

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101018\
 Data File : BF109742.D
 Acq On : 10 Oct 2018 15:09
 Operator : JU/SJ
 Sample : J5326-33
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FL-PH-2-STONE

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-BF100818.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	474	478	490	rBV	49982	78698	2.49%	0.320%
2	5.316	545	549	573	rBV	1488978	1920554	60.77%	7.807%
3	6.345	720	724	741	rBV	1684433	2212569	70.01%	8.994%
4	6.469	741	745	769	rVB	1992461	2294998	72.62%	9.329%
5	6.692	780	783	794	rBV	318433	466980	14.78%	1.898%
6	6.851	806	810	834	rBV	1663783	1724551	54.57%	7.010%
7	7.257	875	879	913	rBV	1061671	1484485	46.97%	6.034%
8	7.975	997	1001	1022	rBV	517679	663767	21.00%	2.698%
9	9.051	1179	1184	1199	rBV	2629743	2859766	90.49%	11.624%
10	9.439	1247	1250	1261	rBV	140105	159627	5.05%	0.649%
11	9.722	1294	1298	1320	rBV	824829	815333	25.80%	3.314%
12	10.510	1428	1432	1450	rBV	1632139	1919152	60.73%	7.801%
13	11.198	1546	1549	1559	rBV	719145	925143	29.27%	3.761%
14	11.739	1638	1641	1648	rBV2	134851	168909	5.34%	0.687%
15	12.410	1753	1755	1760	rBV	28060	37225	1.18%	0.151%
16	12.521	1772	1774	1781	rBV3	40607	53143	1.68%	0.216%
17	12.786	1814	1819	1835	rBV	2927447	3160372	100.00%	12.846%
18	13.021	1856	1859	1861	rVB	46167	43238	1.37%	0.176%
