

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090718\
 Data File : BF108853.D
 Acq On : 7 Sep 2018 11:58
 Operator : JU/SJ
 Sample : J4803-13
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-Q2-I5

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-BF090518.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	4.925	436	440	448	rVB	134253	171753	3.49%	0.344%
2	5.343	506	511	514	rBV	3852513	3813186	77.39%	7.648%
3	6.366	680	685	688	rBV	3954872	4177499	84.78%	8.378%
4	6.501	704	708	711	rBV	4396602	4061955	82.44%	8.147%
5	6.566	716	719	722	rBV	145312	110913	2.25%	0.222%
6	6.737	744	748	751	rBV	1890468	1571926	31.90%	3.153%
7	6.890	770	774	778	rBV	3437516	3184080	64.62%	6.386%
8	7.295	837	843	846	rBV	2921642	2660648	54.00%	5.336%
9	8.019	961	966	969	rBV	2357217	2091890	42.45%	4.195%
10	9.095	1144	1149	1152	rBV	5352585	4927429	100.00%	9.882%
11	9.219	1167	1170	1173	rVB	83761	69252	1.41%	0.139%
12	9.483	1211	1215	1218	rBV	1728922	1394321	28.30%	2.796%
13	9.766	1259	1263	1267	rBV2	2853083	2385130	48.41%	4.784%
14	10.548	1392	1396	1399	rBV	3197607	2901669	58.89%	5.819%
15	10.648	1410	1413	1416	rBV	147401	125461	2.55%	0.252%
16	10.925	1457	1460	1463	rBV3	84312	83219	1.69%	0.167%
17	11.242	1510	1514	1517	rBV	2784296	2299695	46.67%	4.612%
18	11.707	1591	1593	1597	rBV2	113821	122940	2.50%	0.247%
19	11.789	1603	1607	1614	rVB	861979	857590	17.40%	1.720%
20	12.448	1717	1719	1721	rVB	97137	63157	1.28%	0.127%
21	12.566	1736	1739	1746	rVB	471995	540010	10.96%	1.083%
