

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092818\
 Data File : BF109438.D
 Acq On : 28 Sep 2018 18:58
 Operator : JU/SJ
 Sample : J5077-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PARCEL-190-092418-2

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-BF092218.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	4.898	475	478	488	rBV	51655	64750	3.79%	0.383%
2	5.322	545	550	553	rBV	1768178	1628853	95.44%	9.637%
3	6.351	720	725	736	rBV	1787567	1684163	98.68%	9.964%
4	6.481	743	747	750	rBV	1961650	1706661	100.00%	10.097%
5	6.710	782	786	789	rBV	710896	564380	33.07%	3.339%
6	6.869	809	813	816	rBV	1491626	1355790	79.44%	8.021%
7	7.269	876	881	884	rBV	1215985	1008324	59.08%	5.965%
8	7.992	1000	1004	1007	rBV	719575	625291	36.64%	3.699%
9	9.063	1183	1186	1194	rBV	1891017	1569572	91.97%	9.286%
10	9.457	1249	1253	1260	rBV	555742	459190	26.91%	2.717%
11	9.739	1297	1301	1306	rBV	728278	602453	35.30%	3.564%
12	10.522	1430	1434	1440	rBV	994876	884533	51.83%	5.233%
13	11.180	1542	1546	1549	rBV3	23780	34889	2.04%	0.206%
14	11.216	1549	1552	1555	rVV	709565	605916	35.50%	3.585%
15	11.239	1555	1556	1559	rVB	54572	30066	1.76%	0.178%
16	11.722	1634	1638	1640	rBV2	15585	18838	1.10%	0.111%
