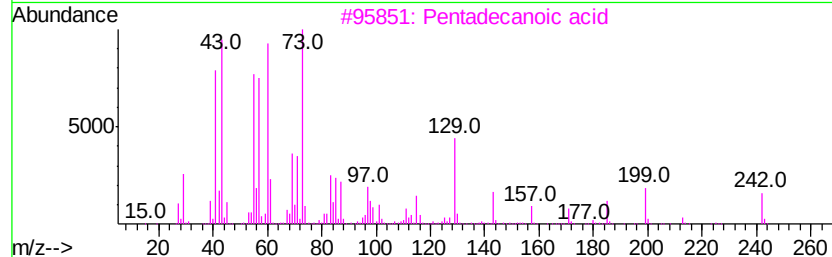
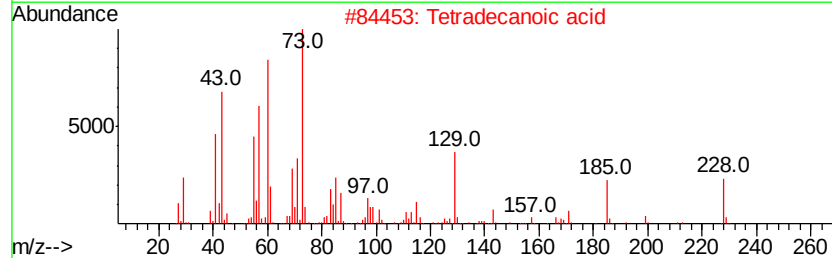
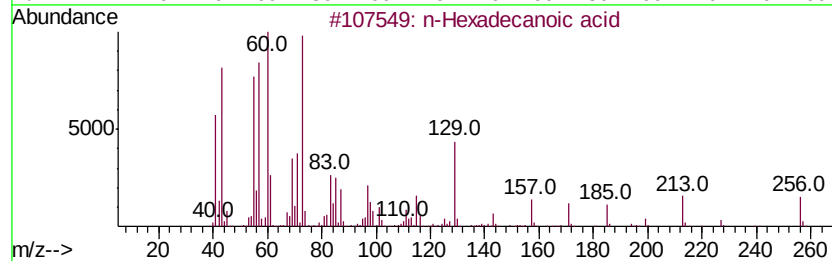
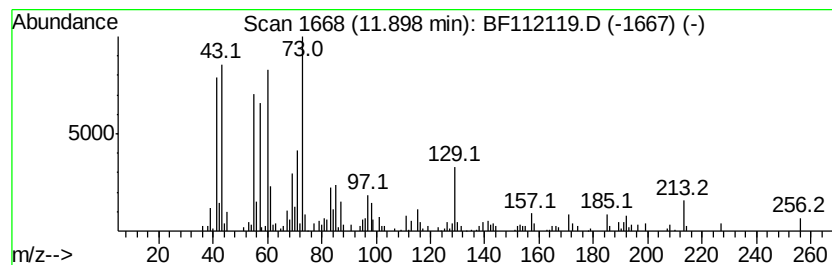
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.96 ng	369434	Phenanthrene-d10	11.38

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		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4		Tridecanoic acid	214	C13H26O2	000638-53-9	70
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



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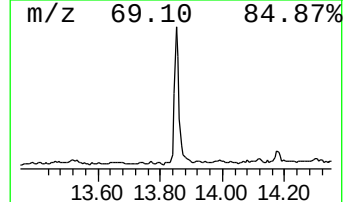
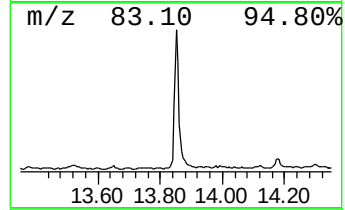
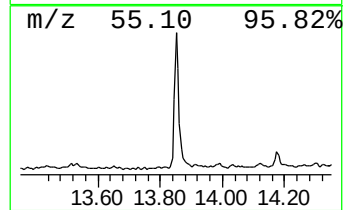
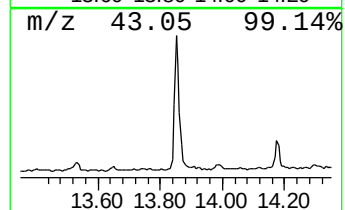
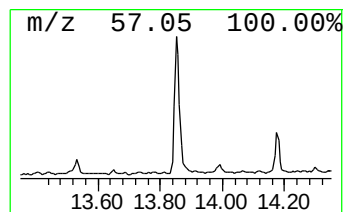
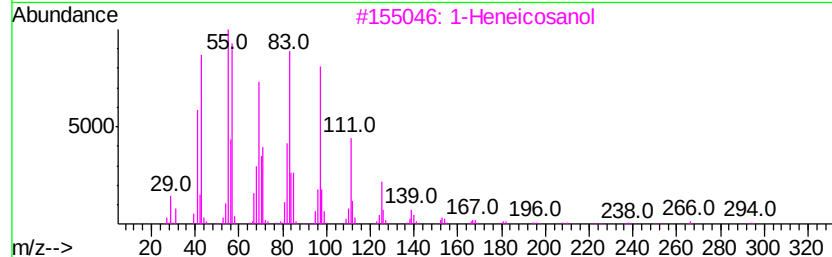
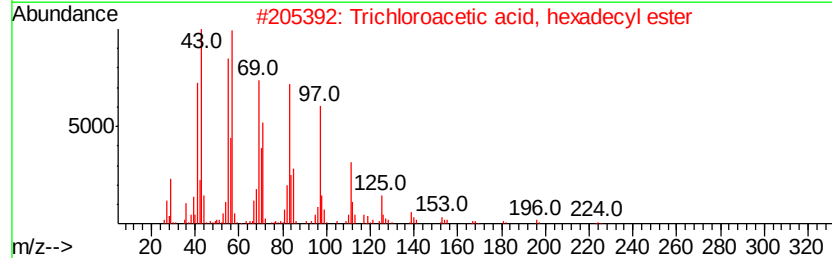
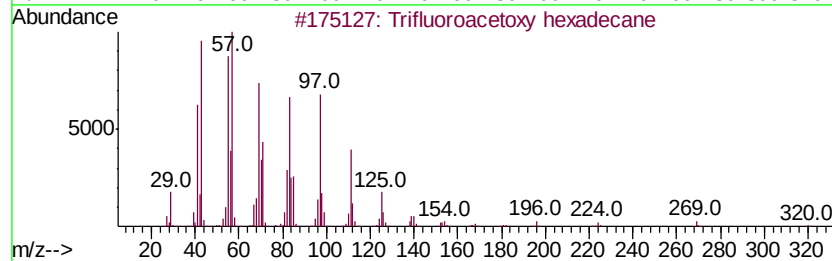
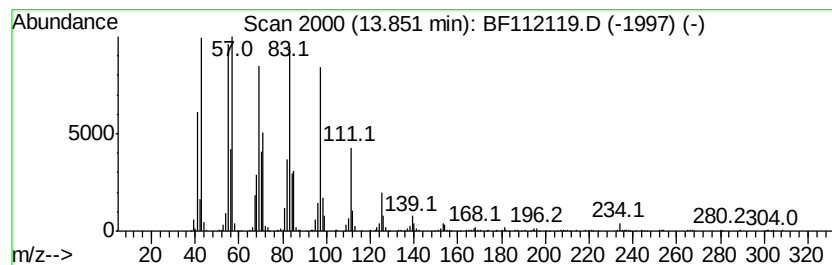