22	12.824	1779	1783	1787	rBV	4289145	4175622	84.74%	8.374%
23	13.730	1934	1937	1943	rVB	379366	400608	8.13%	0.803%
24	13.866	1956	1960	1963	rBV	1913014	1744242	35.40%	3.498%
25	14.360	2042	2044	2049	rVB	169350	173507	3.52%	0.348%
26	14.630	2087	2090	2092	rBV	247872	256086	5.20%	0.514%
27	14.654	2092	2094	2099	rVV	351437	367977	7.47%	0.738%
28	14.724	2103	2106	2110	rVB	865573	834827	16.94%	1.674%
29	14.977	2145	2149	2155	rVB	595121	673140	13.66%	1.350%
30	15.277	2195	2200	2204	rVV	1352840	1567221	31.81%	3.143%
31	15.336	2205	2210	2218	rVB	666583	892029	18.10%	1.789%
32	15.742	2274	2279	2284	rVB	507042	722312	14.66%	1.449%
33	16.212	2355	2359	2368	rVB2	259760	439932	8.93%	0.882%

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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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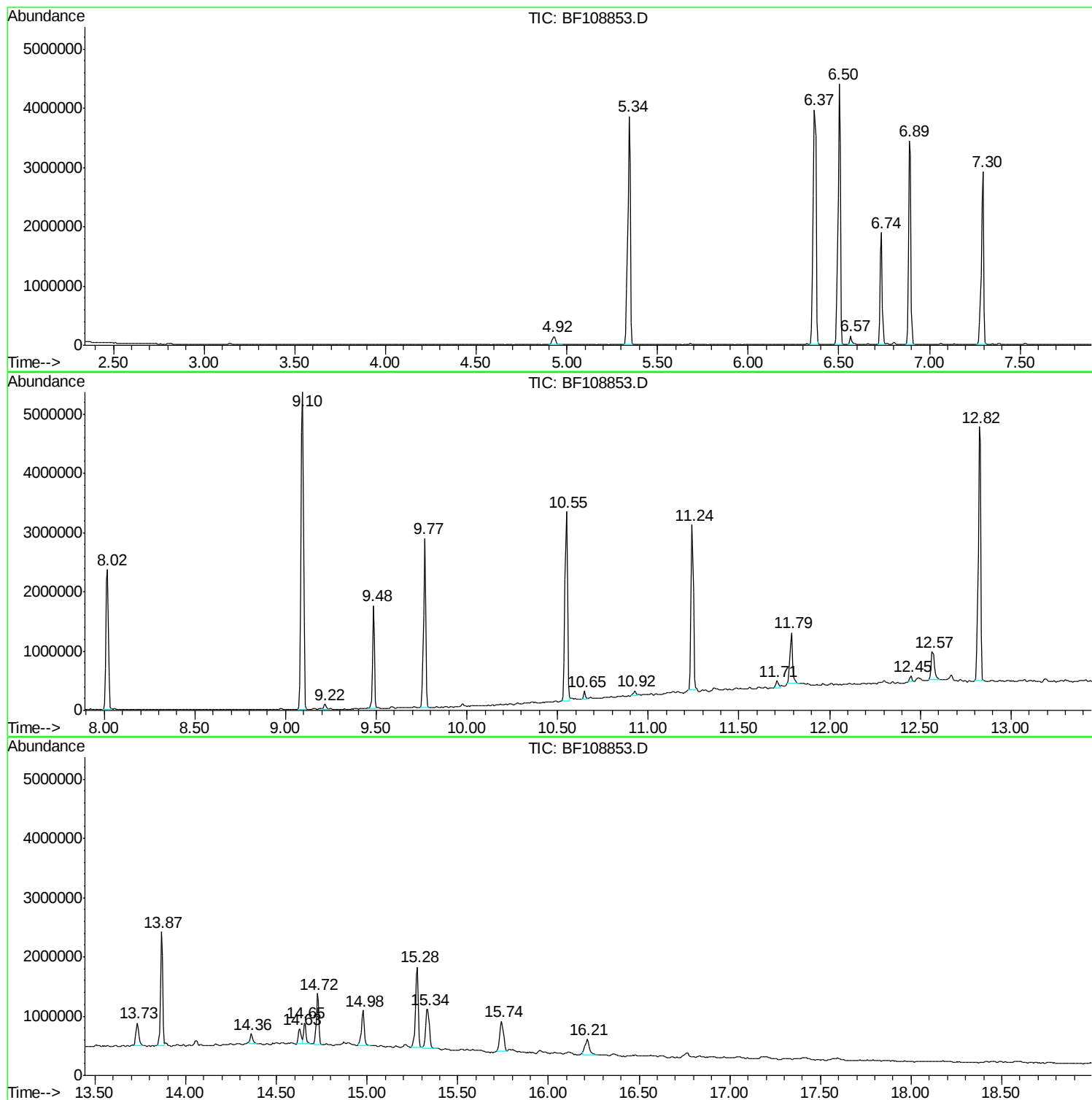
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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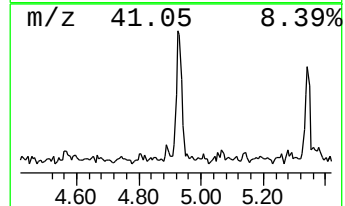
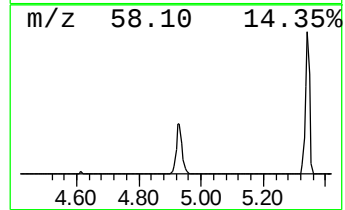
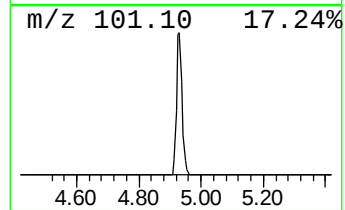
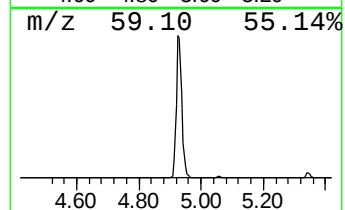
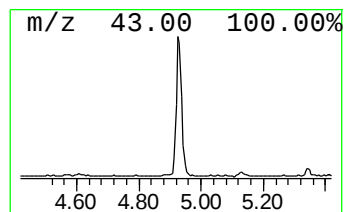
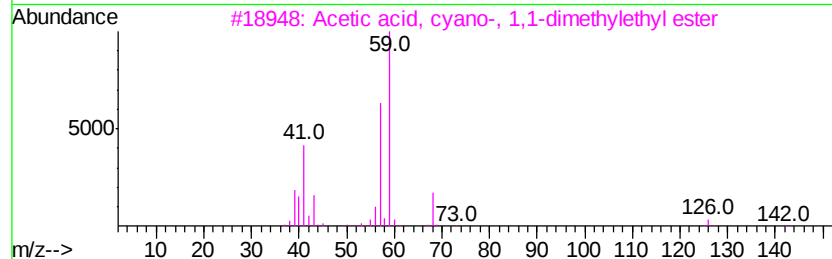
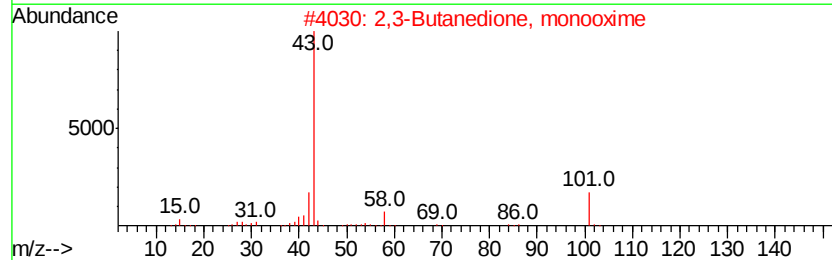
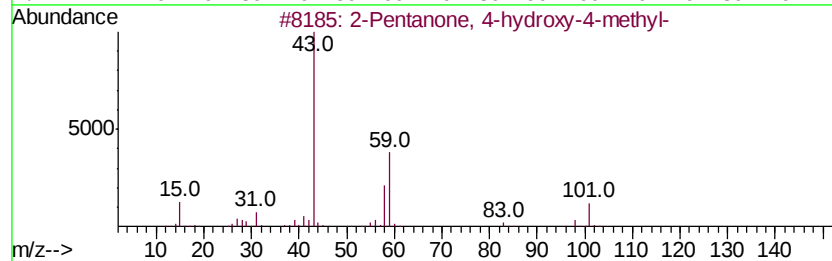
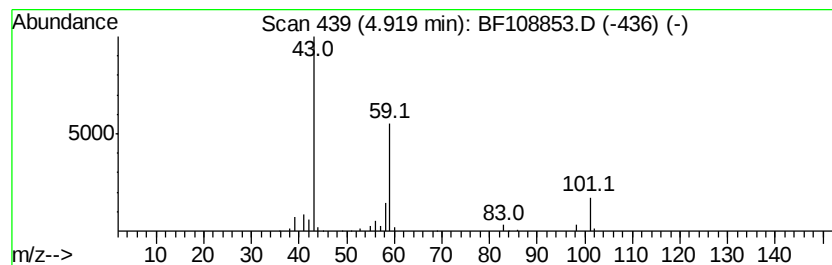