17	11.757	1640	1644	1648	rBV2	222459	227166	13.31%	1.344%
18	12.033	1684	1691	1695	rBV9	18930	33592	1.97%	0.199%
19	12.345	1742	1744	1748	rBV	21428	22237	1.30%	0.132%
20	12.422	1754	1757	1760	rBV	184611	168363	9.87%	0.996%
21	12.539	1774	1777	1783	rBV3	65979	84617	4.96%	0.501%
22	12.651	1791	1796	1799	rBV	148170	151791	8.89%	0.898%
23	12.798	1817	1821	1824	rBV	1589421	1306639	76.56%	7.730%
24	12.980	1850	1852	1855	rVB3	31332	27312	1.60%	0.162%
25	13.710	1973	1976	1983	rBV	130891	200703	11.76%	1.187%
26	13.845	1995	1999	2002	rBV2	626090	639539	37.47%	3.784%
27	14.621	2129	2131	2134	rBV	95496	110128	6.45%	0.652%
28	14.692	2141	2143	2147	rVB	158222	133775	7.84%	0.791%
29	14.939	2183	2185	2190	rVB2	179341	189092	11.08%	1.119%
30	15.251	2235	2238	2241	rBV	281618	301160	17.65%	1.782%
31	15.292	2242	2245	2249	rVB	193493	245865	14.41%	1.455%
32	15.698	2310	2314	2318	rBV	163775	217268	12.73%	1.285%

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

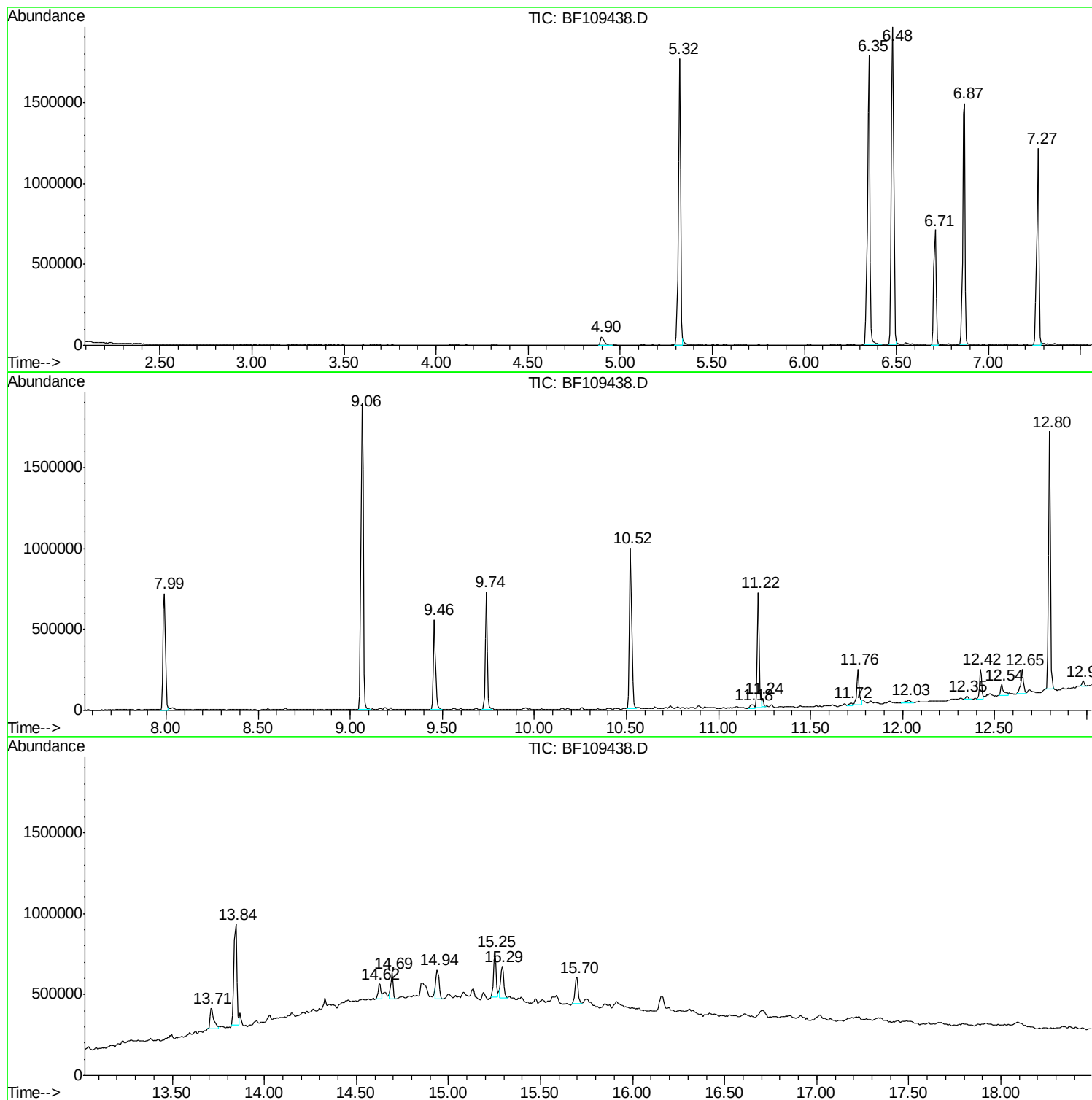
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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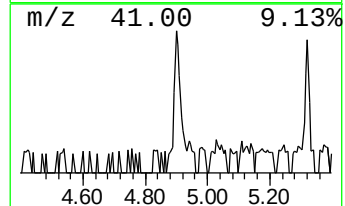