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.85	9.70 ng	1110940	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
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Operator : JU/SJ
Sample : K1157-07
Misc :
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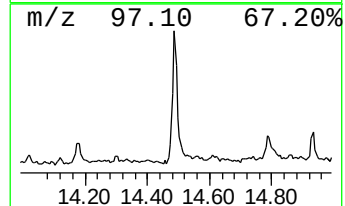
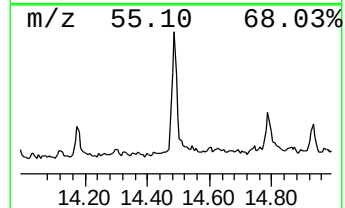
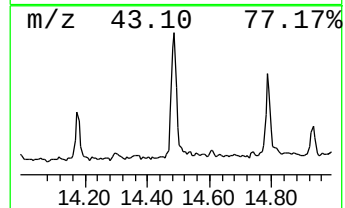
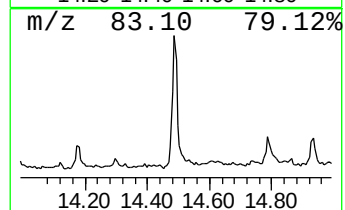
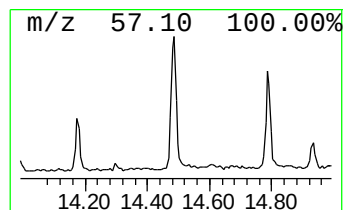
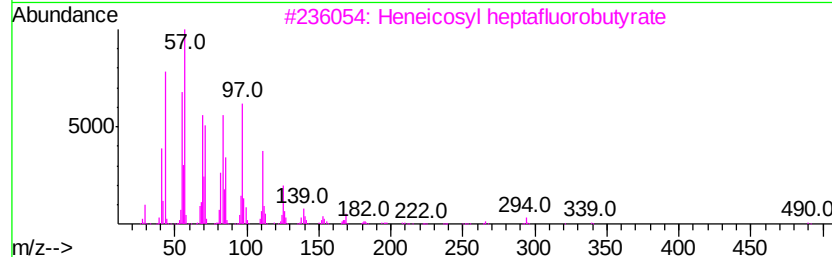
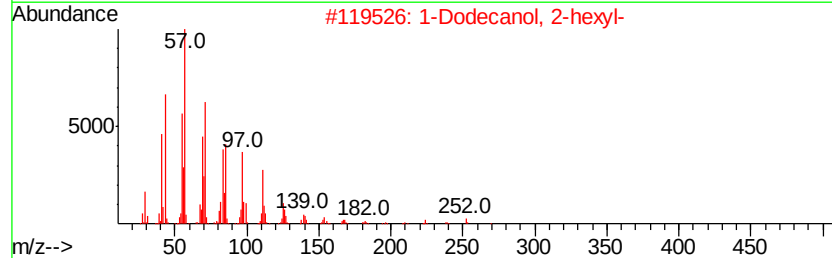
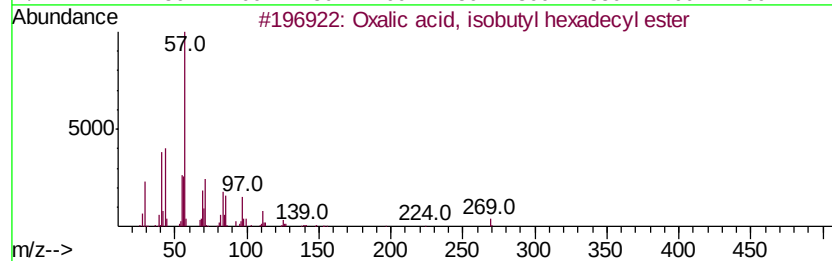
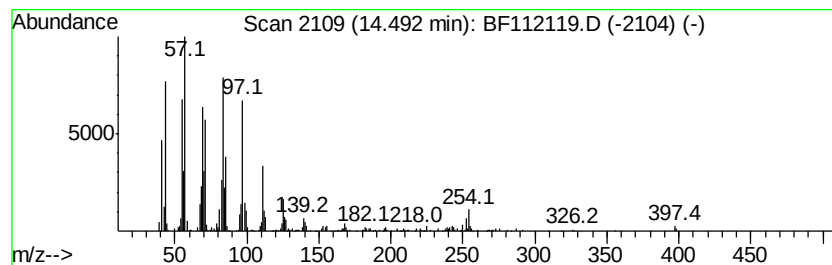
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxalic acid, isobutyl hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.49	5.06 ng	579410	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
2	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	81