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.19 ng	171753	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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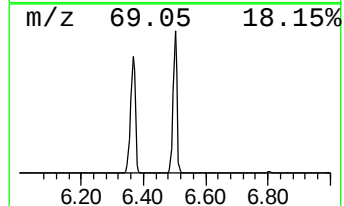
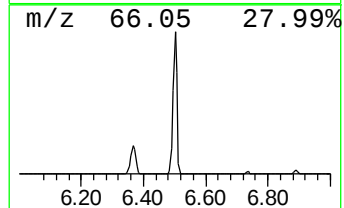
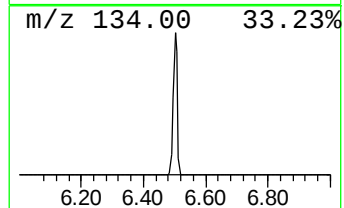
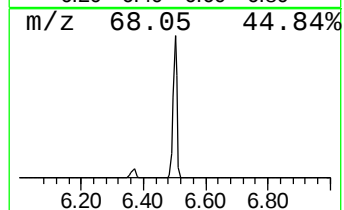
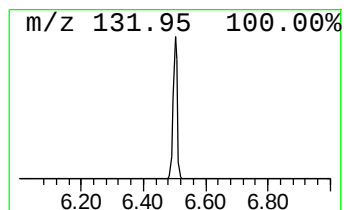
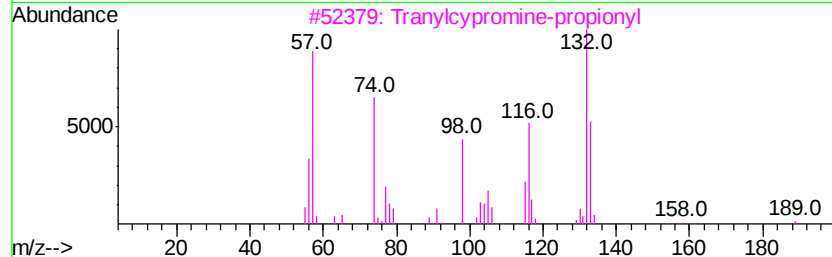
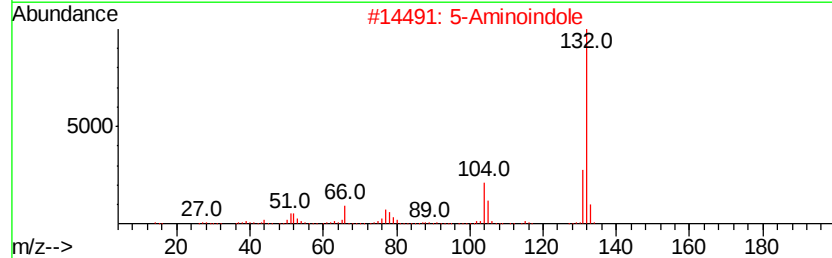
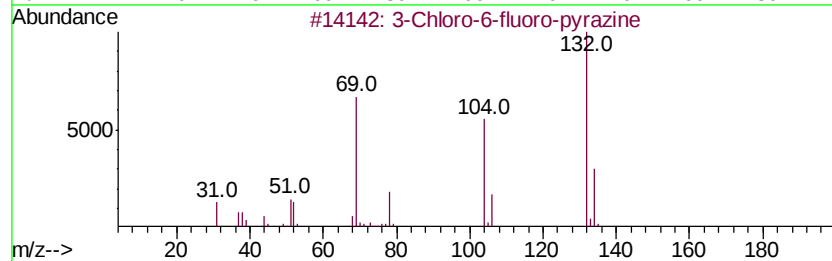
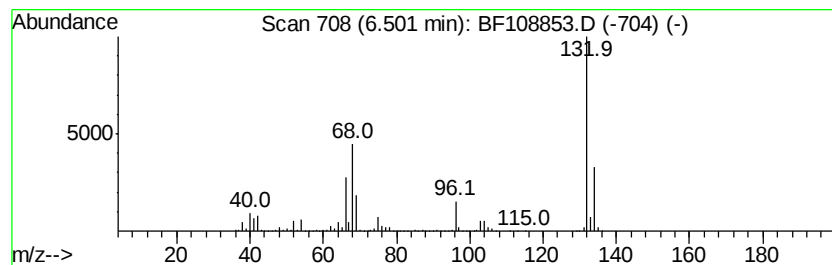
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	51.68 ng	4061960	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5		Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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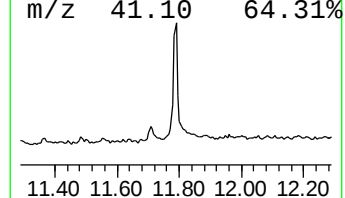
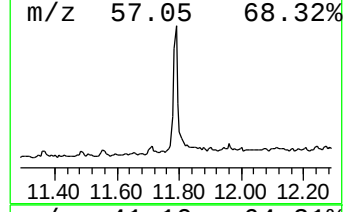
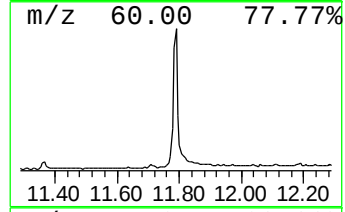
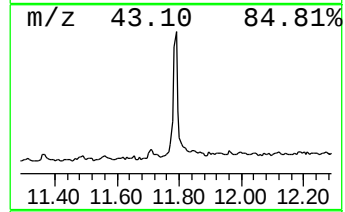
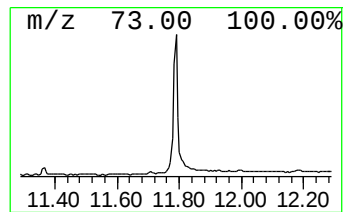
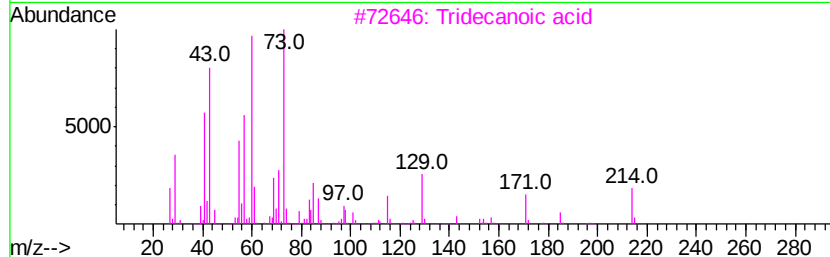
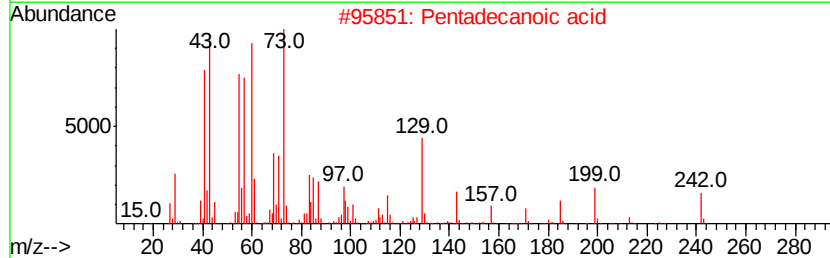
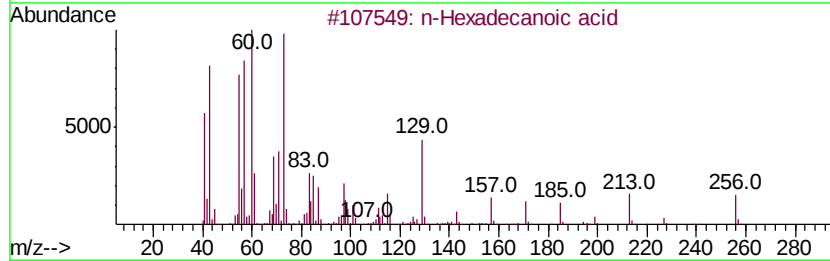
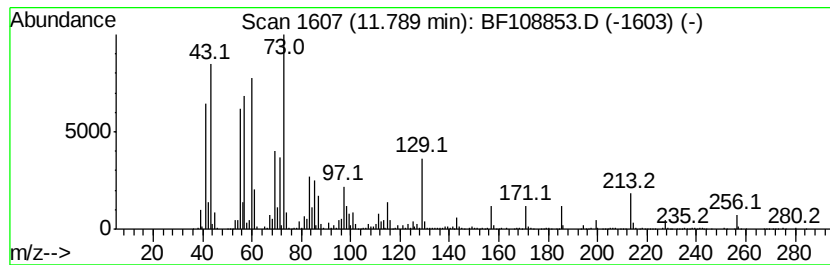
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.79	7.46 ng	857590	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	59



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q2-I5

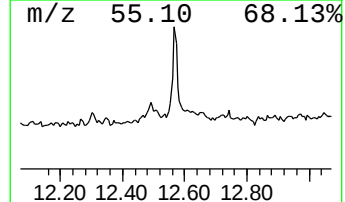
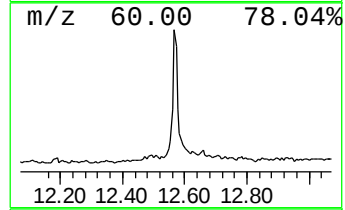
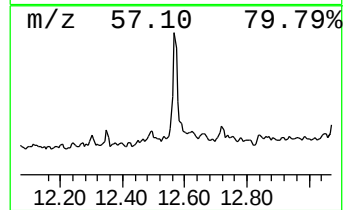
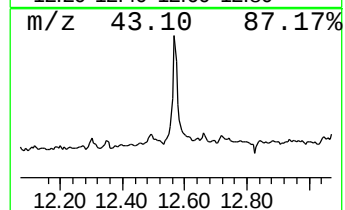
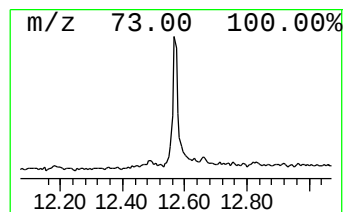
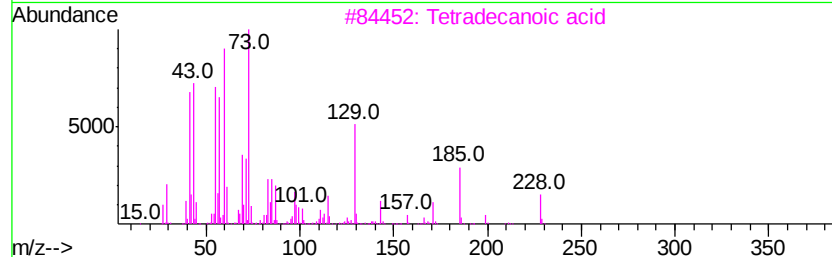