19	13.357	1914	1916	1925	rVB	70103	83582	2.64%	0.340%
20	13.686	1969	1972	1984	rVB	330168	432526	13.69%	1.758%
21	13.827	1992	1996	2009	rVB	830130	971784	30.75%	3.950%
22	13.998	2022	2025	2033	rVB	94218	104947	3.32%	0.427%
23	14.304	2074	2077	2079	rBV	96449	85845	2.72%	0.349%
24	14.598	2123	2127	2130	rBV	112358	108998	3.45%	0.443%
25	14.904	2175	2179	2183	rVB	183145	184191	5.83%	0.749%
26	15.227	2229	2234	2249	rVB	579689	934465	29.57%	3.798%
27	15.433	2266	2269	2274	rVB3	33640	43167	1.37%	0.175%
28	15.651	2301	2306	2310	rVB	106852	151299	4.79%	0.615%
29	15.709	2311	2316	2327	rVV4	56178	141191	4.47%	0.574%
30	16.104	2378	2383	2394	rVB3	63310	136312	4.31%	0.554%
31	16.362	2422	2427	2433	rBV4	29679	54224	1.72%	0.220%
32	16.639	2469	2474	2481	rVB2	32122	64815	2.05%	0.263%
33	16.862	2508	2512	2518	rVB6	21763	37654	1.19%	0.153%
34	17.103	2547	2553	2562	rBV10	30574	77734	2.46%	0.316%

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Misc :
ALS Vial : 6 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

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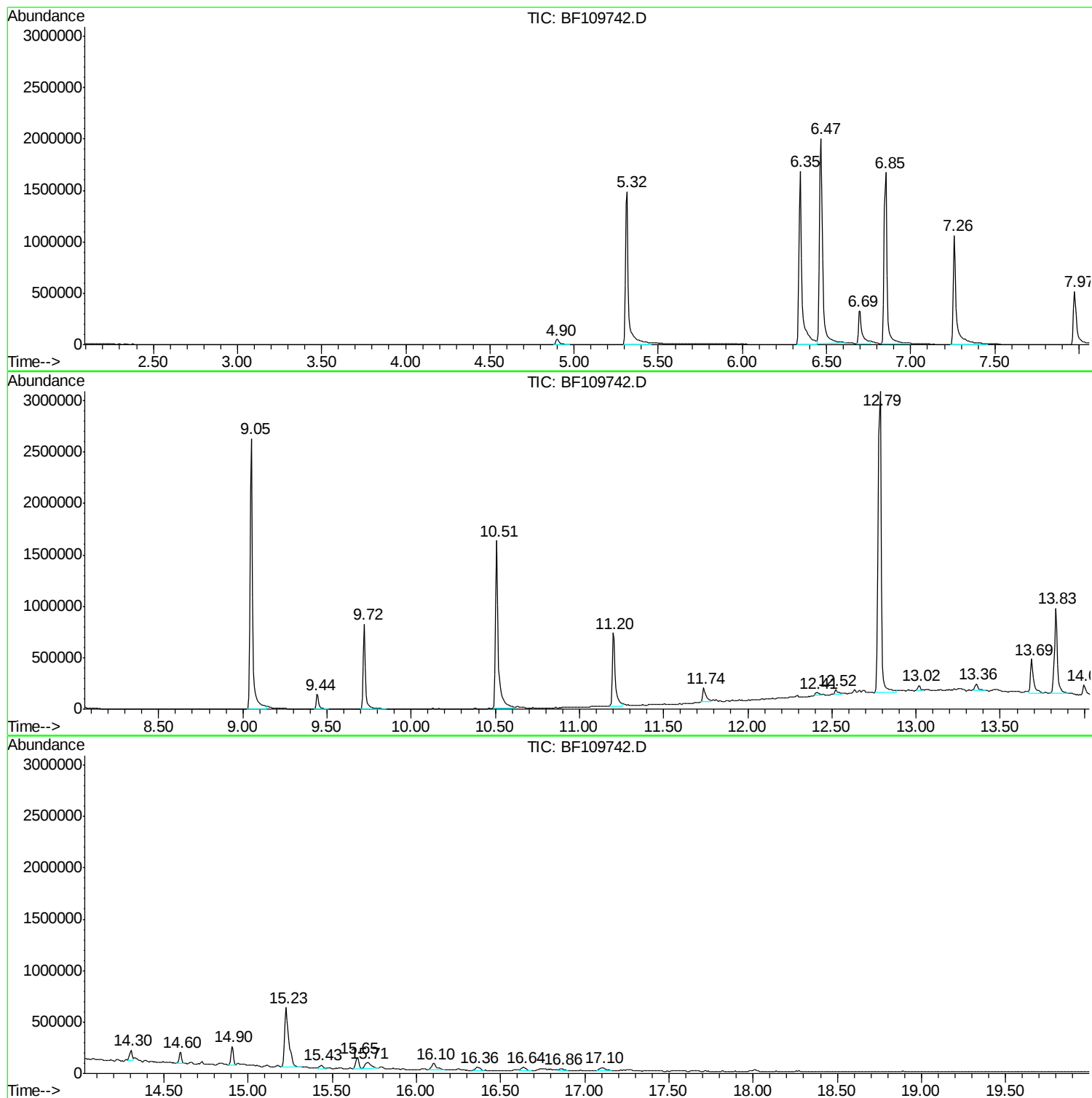
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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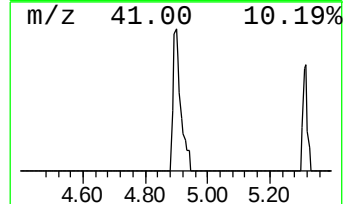
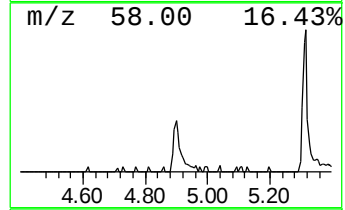
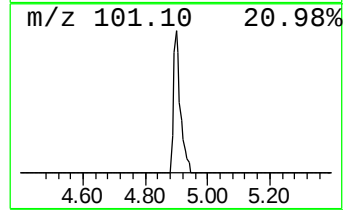