3	Heneicosyl heptafluorobutyrte	508	C25H43F7O2	1000351-83-8	76
4	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	76
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
Data File : BF112119.D
Acq On : 18 Jan 2019 11:30
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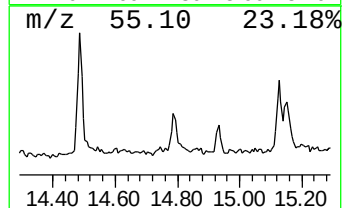
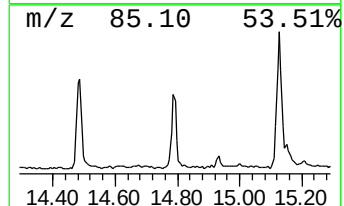
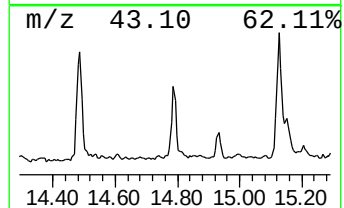
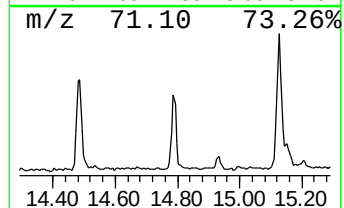
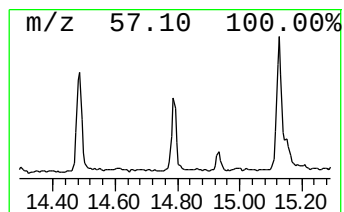
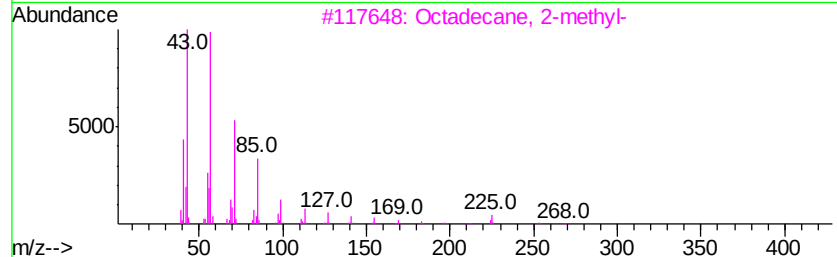
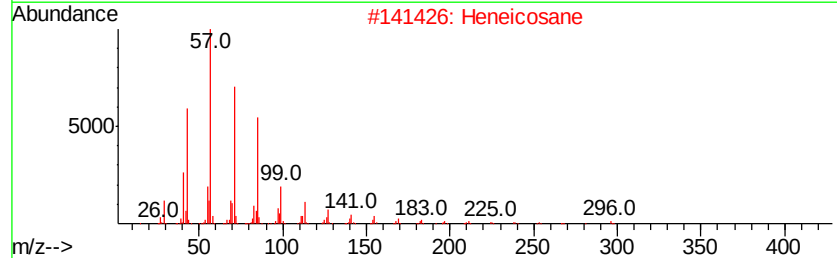
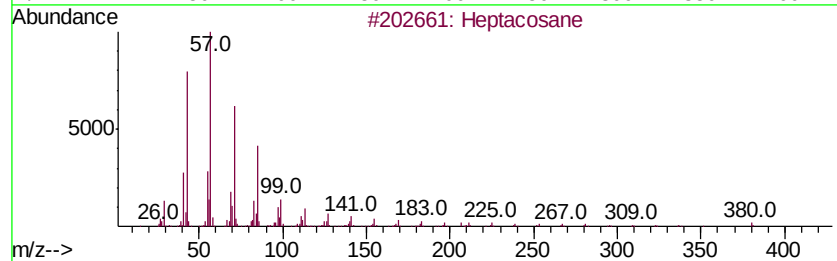
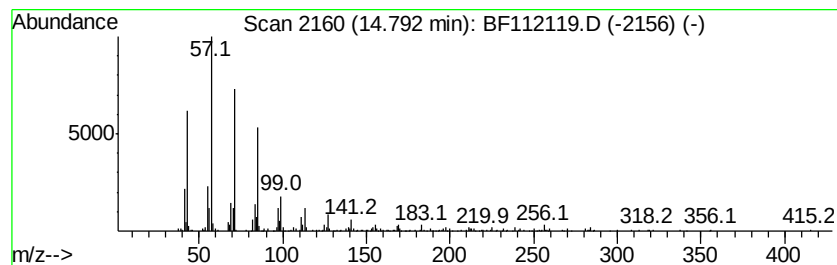
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.27 ng	278829	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Heneicosane		296	C21H44	000629-94-7	90
3	Octadecane, 2-methyl-		268	C19H40	001560-88-9	89