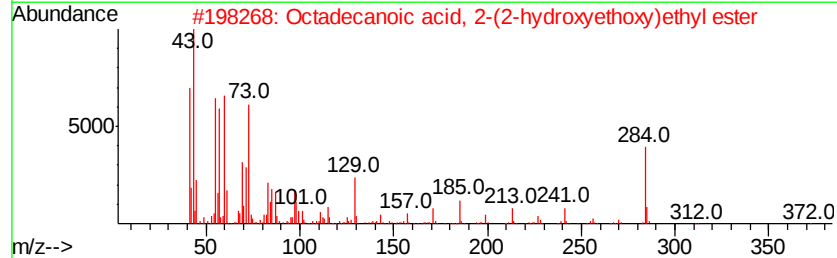
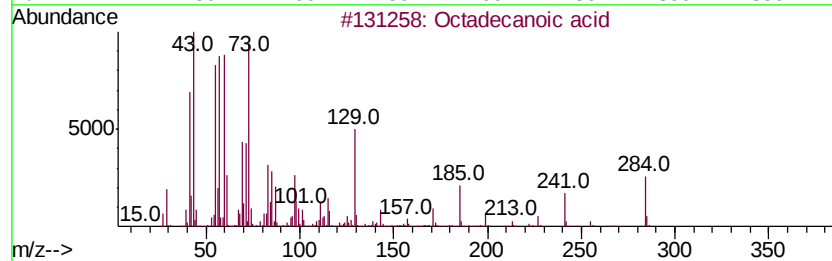
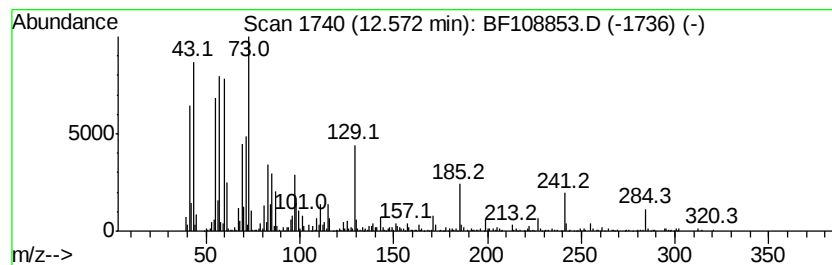
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	6.19 ng	540010	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	80
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



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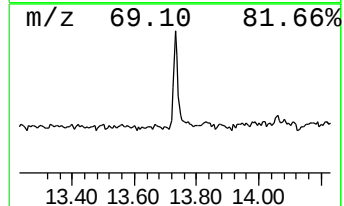
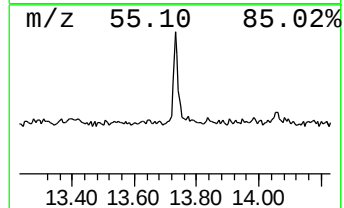
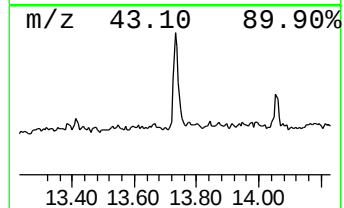
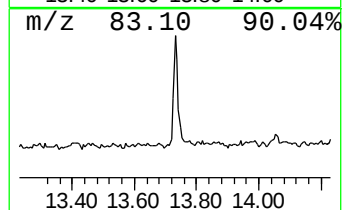
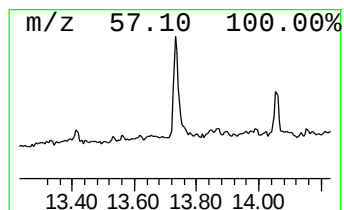
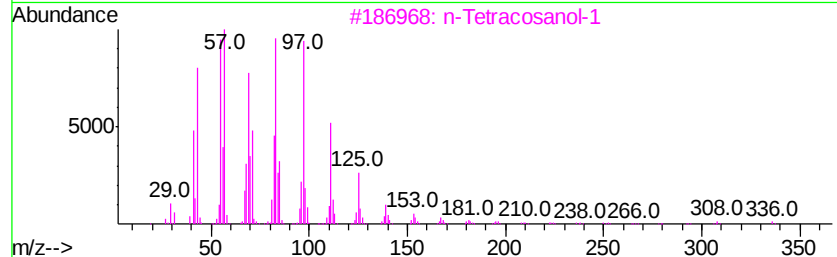
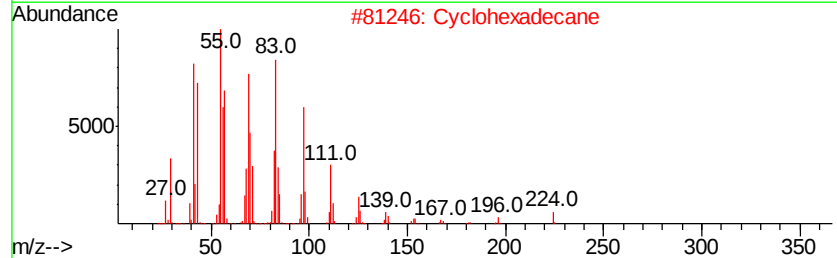
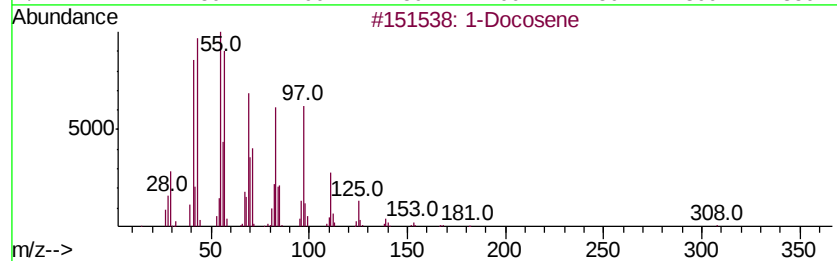
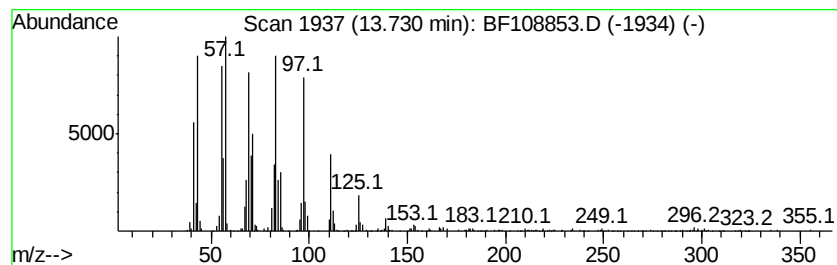
Instrument :
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ClientSampleId :
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Docosene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.59 ng	400608	Chrysene-d12	13.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene	308 C22H44	001599-67-3	99
2	Cyclohexadecane	224 C16H32	000295-65-8	94
3	n-Tetracosanol-1	354 C24H50O	000506-51-4	94
4	Behenic alcohol	326 C22H46O	000661-19-8	94
5	1-Heneicosanol	312 C21H44O	015594-90-8	94



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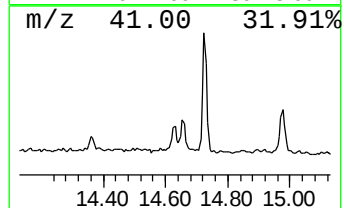
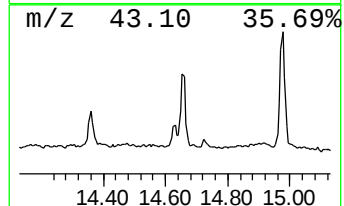
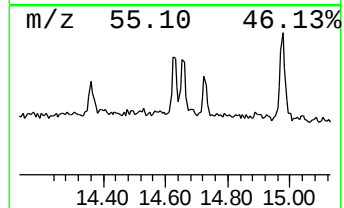
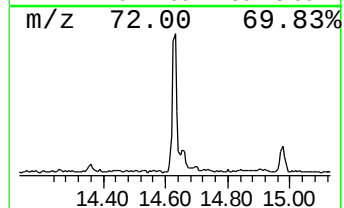
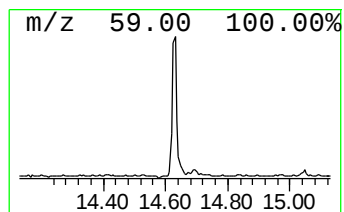