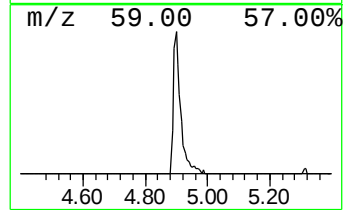
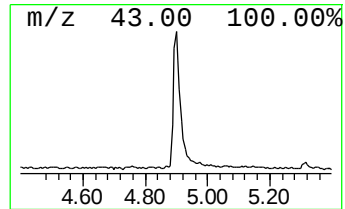
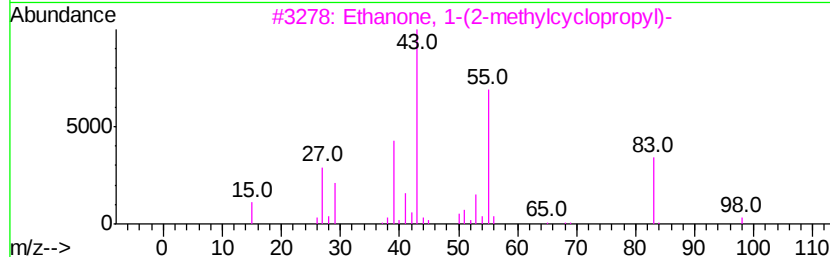
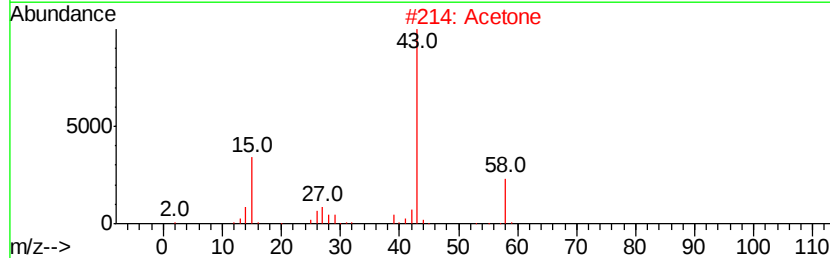
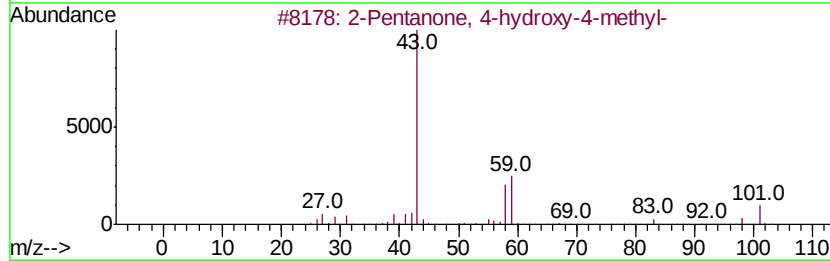
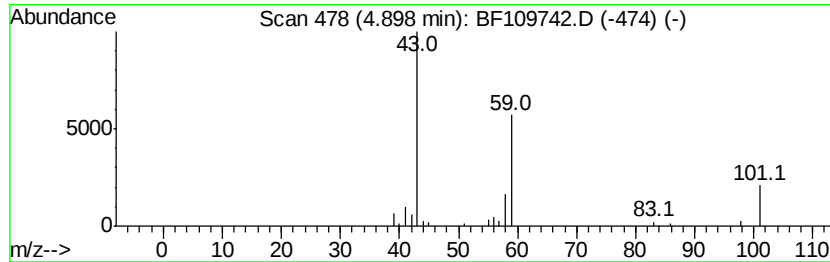
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.37 ng	78698	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetone	58	C3H6O	000067-64-1	10		
3	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9		
4	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9		
5	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	9		



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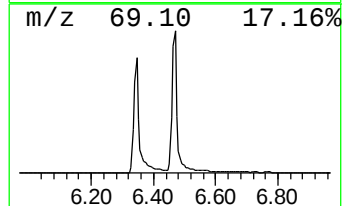
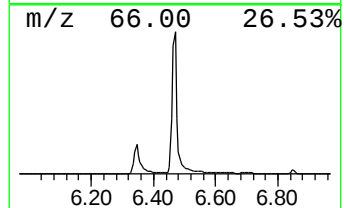
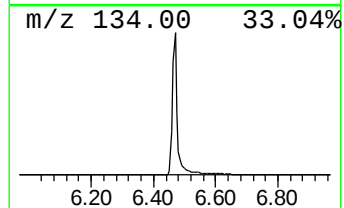
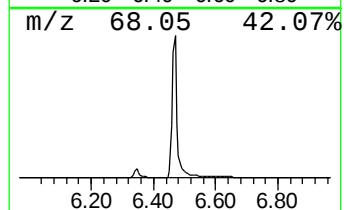
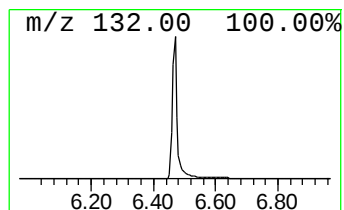
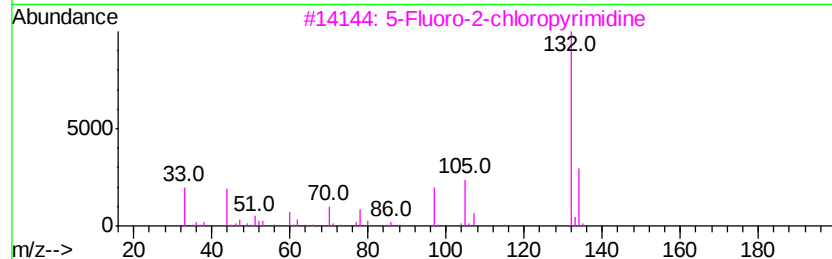
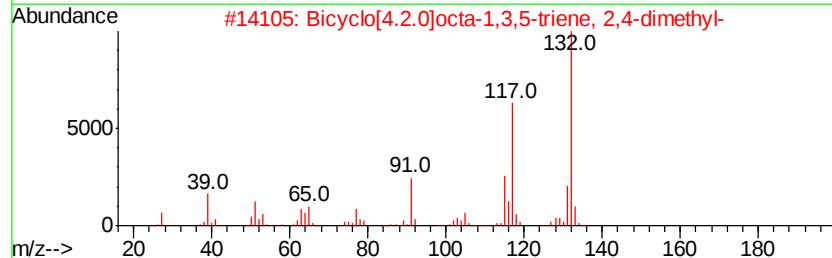
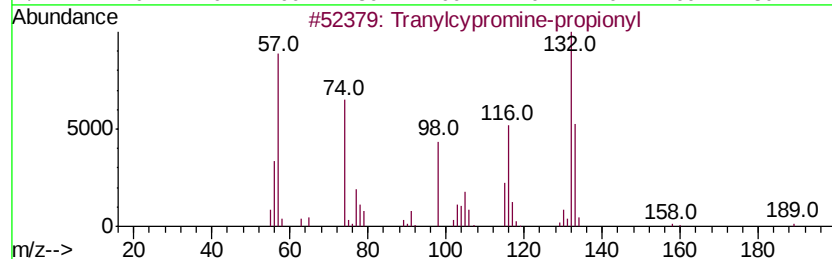
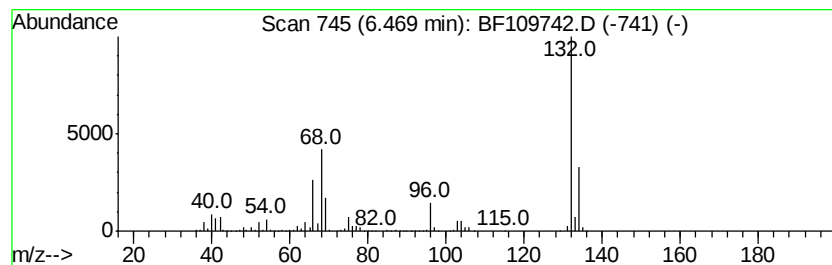
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	98.29 ng	2295000	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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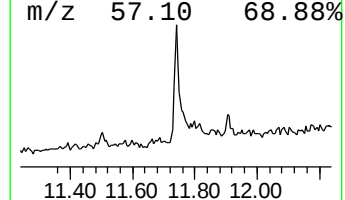
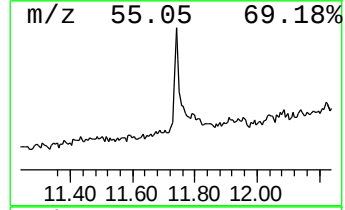
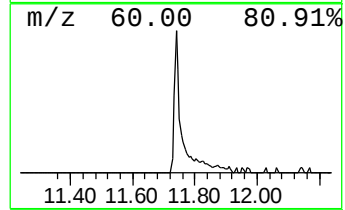
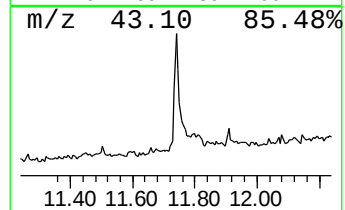