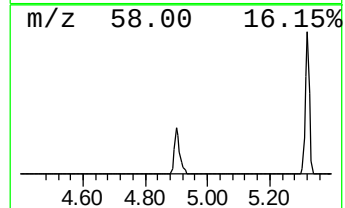
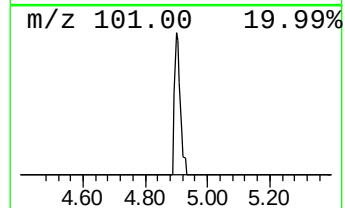
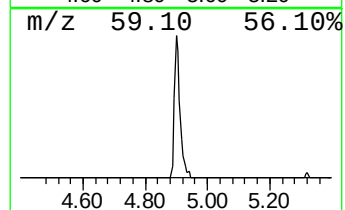
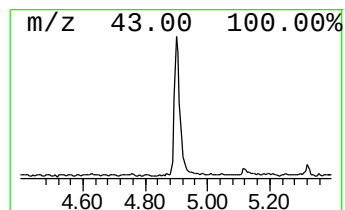
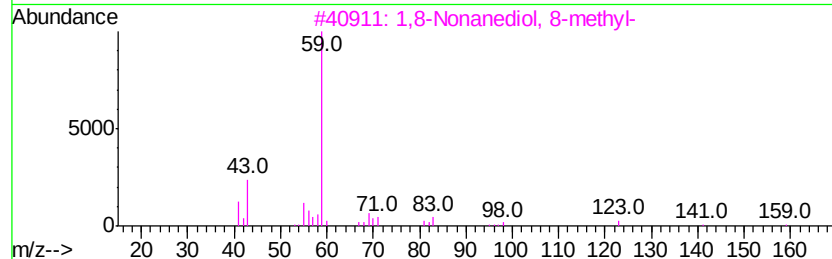
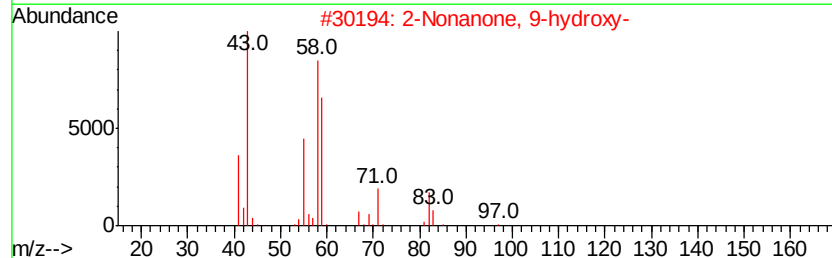
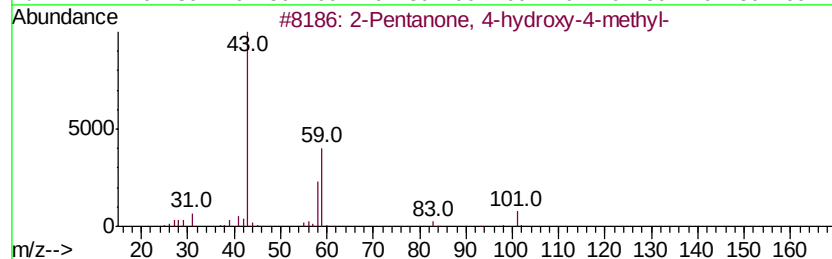
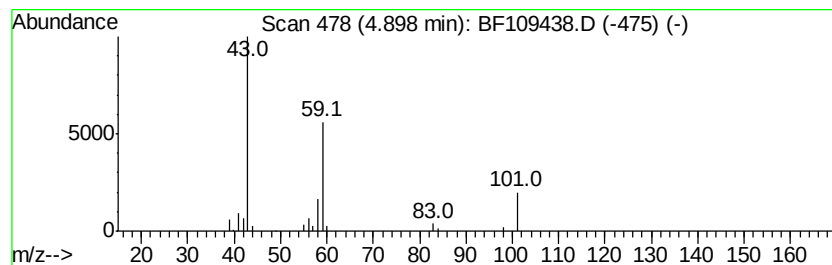
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.29 ng	64750	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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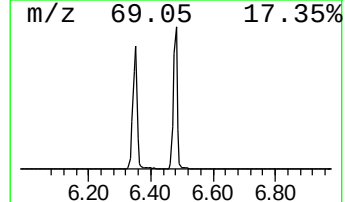
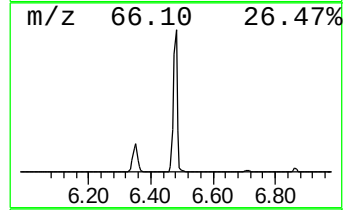
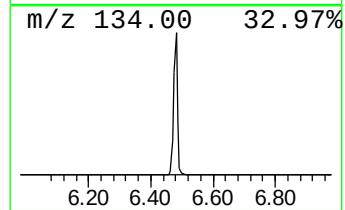
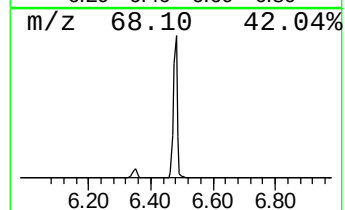
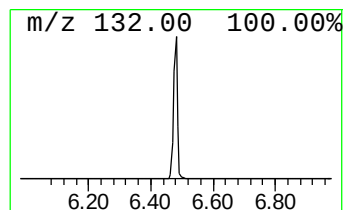
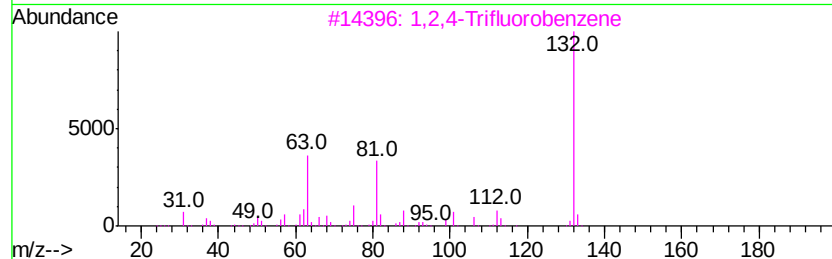
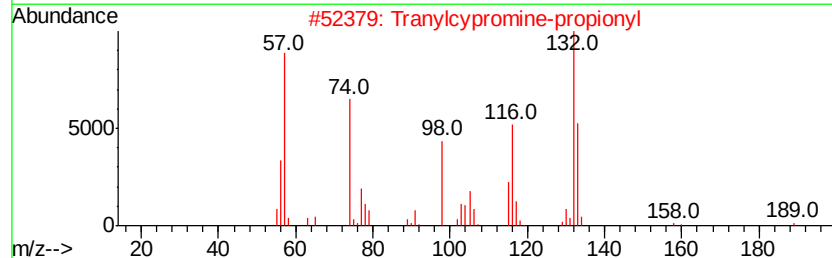
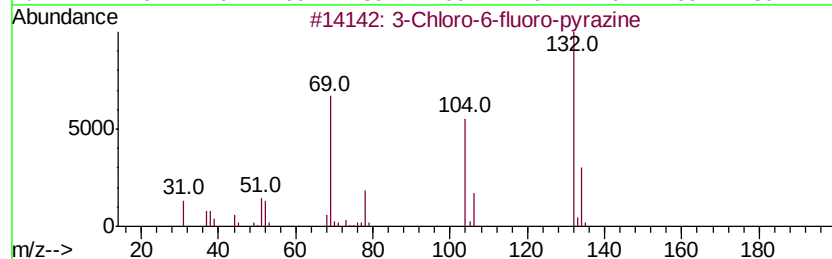
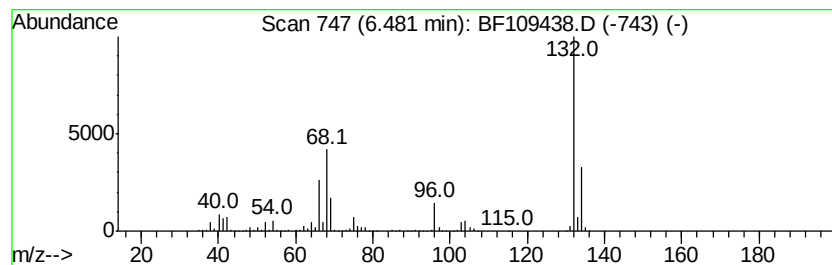
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	60.48 ng	1706660	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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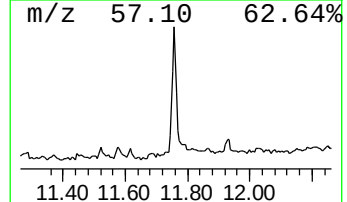
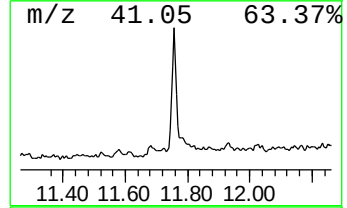
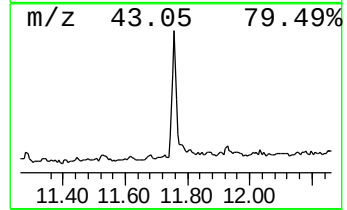
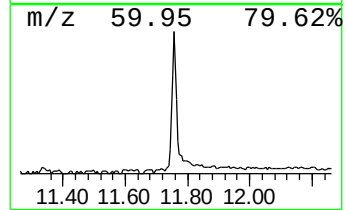