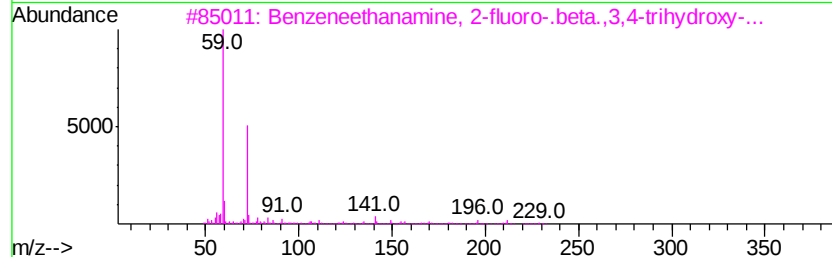
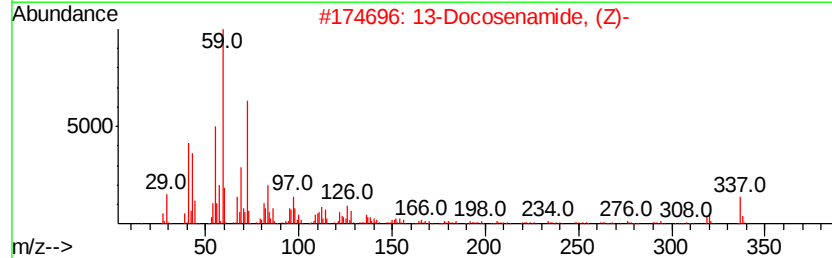
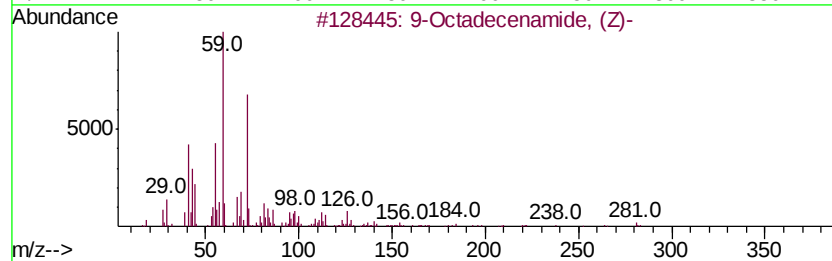
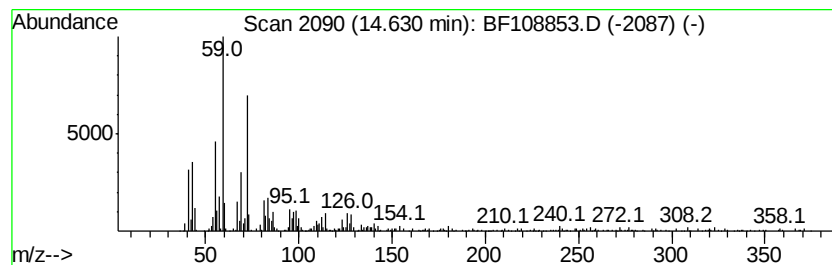
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	3.27 ng	256086	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
4		Octadecanamide	283	C18H37NO	000124-26-5	59
5		Hexadecanamide	255	C16H33NO	000629-54-9	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
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Acq On : 7 Sep 2018 11:58
Operator : JU/SJ
Sample : J4803-13
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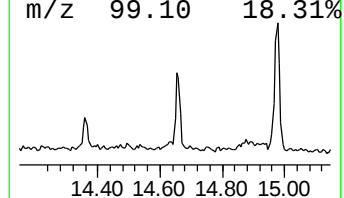
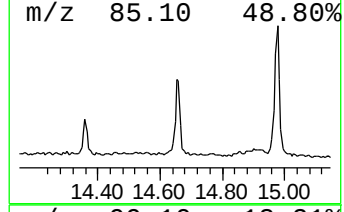
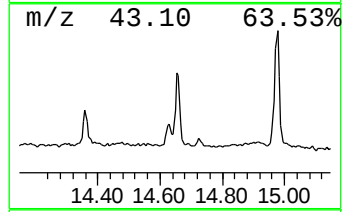
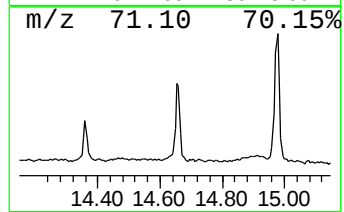
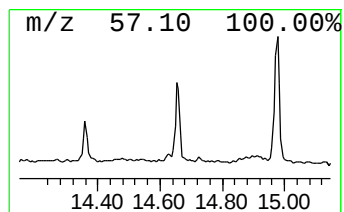
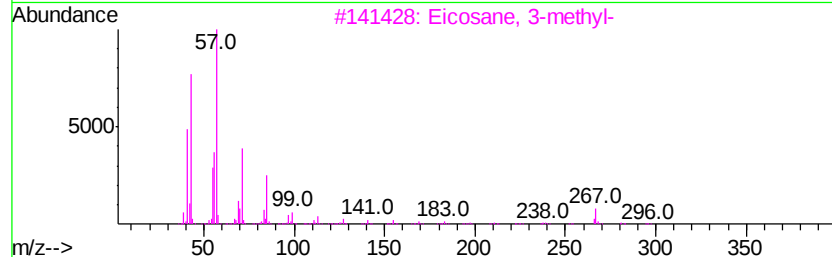
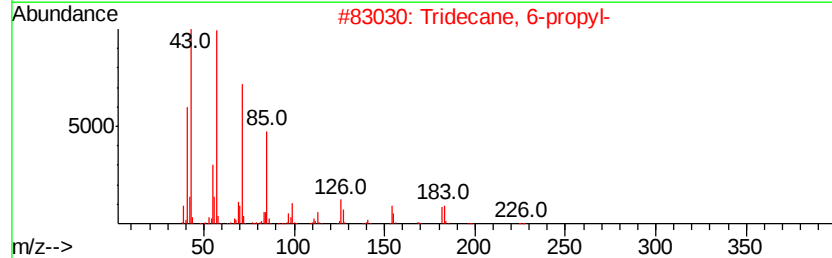
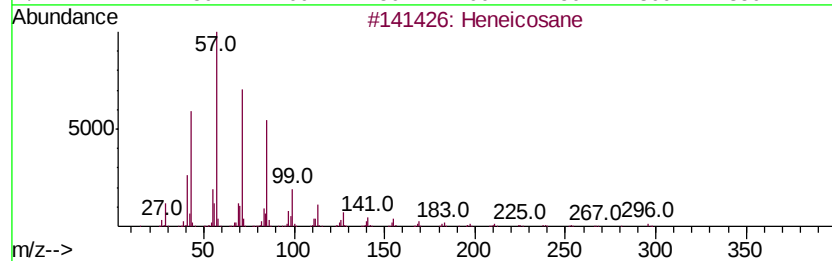
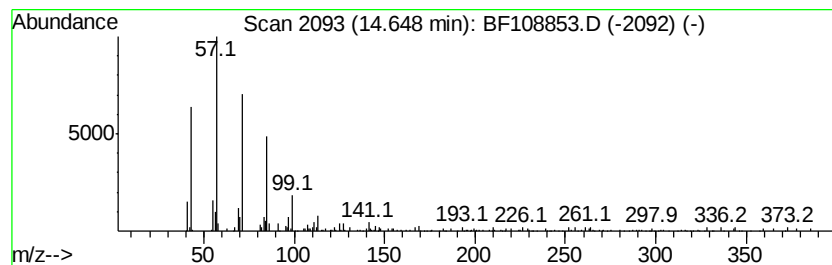
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane, 6-propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	4.70 ng	367977	Perylene-d12	15.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Heneicosane	296 C21H44	000629-94-7 90
2		Tridecane, 6-propyl-	226 C16H34	055045-10-8 87
3		Eicosane, 3-methyl-	296 C21H44	006418-46-8 80
4		Heptacosane	380 C27H56	000593-49-7 80
5		Tetracosane	338 C24H50	000646-31-1 72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