4	Tetracosane		338	C24H50	000646-31-1	87
5	2-methyloctacosane		408	C29H60	1000376-72-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
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Sample : K1157-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

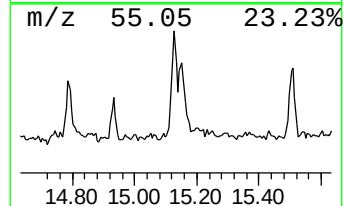
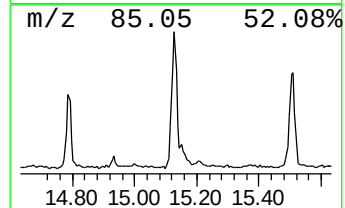
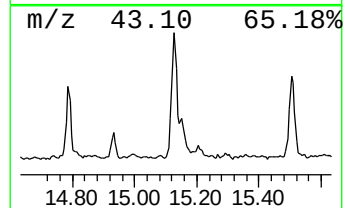
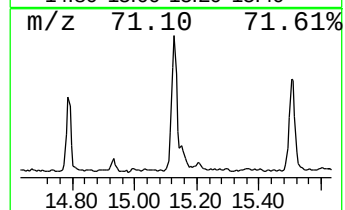
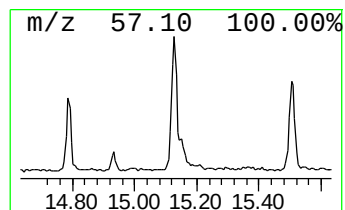
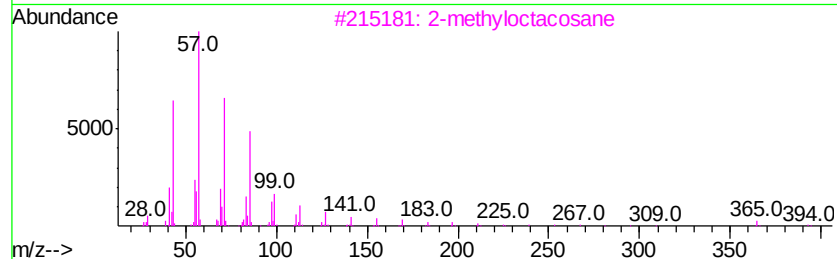
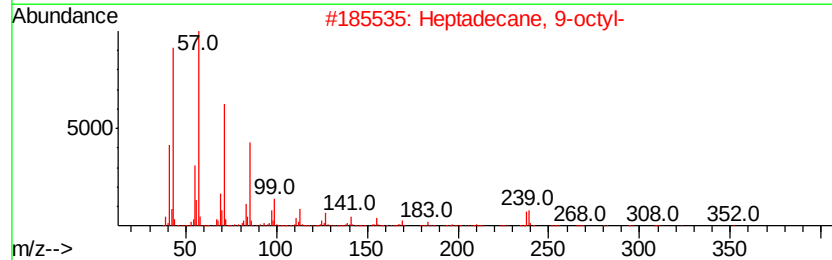
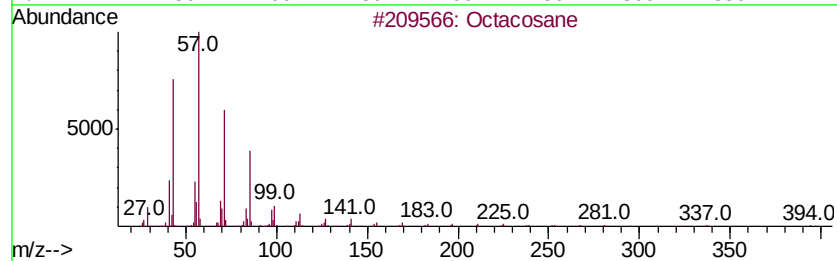
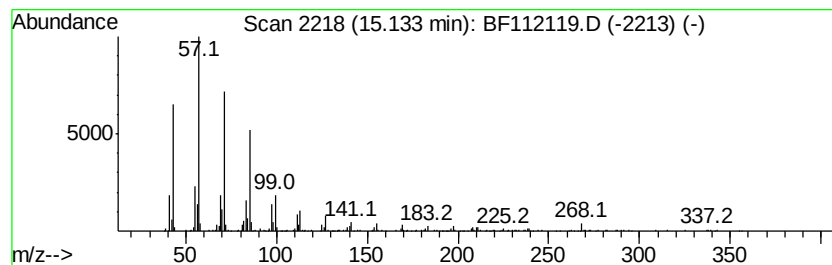
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.13	4.55 ng	558763	Perylene-d12		15.49
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
Data File : BF112119.D
Acq On : 18 Jan 2019 11:30
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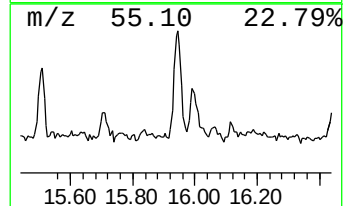