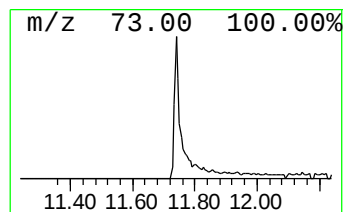
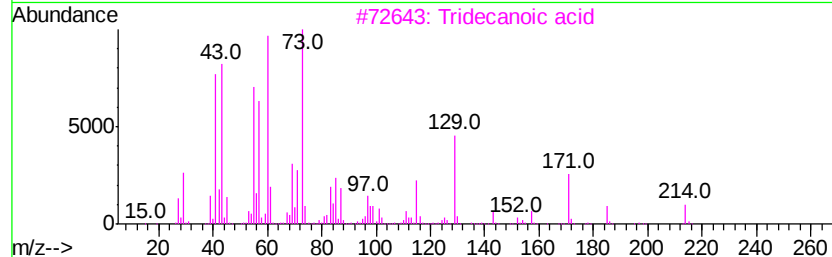
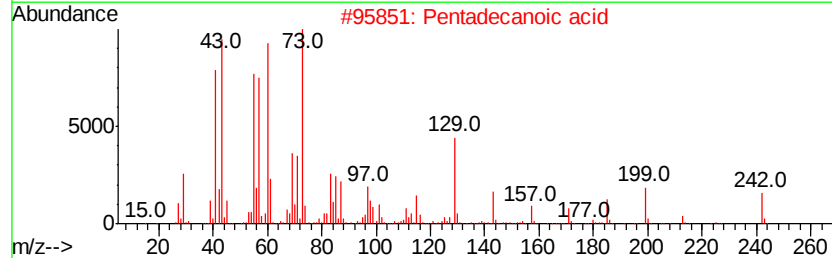
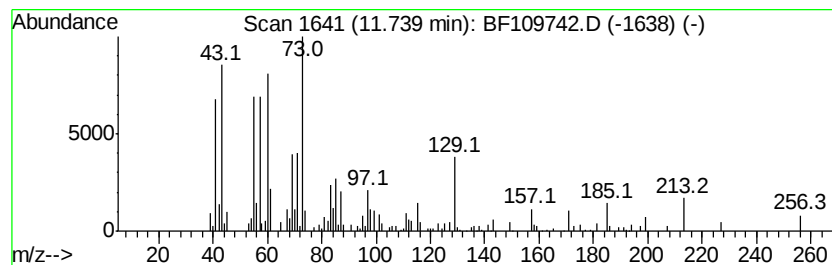
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	3.65 ng	168909	Phenanthrene-d10	11.20

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	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	30



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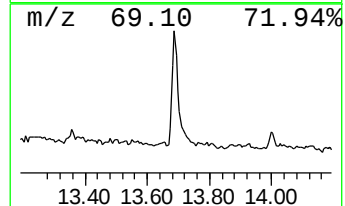
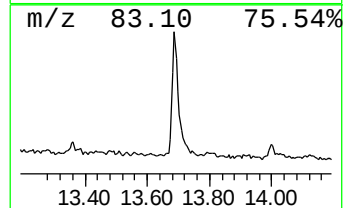
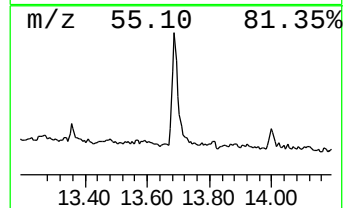
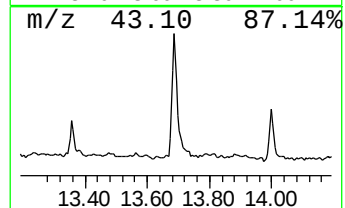
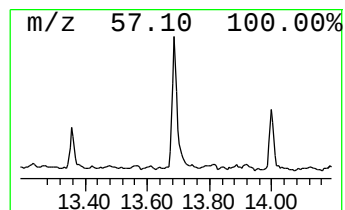
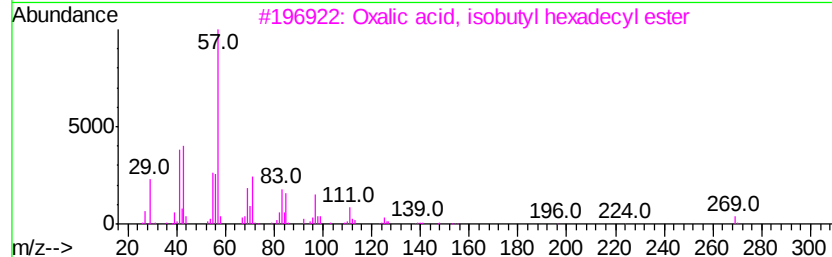
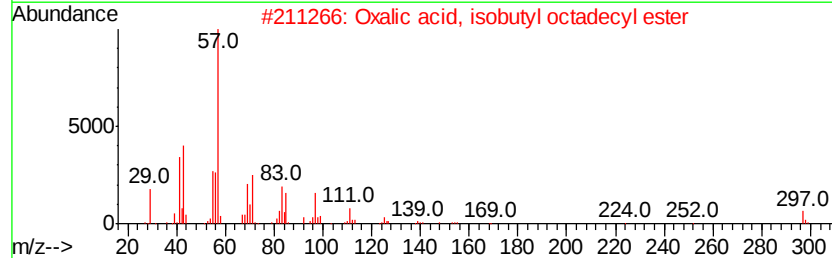
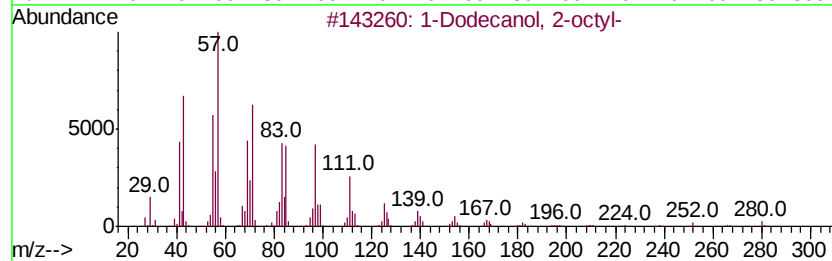
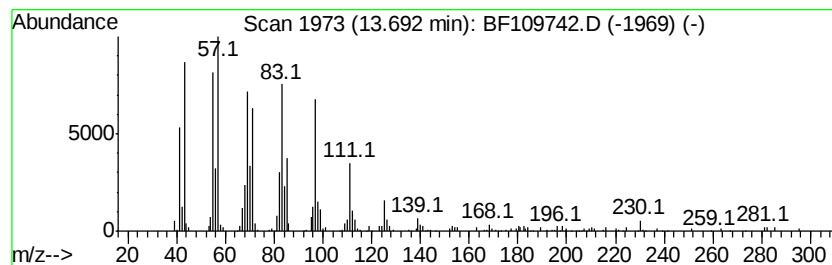
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Dodecanol, 2-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.69	8.90 ng	432526	Chrysene-d12	13.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2		Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
3		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	76
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	76



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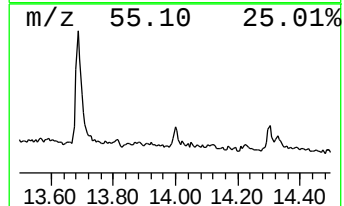
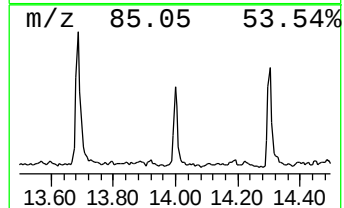
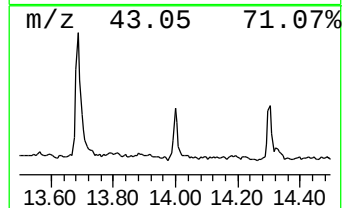