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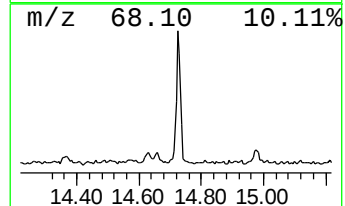
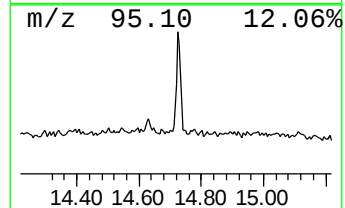
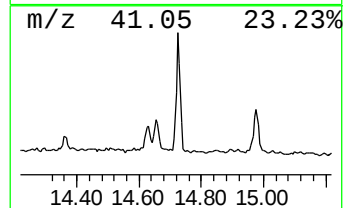
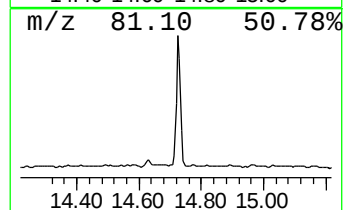
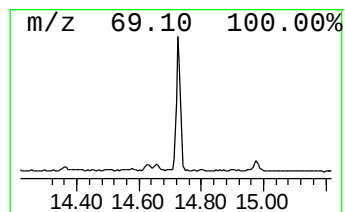
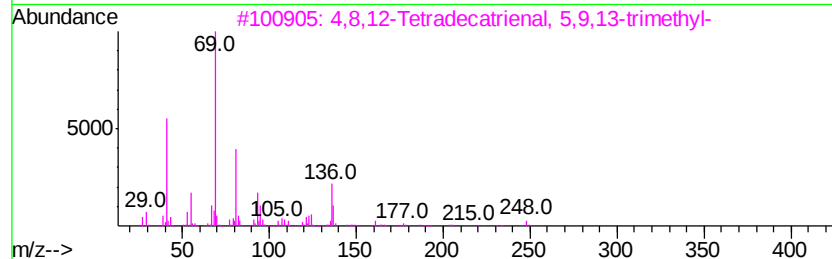
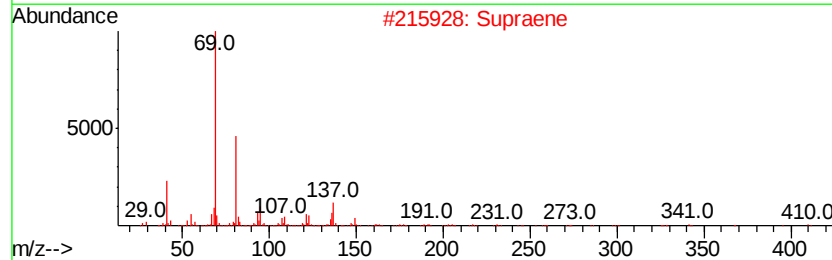
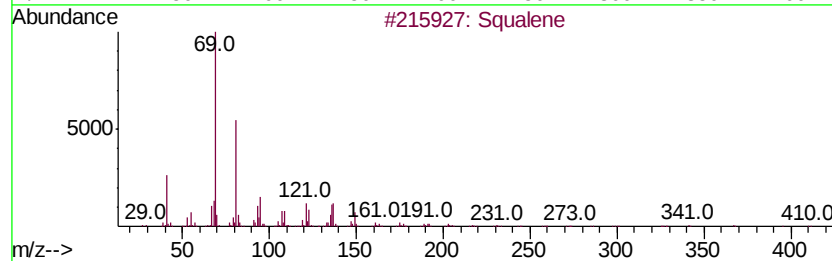
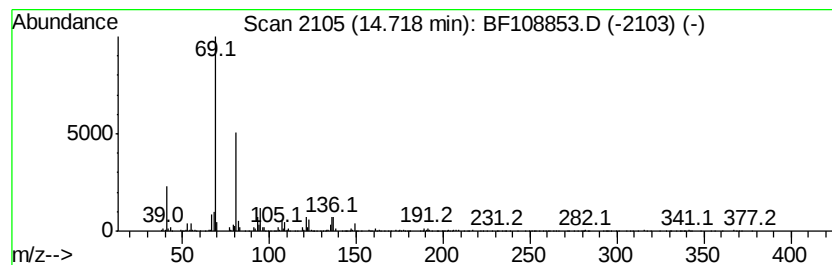
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	10.65 ng	834827	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	97
2		Supraene	410	C30H50	007683-64-9	91
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58
5		2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
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Acq On : 7 Sep 2018 11:58
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ClientSampleId :
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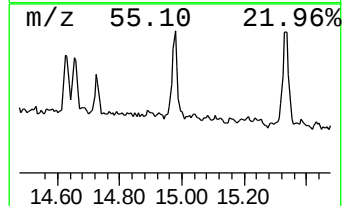
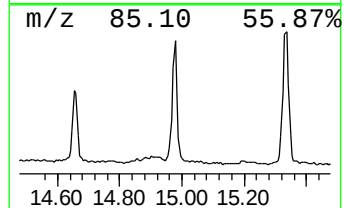
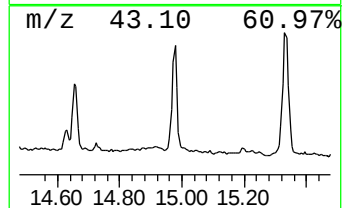
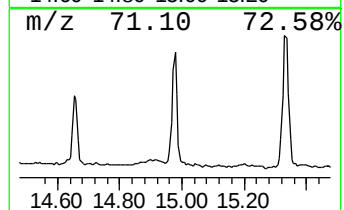
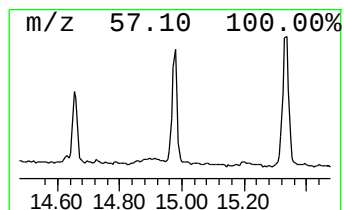
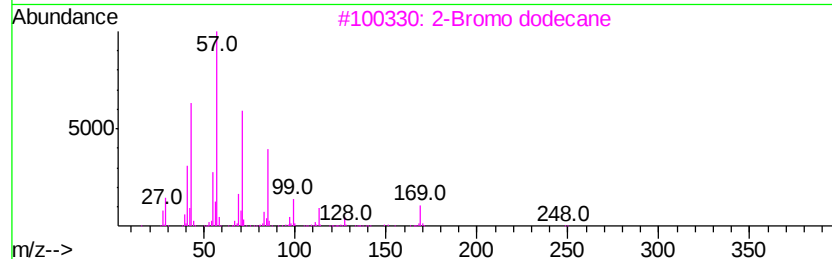
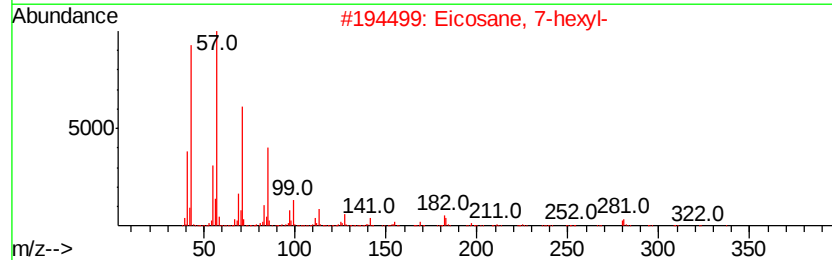
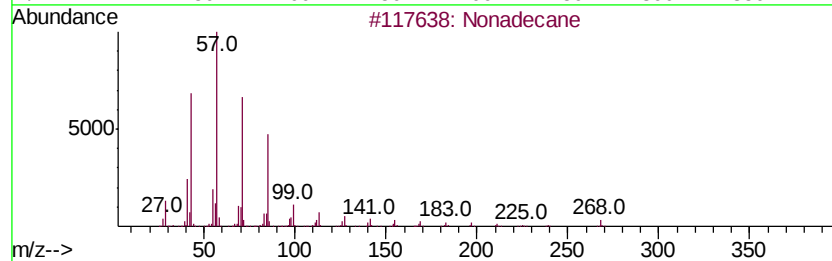
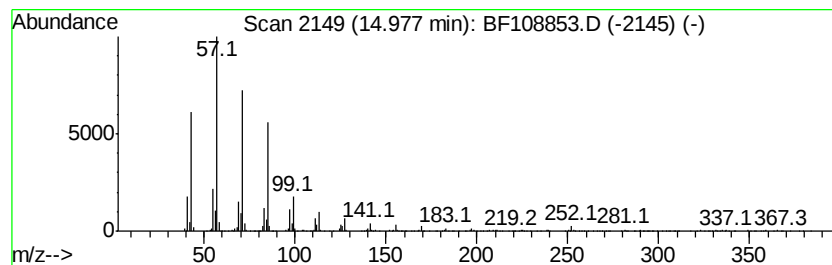
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	8.59 ng	673140	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	86
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	76
4		Eicosane, 2-methyl-	296	C21H44	001560-84-5	72