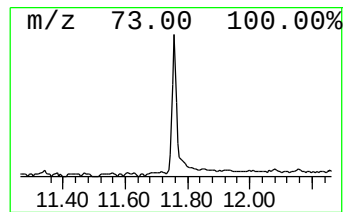
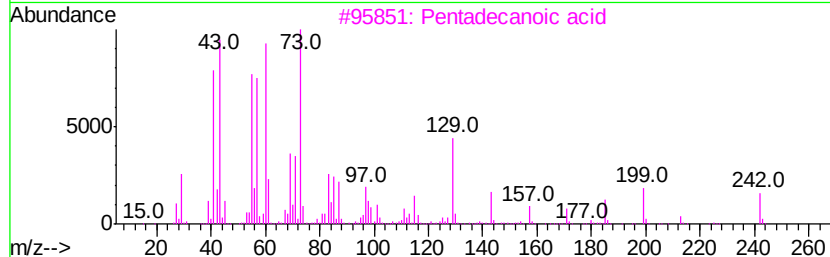
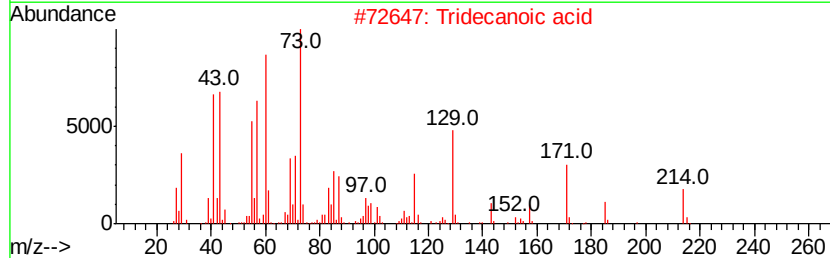
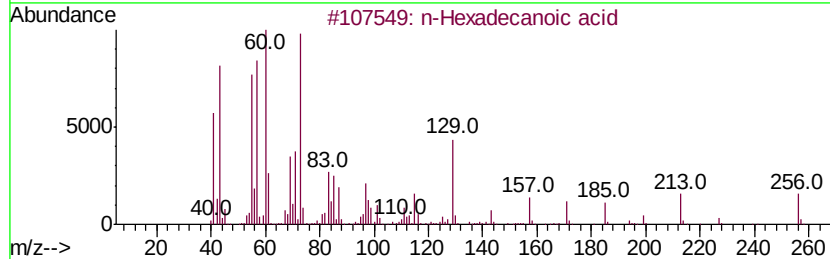
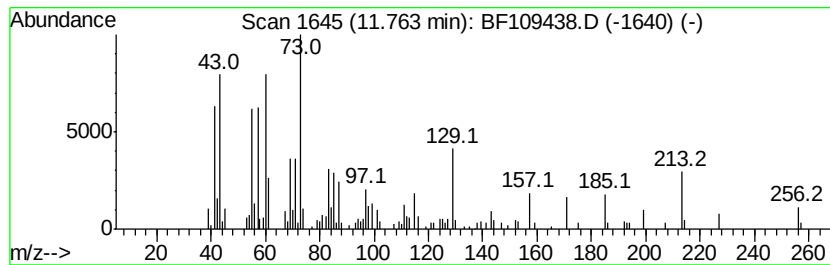
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	7.50 ng	227166	Phenanthrene-d10	11.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5		n-Decanoic acid	172	C10H20O2	000334-48-5	58



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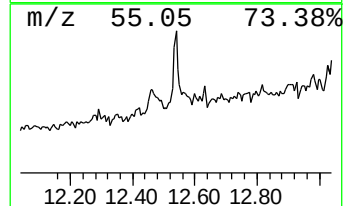
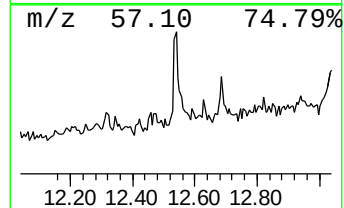
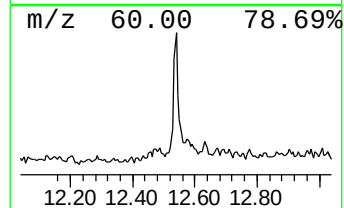
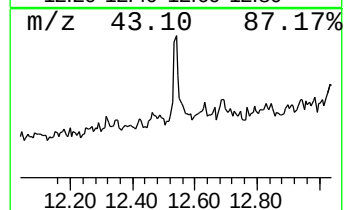
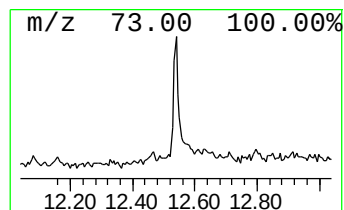
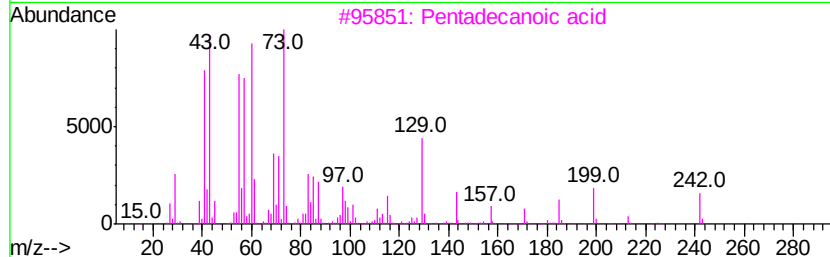
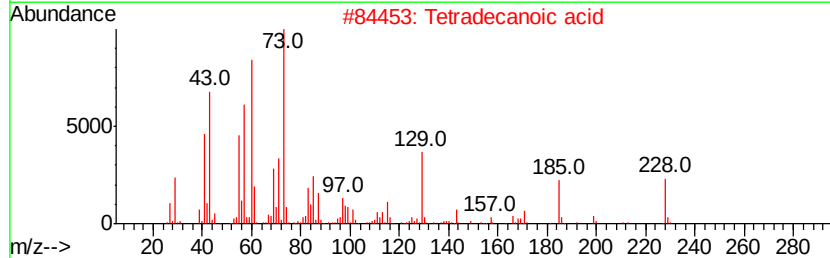
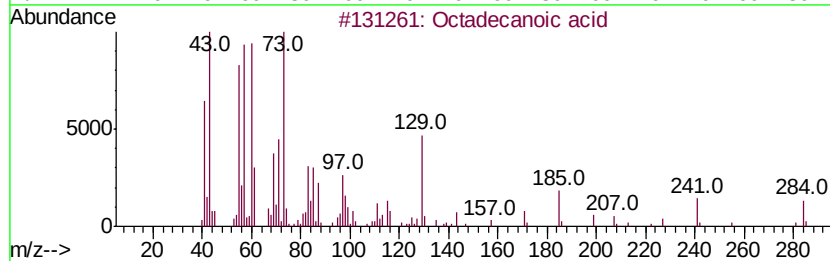
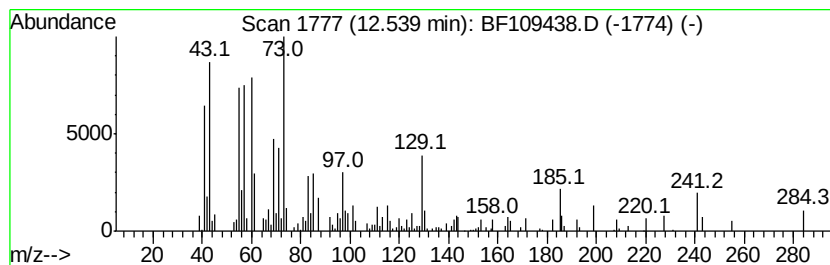
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.54	2.65 ng	84617	Chrysene-d12	13.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
4	Undecanoic acid	186	C11H22O2	000112-37-8	46
5	.alpha.-d-Riboside, 1-O-dodecyl-	318	C17H34O5	1000154-76-8	38



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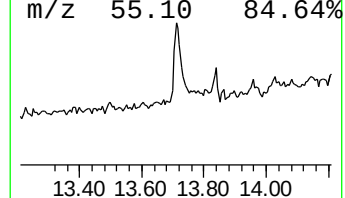