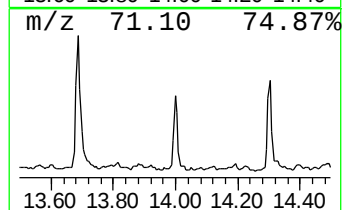
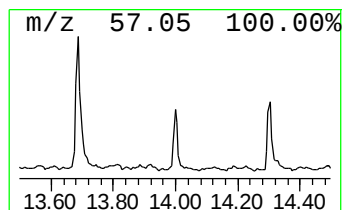
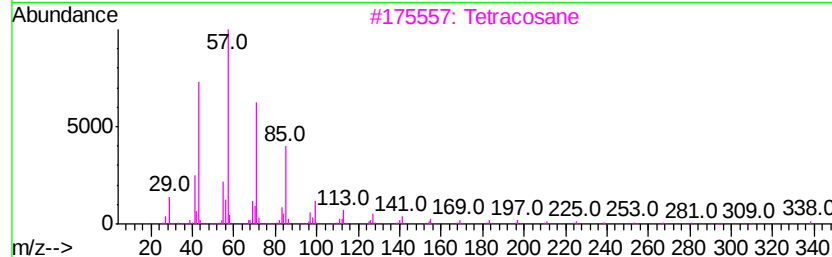
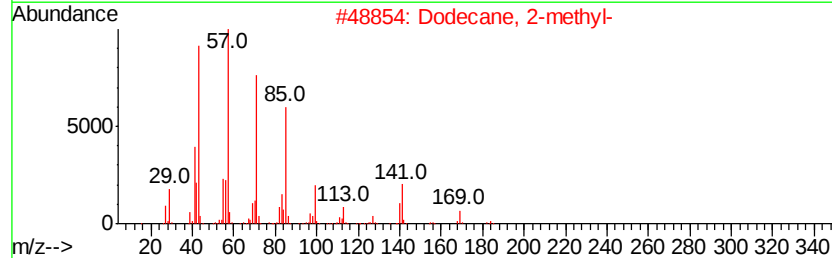
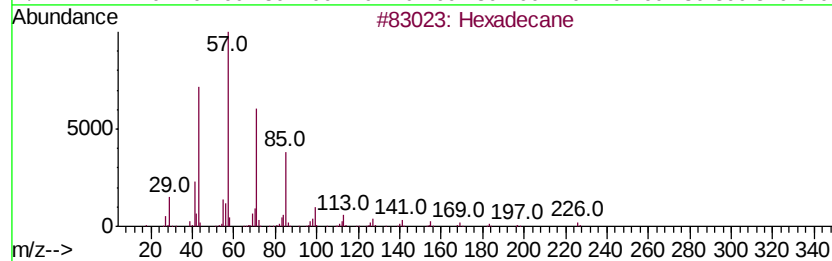
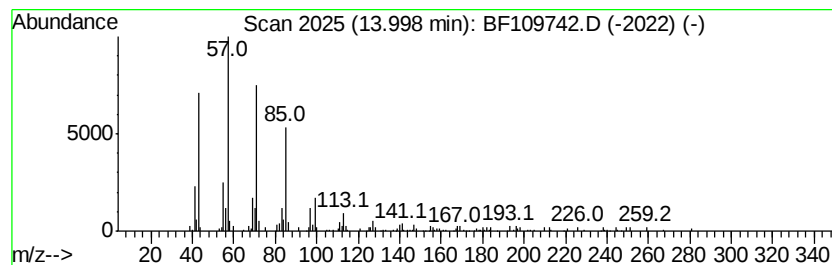
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Peak Number 6 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	2.16 ng	104947	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	93
2		Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
3		Tetracosane	338	C24H50	000646-31-1	90
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86



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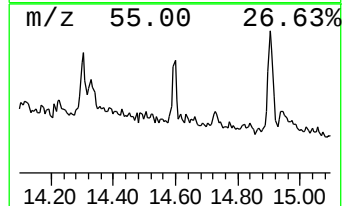
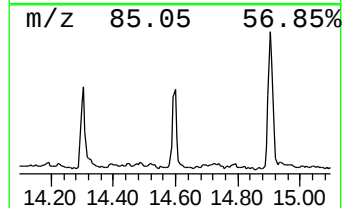
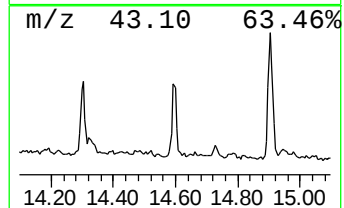
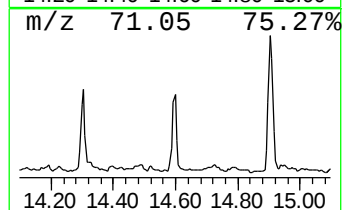
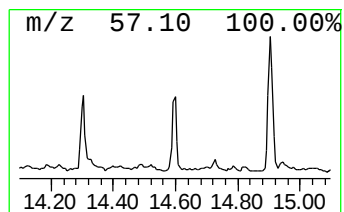
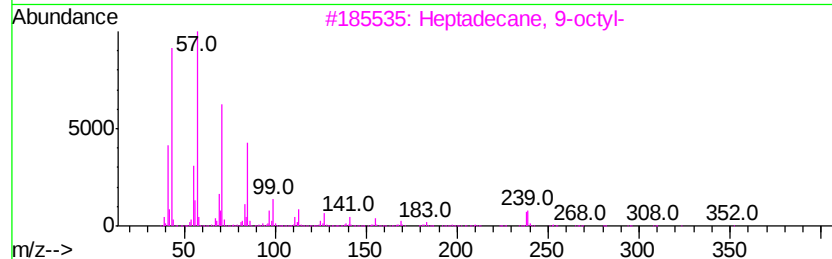
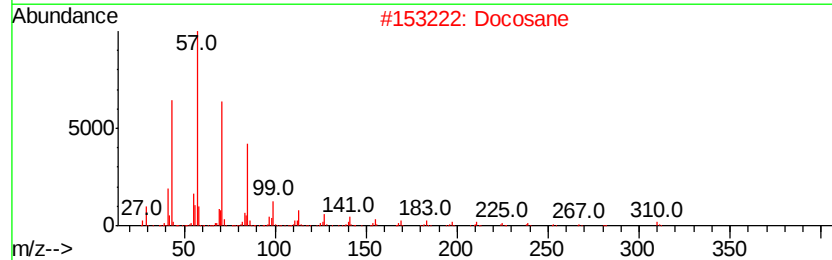
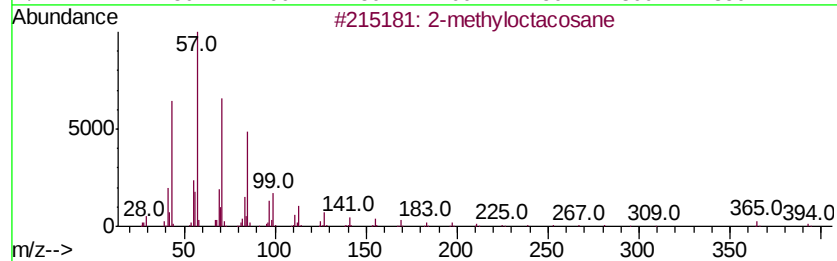
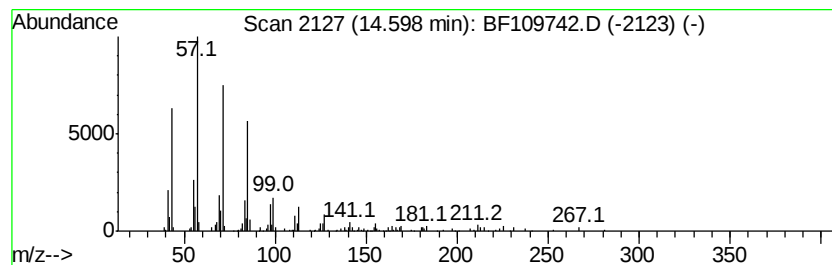
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyloctacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.33 ng	108998	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	91
2	Docosane		310	C22H46	000629-97-0	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	91