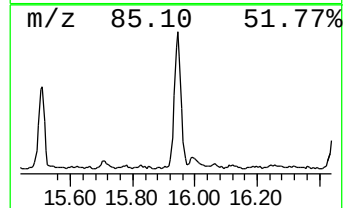
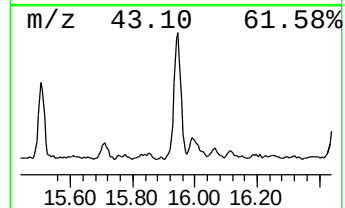
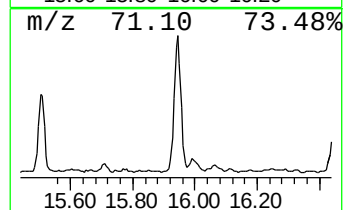
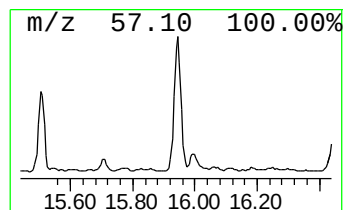
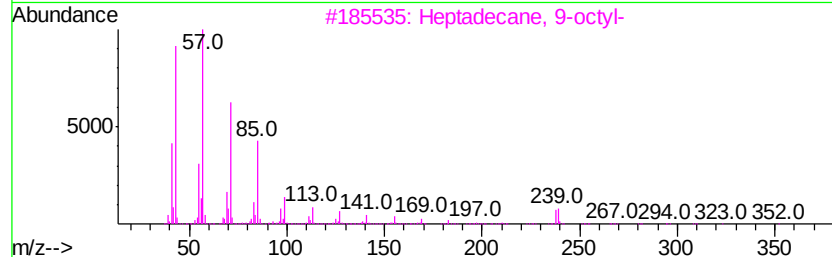
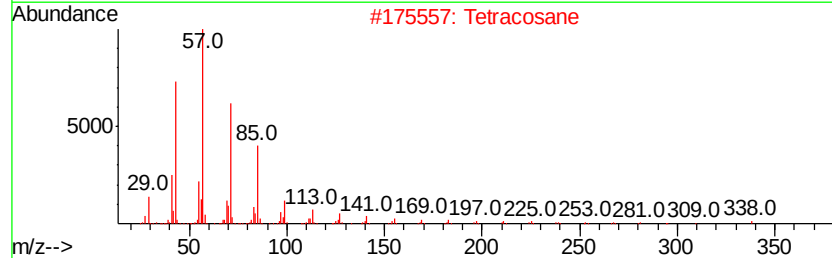
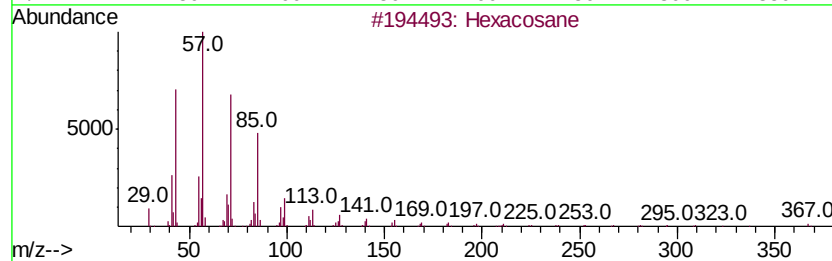
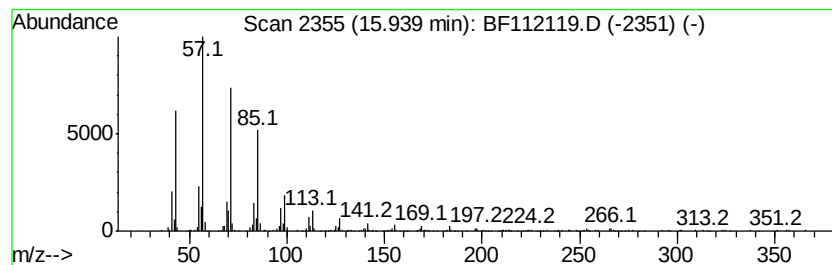
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.94	6.05 ng	742430	Perylene-d12	15.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
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Acq On : 18 Jan 2019 11:30
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Misc :
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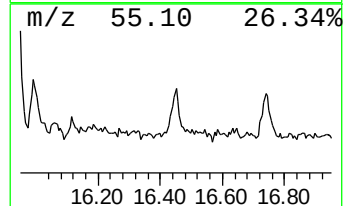
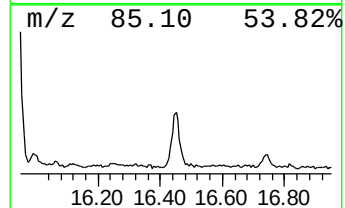
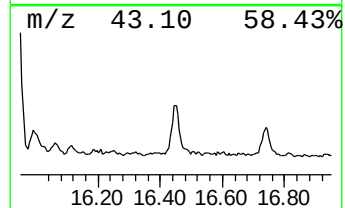
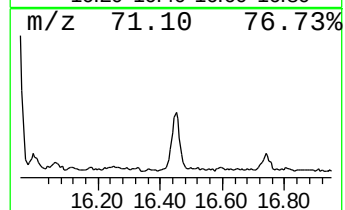