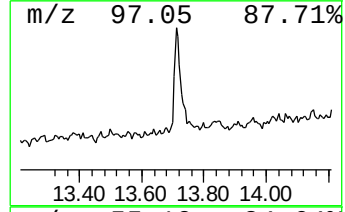
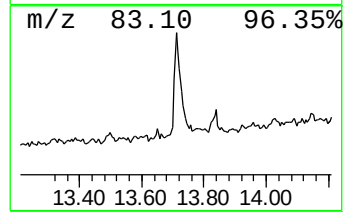
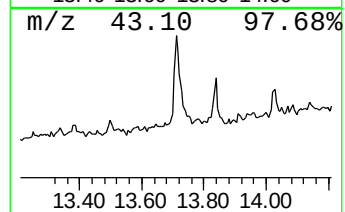
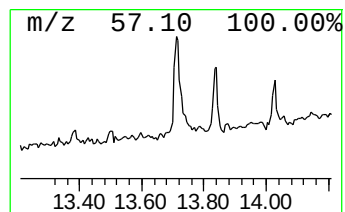
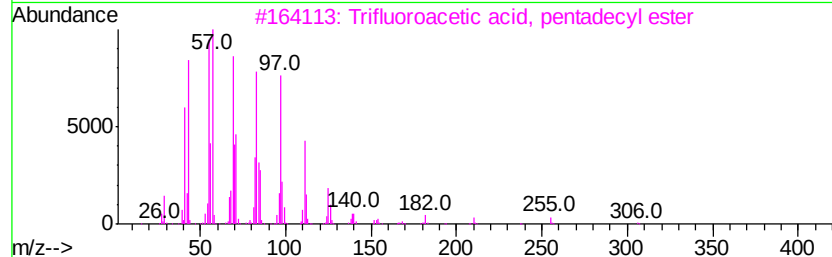
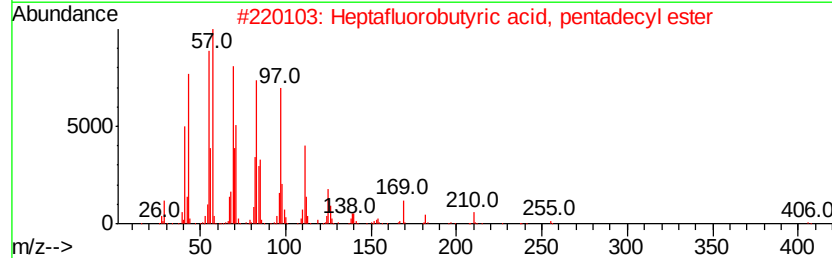
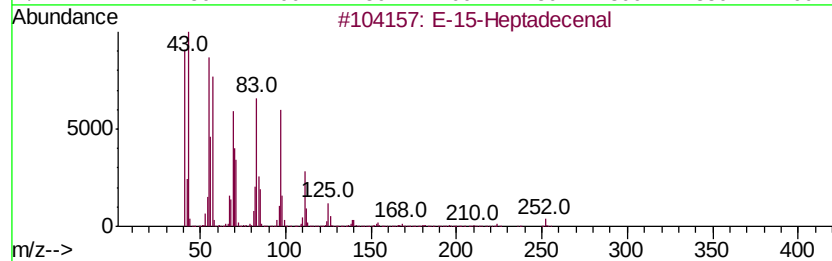
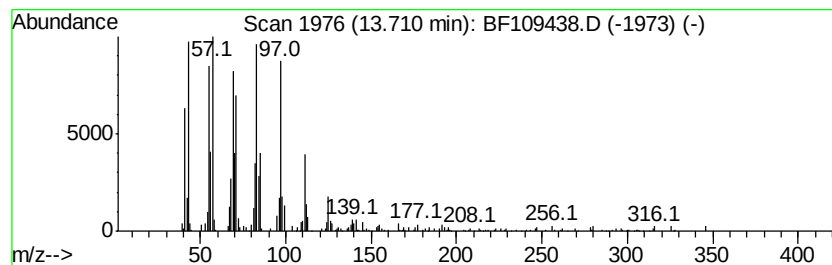
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 E-15-Heptadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	6.28 ng	200703	Chrysene-d12	13.84
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	E-15-Heptadecenal	252 C17H32O	1000130-97-9	96
2	Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5	94
3	Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2	91
4	1-Heneicosyl formate	340 C22H44O2	077899-03-7	91
5	Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1	91



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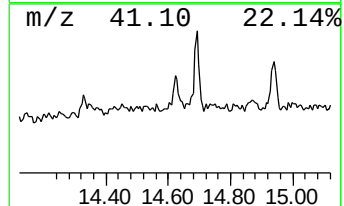
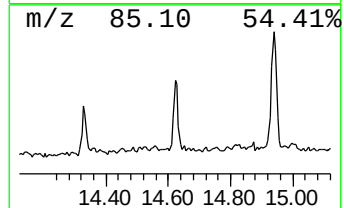
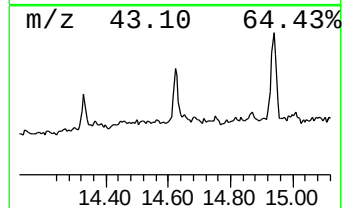
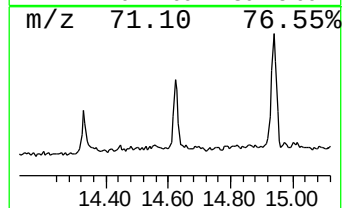
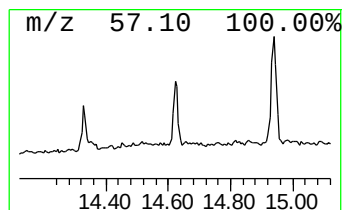
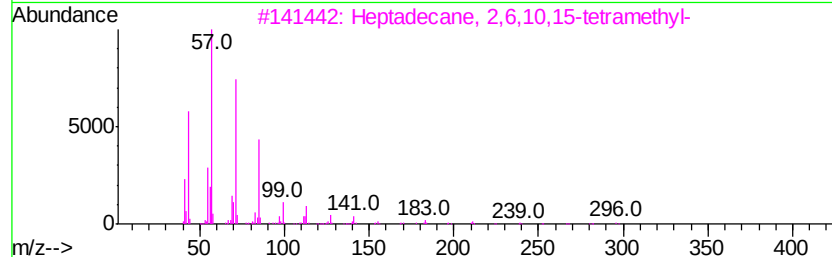
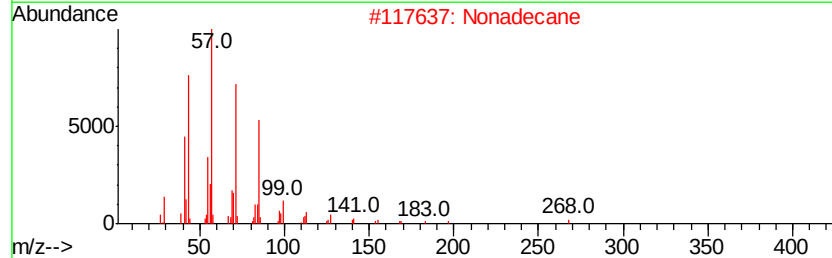
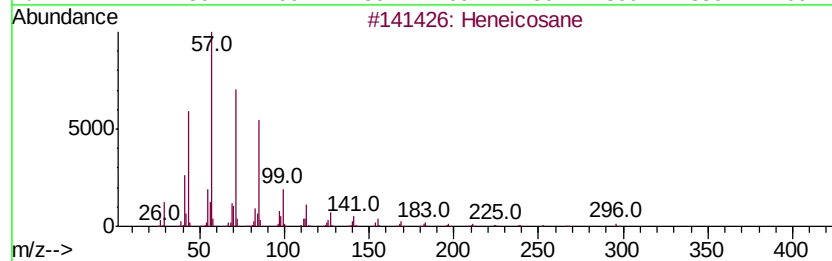