5	Heptadecane		240	C17H36	000629-78-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109742.D
Acq On : 10 Oct 2018 15:09
Operator : JU/SJ
Sample : J5326-33
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FL-PH-2-STONE

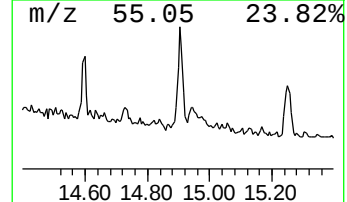
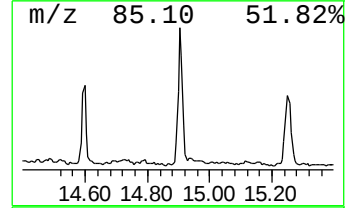
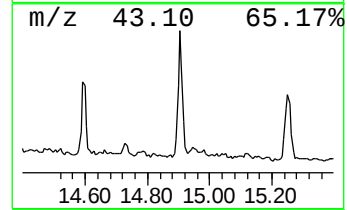
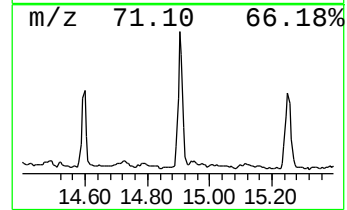
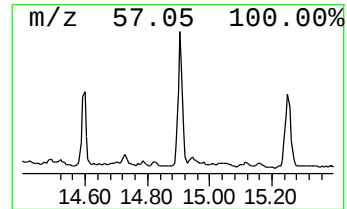
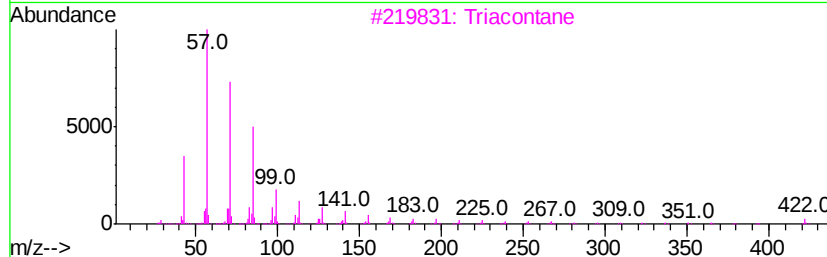
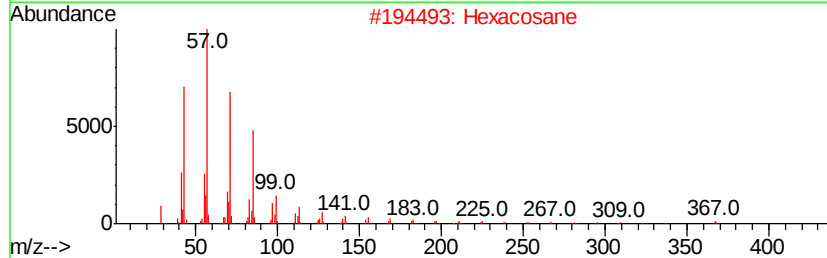
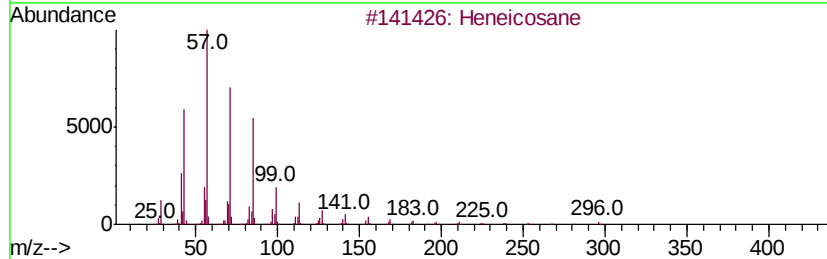
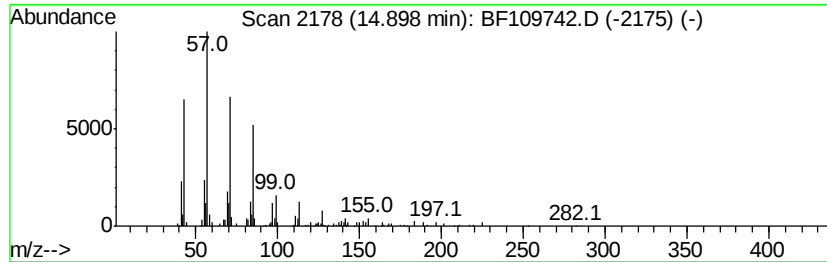
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	3.94 ng	184191	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	triacontane		422	C30H62	000638-68-6	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	Heptacosane		380	C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109742.D
Acq On : 10 Oct 2018 15:09
Operator : JU/SJ
Sample : J5326-33
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FL-PH-2-STONE

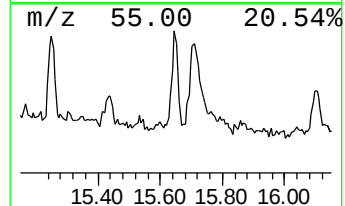
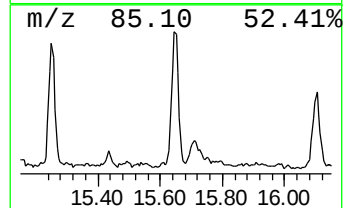
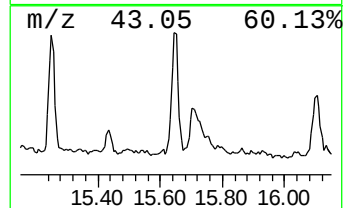
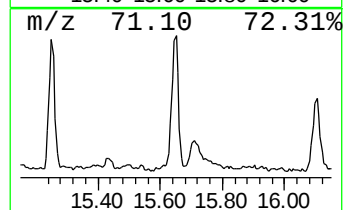
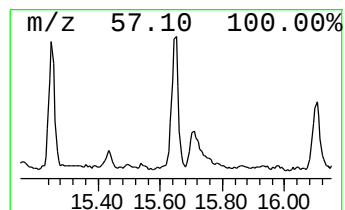
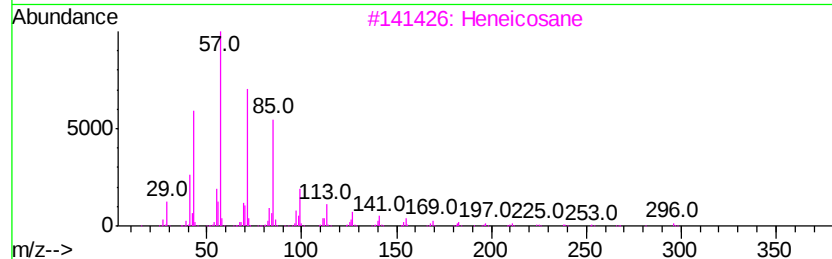
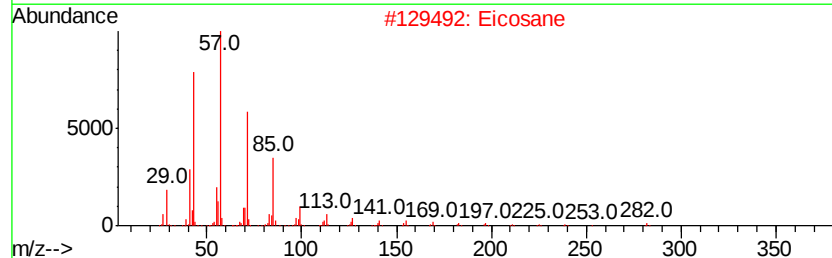
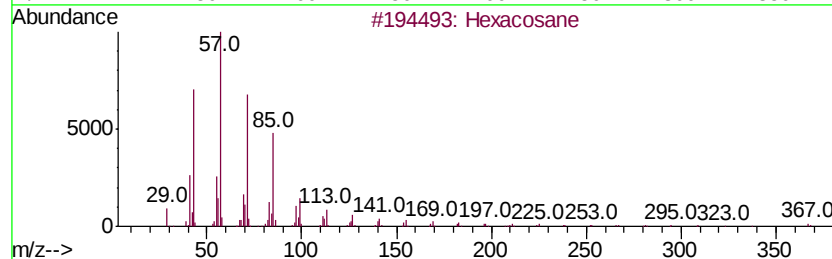