5		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
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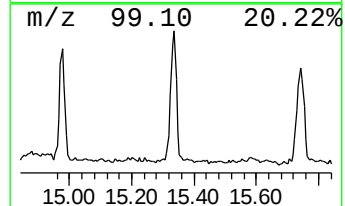
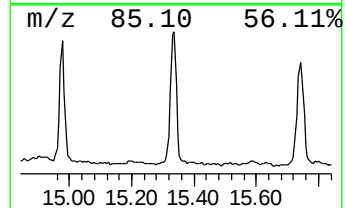
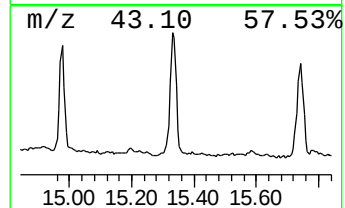
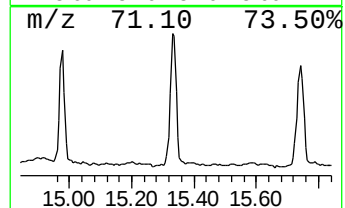
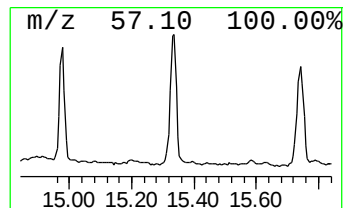
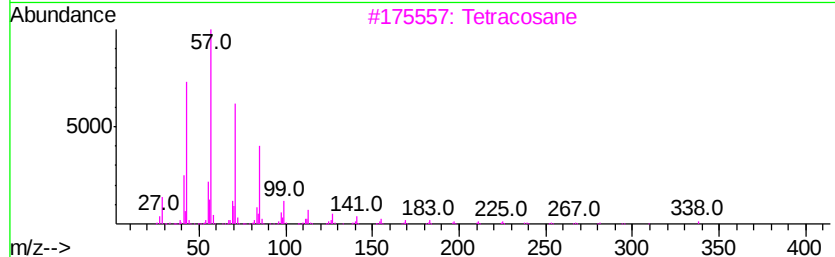
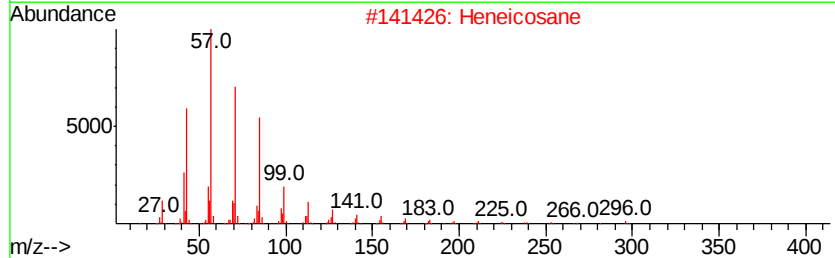
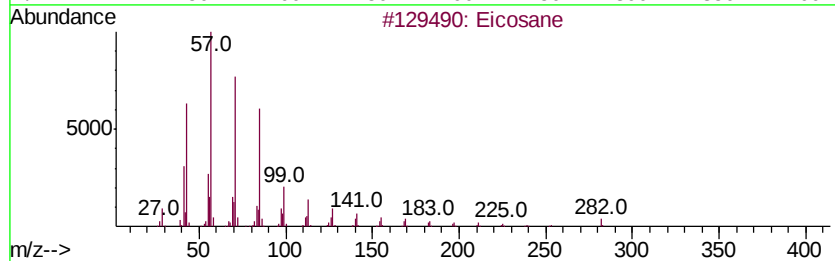
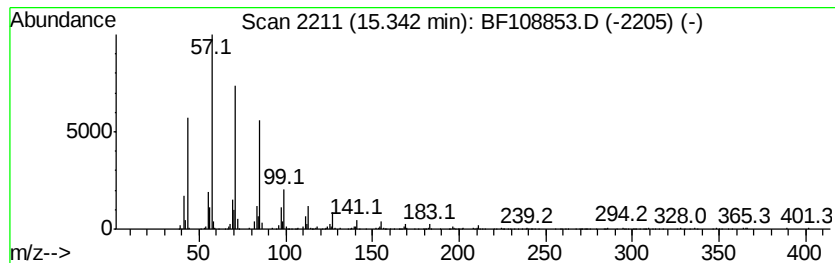
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	11.38 ng	892029	Perylene-d12	15.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Heneicosane	296 C21H44	000629-94-7	91
3	Tetracosane	338 C24H50	000646-31-1	90
4	Hexadecane	226 C16H34	000544-76-3	87
5	Octadecane, 1-iodo-	380 C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
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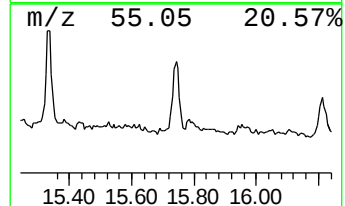
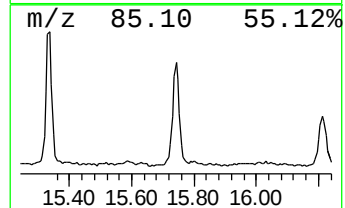
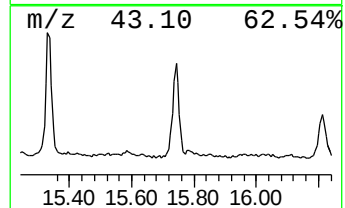
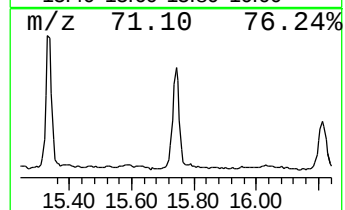
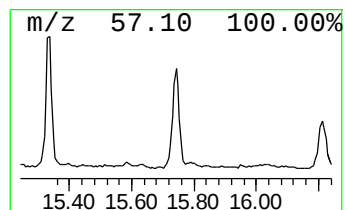
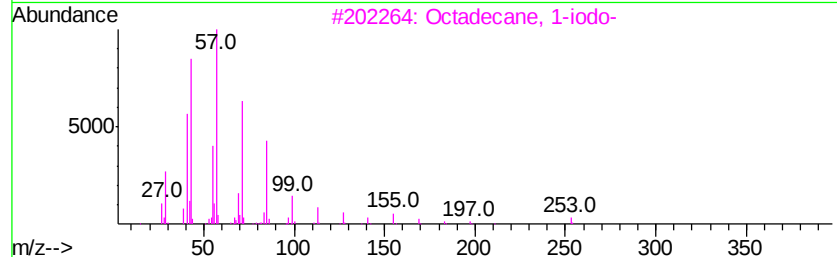
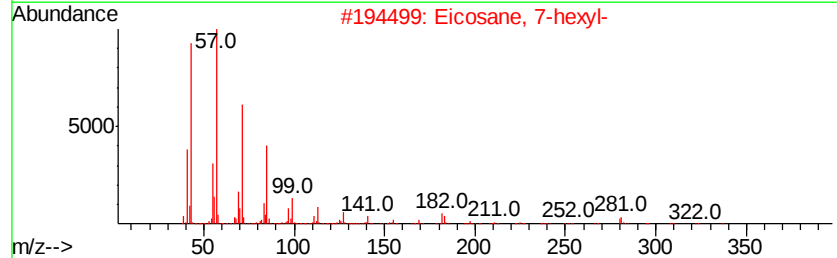
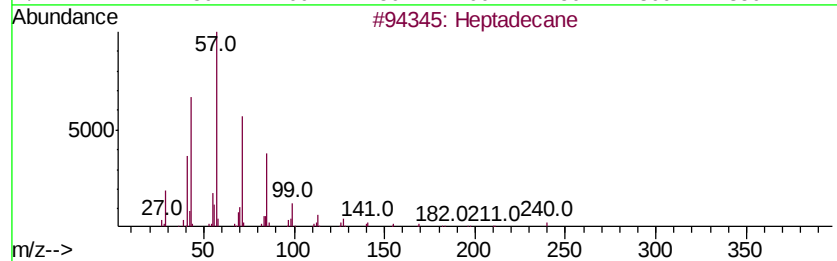
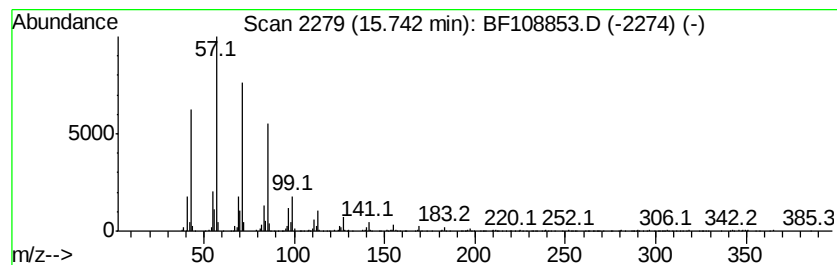
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	9.22 ng	722312	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	90
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4		Octadecane	254	C18H38	000593-45-3	87
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