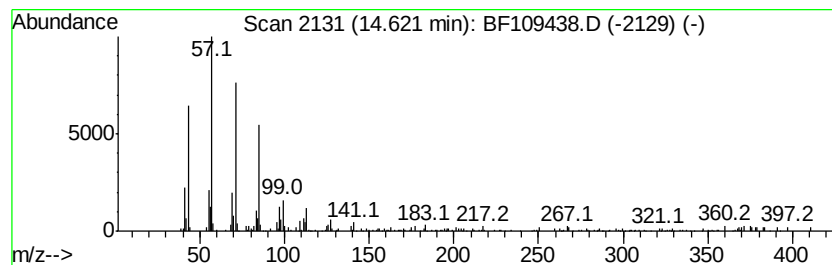
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	7.31 ng	110128	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	94
2	Nonadecane		268	C19H40	000629-92-5	90
3	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	90
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87
5	Octacosane		394	C28H58	000630-02-4	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092818\
Data File : BF109438.D
Acq On : 28 Sep 2018 18:58
Operator : JU/SJ
Sample : J5077-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PARCEL-190-092418-2

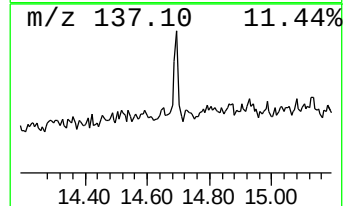
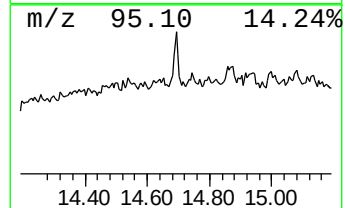
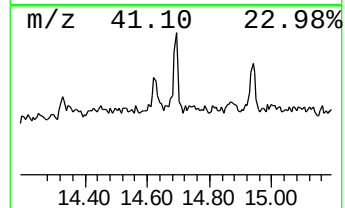
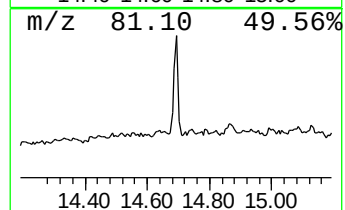
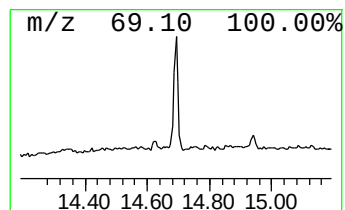
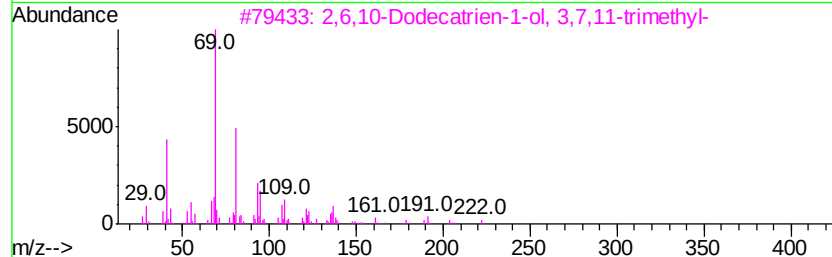
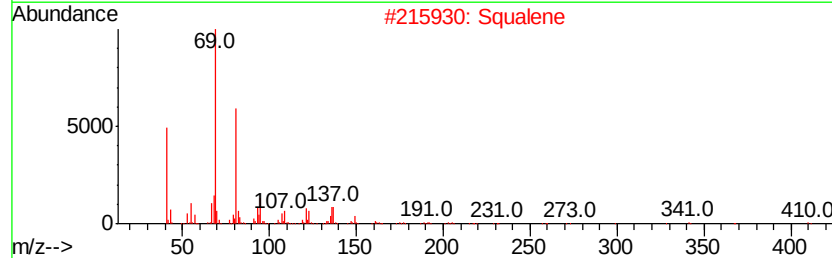
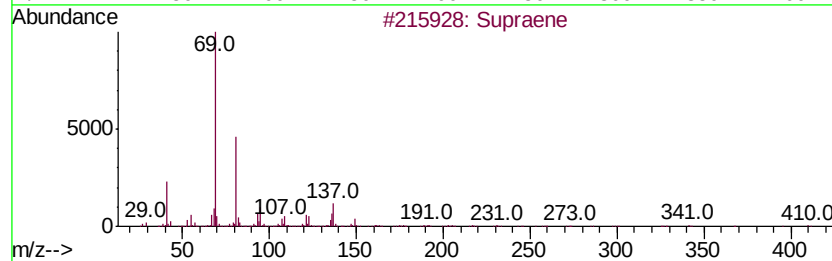
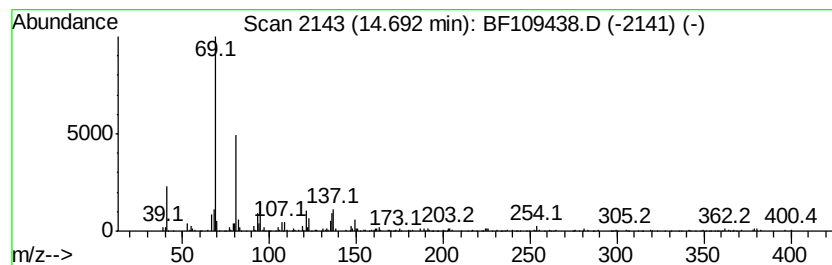
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	8.88 ng	133775	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	90
2		Squalene	410	C30H50	000111-02-4	87
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092818\
Data File : BF109438.D