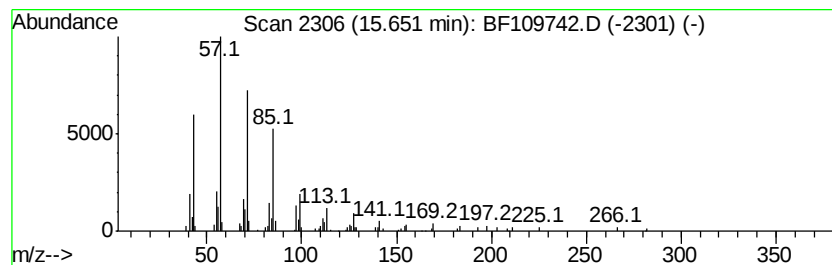
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	3.24 ng	151299	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Eicosane		282	C20H42	000112-95-8	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Hentriacontane		437	C31H64	000630-04-6	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109742.D
Acq On : 10 Oct 2018 15:09
Operator : JU/SJ
Sample : J5326-33
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FL-PH-2-STONE

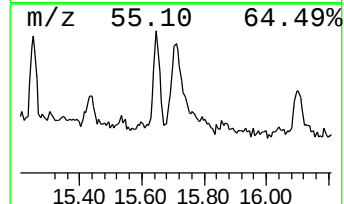
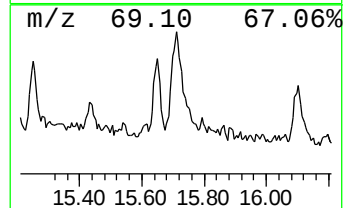
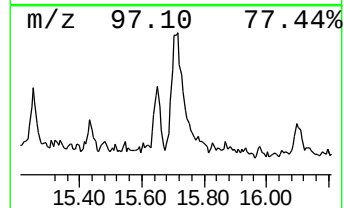
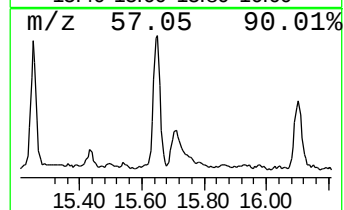
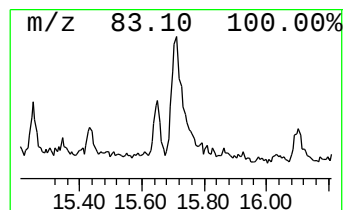
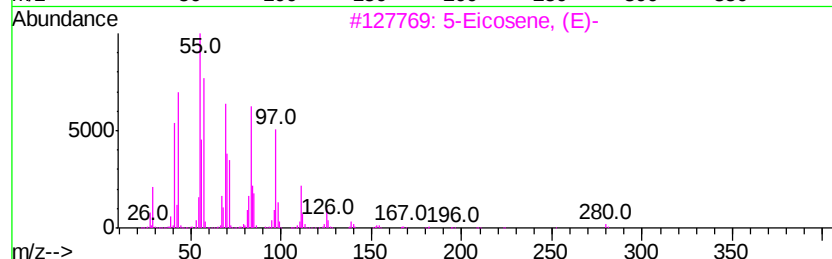
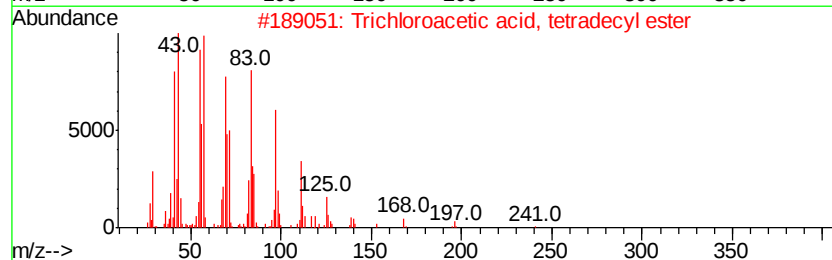
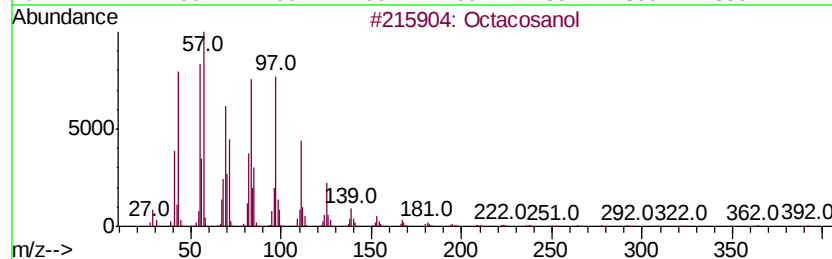
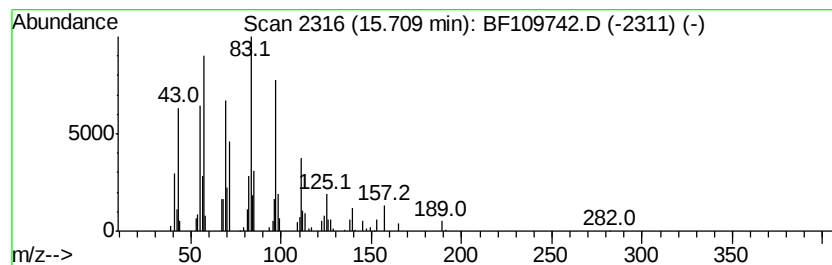
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.02 ng	141191	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosanol	410	C28H58O	000557-61-9	93
2		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	86
4		1-Docosene	308	C22H44	001599-67-3	86
5		Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109742.D
Acq On : 10 Oct 2018 15:09
Operator : JU/SJ
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ALS Vial : 6 Sample Multiplier: 1

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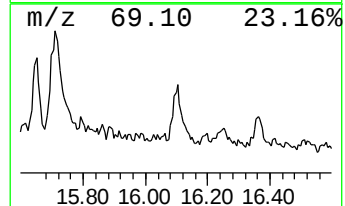