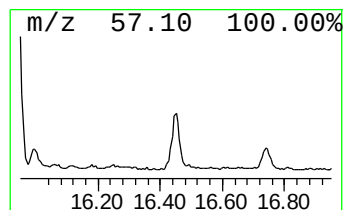
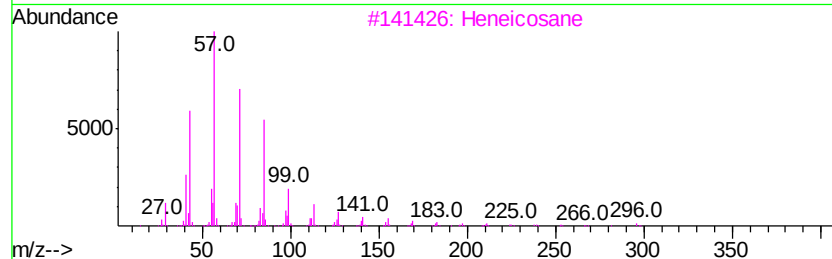
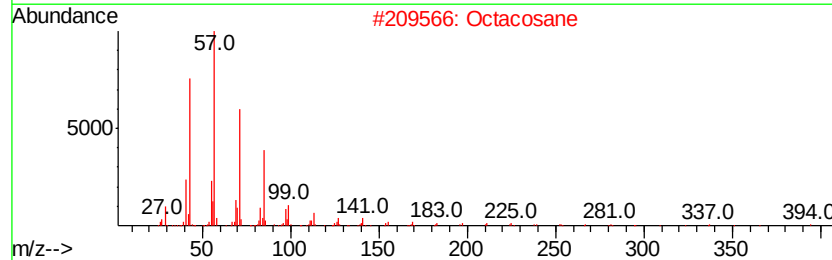
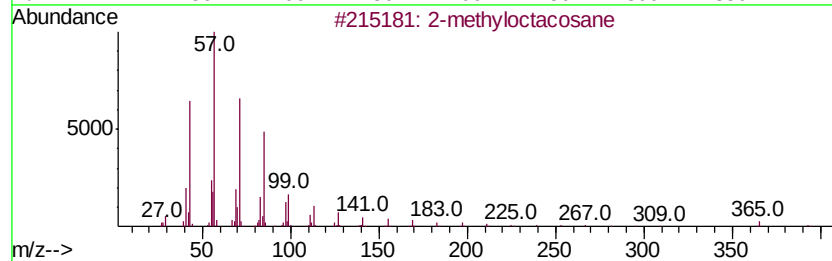
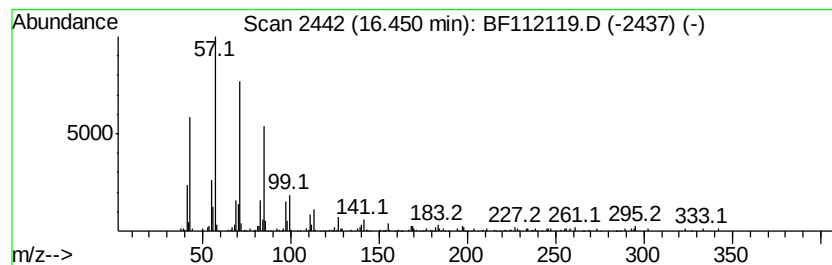
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	2.14 ng	262278	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
Data File : BF112119.D
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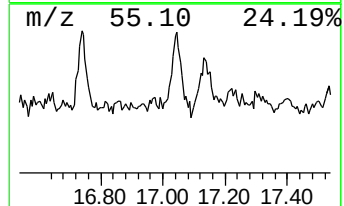
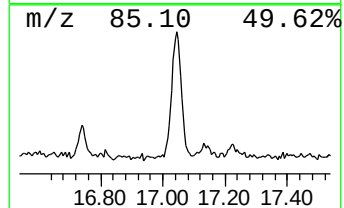
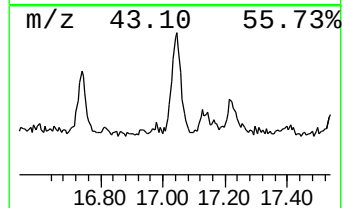
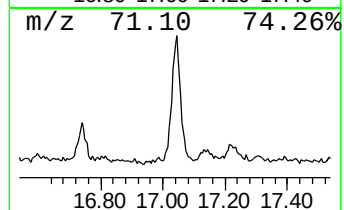
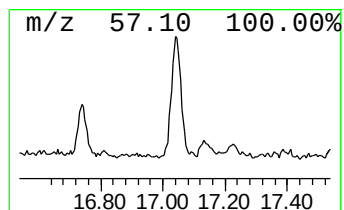
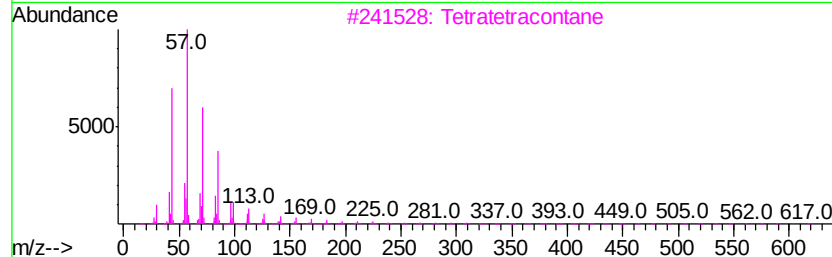
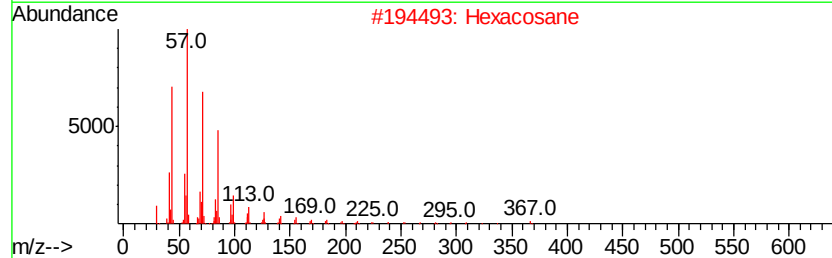
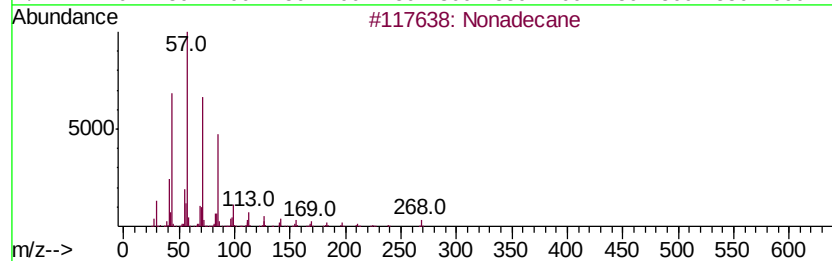
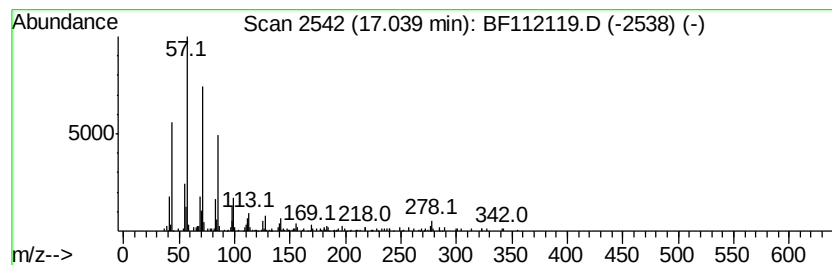
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.04	2.76 ng	339218	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5		Eicosane	282	C20H42	000112-95-8	90