Acq On : 28 Sep 2018 18:58
Operator : JU/SJ
Sample : J5077-04
Misc :
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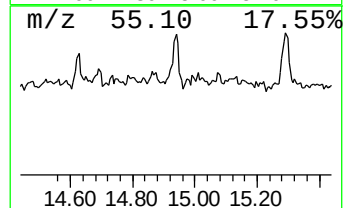
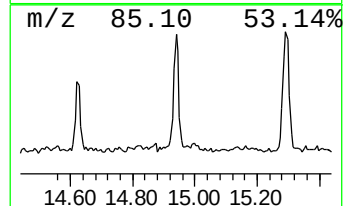
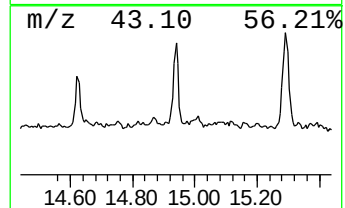
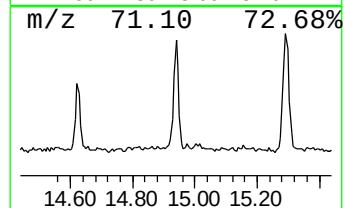
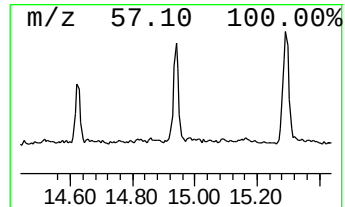
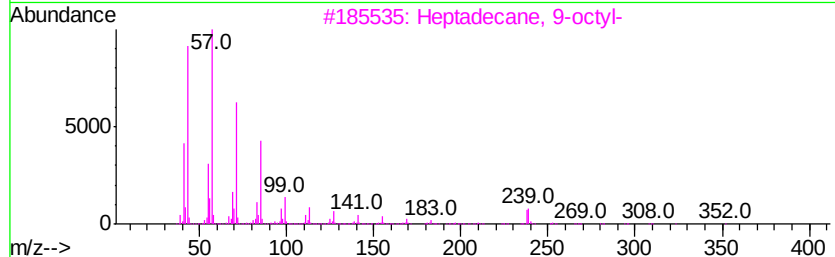
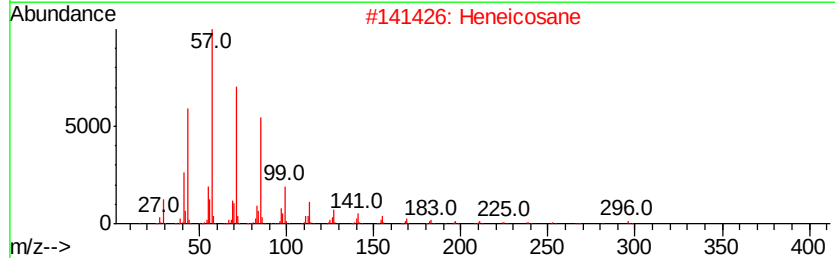
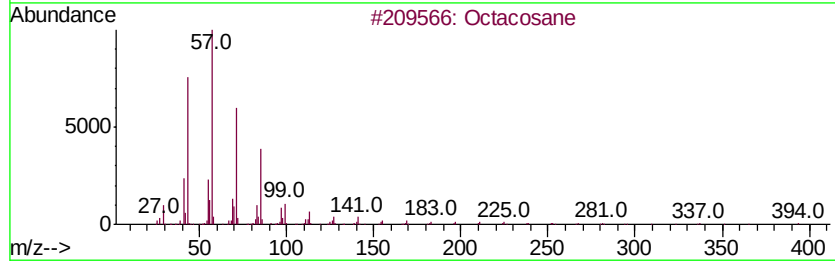
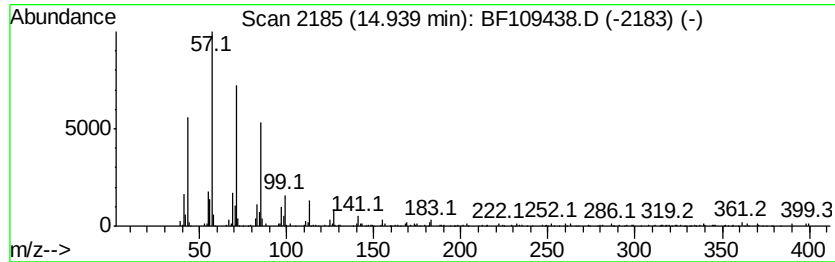
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	12.56 ng	189092	Perylene-d12	15.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394 C28H58	000630-02-4	90
2	Heneicosane	296 C21H44	000629-94-7	87
3	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	87
4	Tetracosane	338 C24H50	000646-31-1	87
5	Hexacosane	366 C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092818\
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Acq On : 28 Sep 2018 18:58
Operator : JU/SJ
Sample : J5077-04
Misc :
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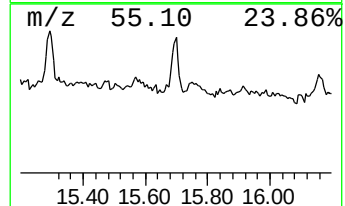
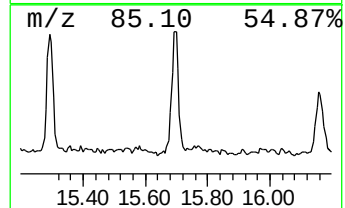
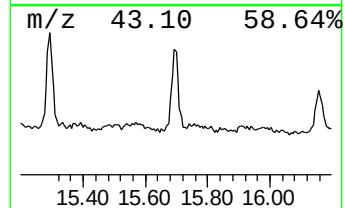