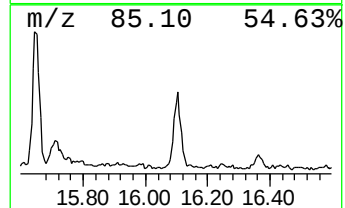
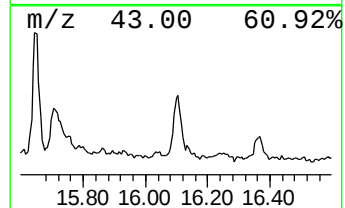
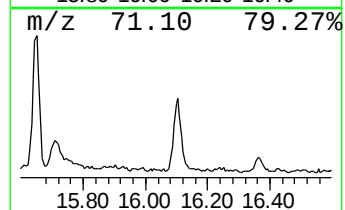
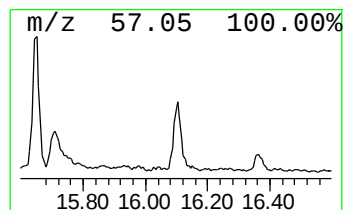
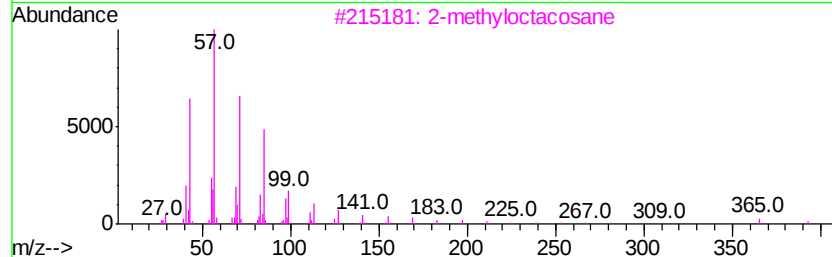
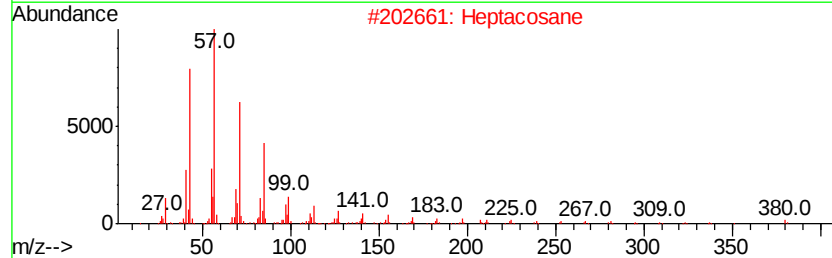
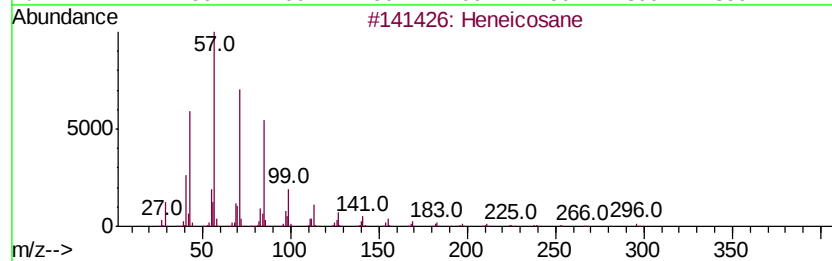
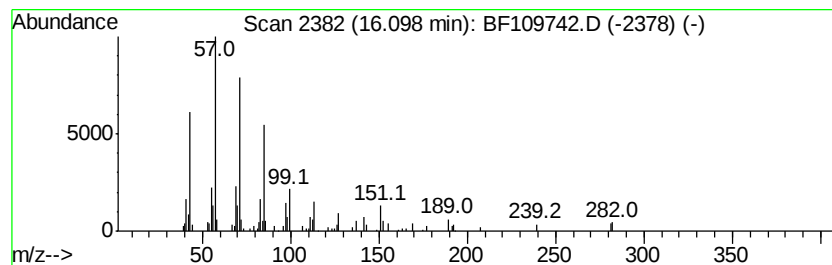
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.92 ng	136312	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heptadecane	240	C17H36	000629-78-7	90
5		triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101018\
 Data File : BF109742.D
 Acq On : 10 Oct 2018 15:09
 Operator : JU/SJ
 Sample : J5326-33
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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
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unknown6.47	6.47	98.3	ng	2295000	1	6.70	466980	20.0
n-Hexadecanoic acid	11.74	3.6	ng	168909	4	11.20	925143	20.0
1-Dodecanol, 2-oc...	13.69	8.9	ng	432526	5	13.83	971784	20.0
Hexadecane	14.00	2.2	ng	104947	5	13.83	971784	20.0
2-methyloctacosane	14.60	2.3	ng	108998	6	15.23	934465	20.0
Heneicosane	14.90	3.9	ng	184191	6	15.23	934465	20.0
Hexacosane	15.65	3.2	ng	151299	6	15.23	934465	20.0
Octacosanol	15.71	3.0	ng	141191	6	15.23	934465	20.0
Heptadecane	16.10	2.9	ng	136312	6	15.23	934465	20.0