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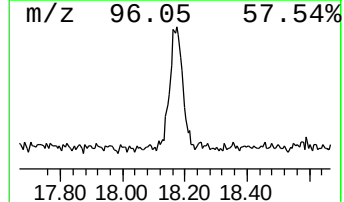
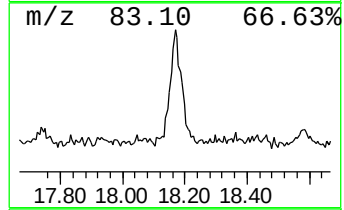
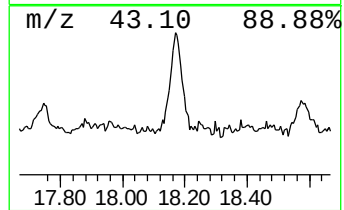
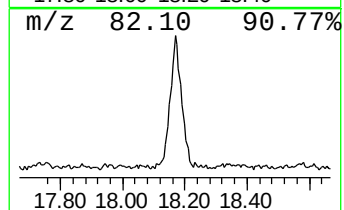
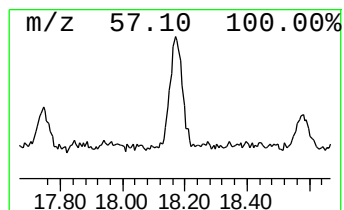
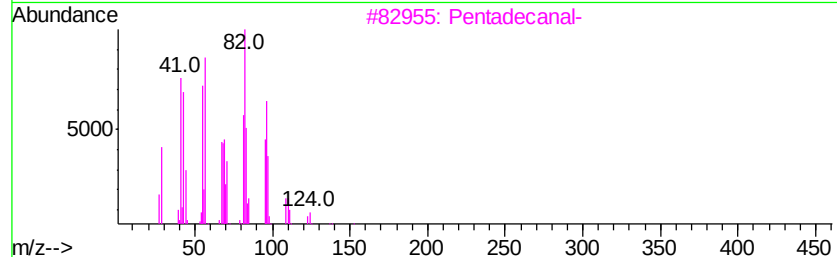
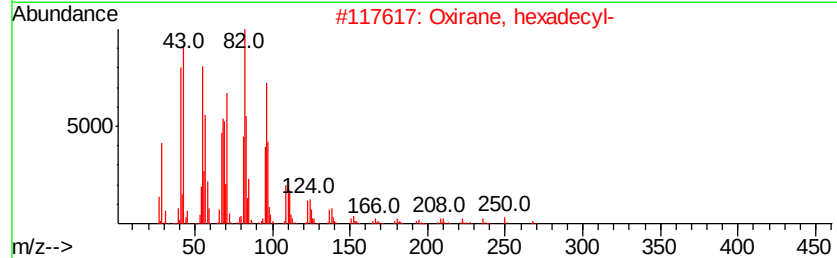
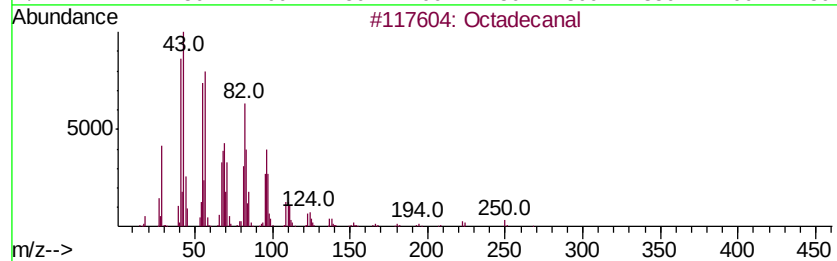
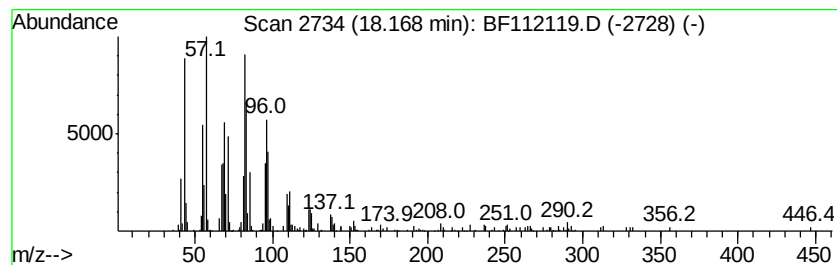
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	4.46 ng	548017	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	90
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	76
3		Pentadecanal-	226	C15H30O	002765-11-9	72
4		1,16-Hexadecanediol	258	C16H34O2	007735-42-4	70
5		1,19-Eicosadiene	278	C20H38	014811-95-1	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011819\
 Data File : BF112119.D
 Acq On : 18 Jan 2019 11:30
 Operator : JU/SJ
 Sample : K1157-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-04-011519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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...	2.16	2.9	ng	281322	1	6.86	1943760	20.0
2-Pentanone, 4-hy...	5.09	5.8	ng	565024	1	6.86	1943760	20.0
unknown6.63	6.63	85.2	ng	8276690	1	6.86	1943760	20.0
n-Hexadecanoic acid	11.90	3.0	ng	369434	4	11.38	2494870	20.0
Trifluoroacetoxy ...	13.85	9.7	ng	1110940	5	14.02	2289500	20.0
Oxalic acid, isob...	14.49	5.1	ng	579410	5	14.02	2289500	20.0
Heptacosane	14.79	2.3	ng	278829	6	15.49	2455060	20.0
Octacosane	15.13	4.5	ng	558763	6	15.49	2455060	20.0
Hexacosane	15.94	6.0	ng	742430	6	15.49	2455060	20.0
2-methyloctacosane	16.45	2.1	ng	262278	6	15.49	2455060	20.0
Nonadecane	17.04	2.8	ng	339218	6	15.49	2455060	20.0
Octadecanal	18.17	4.5	ng	548017	6	15.49	2455060	20.0