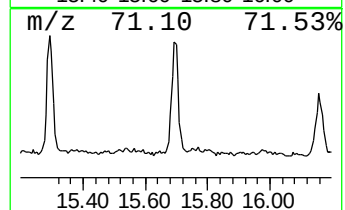
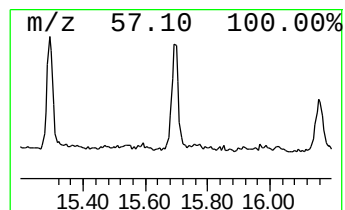
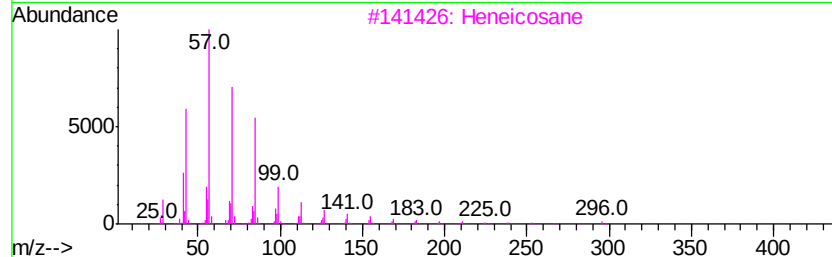
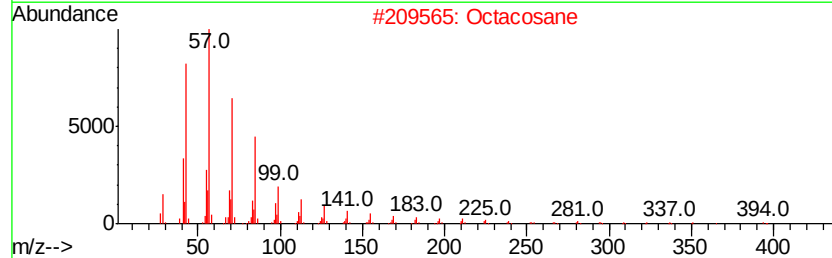
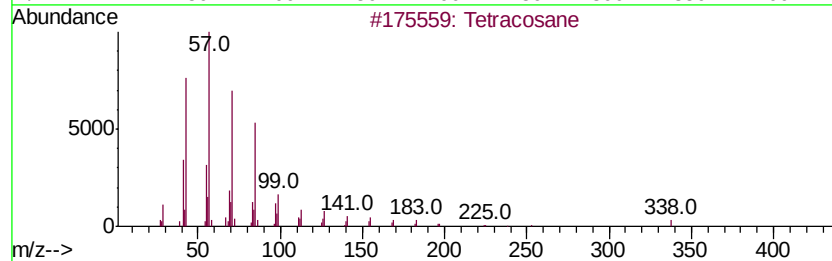
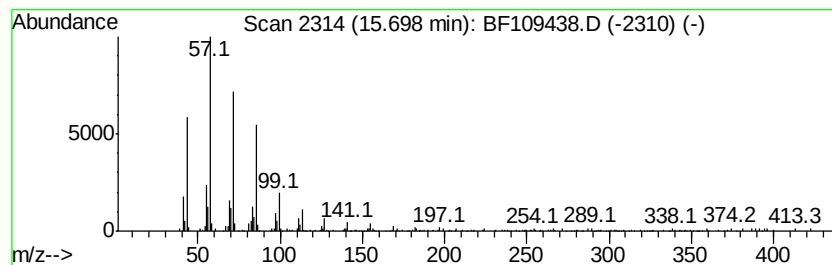
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	14.43 ng	217268	Perylene-d12	15.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetracosane	338 C24H50	000646-31-1 93
2		Octacosane	394 C28H58	000630-02-4 93
3		Heneicosane	296 C21H44	000629-94-7 90
4		Heptadecane	240 C17H36	000629-78-7 87
5		Octadecane	254 C18H38	000593-45-3 86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092818\
Data File : BF109438.D
Acq On : 28 Sep 2018 18:58
Operator : JU/SJ
Sample : J5077-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.48	6.48	60.5	ng	1706660	1	6.71	564380	20.0
n-Hexadecanoic acid	11.76	7.5	ng	227166	4	11.22	605916	20.0
Octadecanoic acid	12.54	2.6	ng	84617	5	13.84	639539	20.0
E-15-Heptadecenal	13.71	6.3	ng	200703	5	13.84	639539	20.0
Heneicosane	14.62	7.3	ng	110128	6	15.25	301160	20.0
Supraene	14.69	8.9	ng	133775	6	15.25	301160	20.0
Octacosane	14.94	12.6	ng	189092	6	15.25	301160	20.0
Tetracosane	15.70	14.4	ng	217268	6	15.25	301160	20.0