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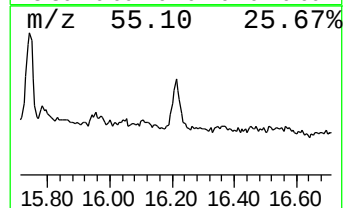
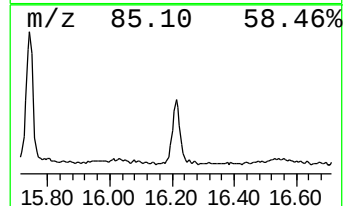
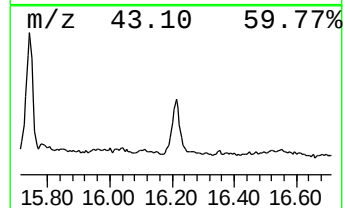
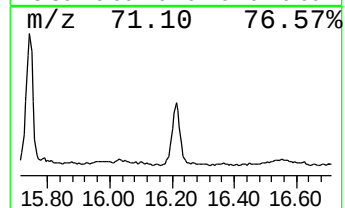
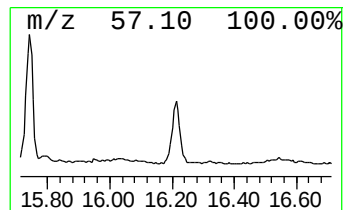
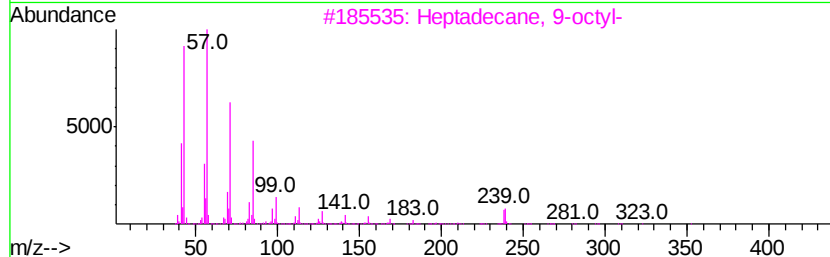
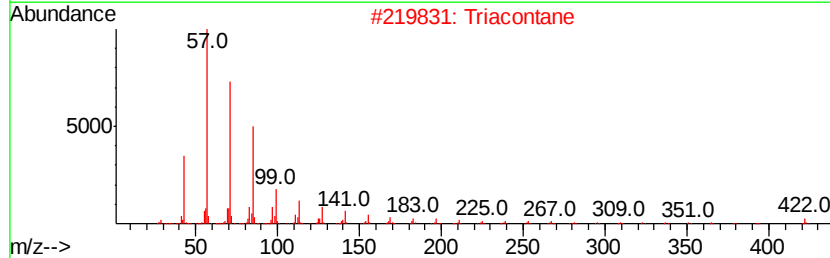
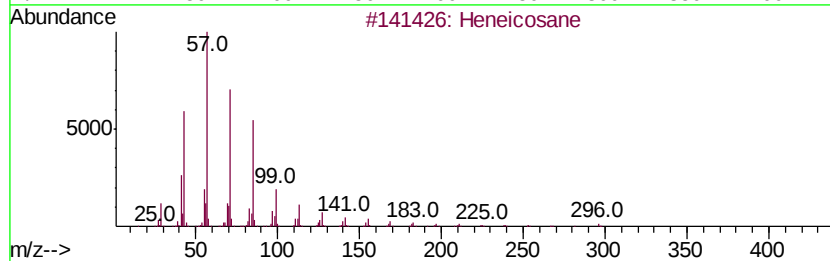
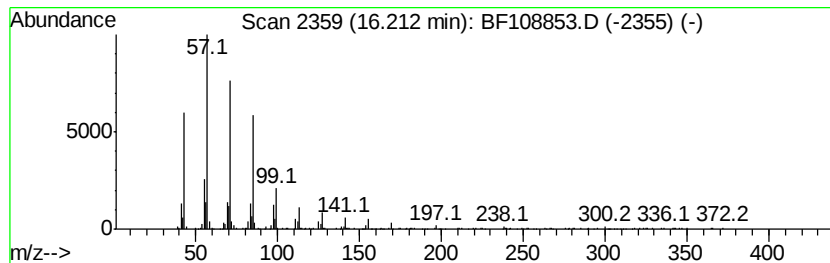
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	5.61 ng	439932	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090718\
Data File : BF108853.D
Acq On : 7 Sep 2018 11:58
Operator : JU/SJ
Sample : J4803-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q2-I5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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
2-Pentanone, 4-hy...	4.92	2.2	ng	171753	1	6.74	1571930	20.0
unknown6.50	6.50	51.7	ng	4061960	1	6.74	1571930	20.0
n-Hexadecanoic acid	11.79	7.5	ng	857590	4	11.24	2299700	20.0
Octadecanoic acid	12.57	6.2	ng	540010	5	13.87	1744240	20.0
1-Docosene	13.73	4.6	ng	400608	5	13.87	1744240	20.0
9-Octadecenamide,...	14.63	3.3	ng	256086	6	15.28	1567220	20.0
Tridecane, 6-propyl-	14.65	4.7	ng	367977	6	15.28	1567220	20.0
Squalene	14.72	10.7	ng	834827	6	15.28	1567220	20.0
Nonadecane	14.98	8.6	ng	673140	6	15.28	1567220	20.0
Eicosane	15.34	11.4	ng	892029	6	15.28	1567220	20.0
Heptadecane	15.74	9.2	ng	722312	6	15.28	1567220	20.0
Heneicosane	16.21	5.6	ng	439932	6	15.28	1567220	20.0