

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110818\
 Data File : BF110608.D
 Acq On : 9 Nov 2018 1:50
 Operator : JU/SJ
 Sample : J5859-05
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-24(0-10)

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-BF110818.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	5.181	523	526	537	rBV	39267	55660	3.27%	0.377%
2	5.569	587	592	613	rBV	1472827	1550646	91.12%	10.498%
3	6.569	757	762	777	rBV	1629422	1701725	100.00%	11.521%
4	6.716	782	787	790	rBV	1797773	1653246	97.15%	11.192%
5	6.945	822	826	832	rBV	521084	443269	26.05%	3.001%
6	7.098	848	852	868	rVB	1431897	1273293	74.82%	8.620%
7	7.510	917	922	933	rBV	1094463	1019522	59.91%	6.902%
8	8.228	1040	1044	1057	rBV	597029	562001	33.03%	3.805%
9	9.298	1222	1226	1229	rBV	2041999	1675463	98.46%	11.343%
10	9.692	1289	1293	1300	rBV	127021	111889	6.58%	0.757%
11	9.986	1339	1343	1354	rVB	615690	548725	32.25%	3.715%
12	10.775	1474	1477	1489	rBV	807180	775715	45.58%	5.252%
13	11.480	1593	1597	1600	rBV	467947	435279	25.58%	2.947%
14	11.980	1679	1682	1688	rBV	66414	68701	4.04%	0.465%
15	12.698	1801	1804	1807	rBV	25541	21880	1.29%	0.148%
16	12.769	1813	1816	1824	rBV4	28147	40271	2.37%	0.273%
17	12.927	1841	1843	1847	rVB	27447	25195	1.48%	0.171%
18	13.057	1861	1865	1869	rBV	1177752	1127607	66.26%	7.634%
19	13.527	1940	1945	1949	rBV	87754	87974	5.17%	0.596%
20	13.610	1956	1959	1962	rBV2	22186	21711	1.28%	0.147%
21	13.939	2012	2015	2029	rBV	123574	186968	10.99%	1.266%
22	14.127	2043	2047	2050	rBV	507302	453511	26.65%	3.070%
23	14.257	2066	2069	2072	rVB	30191	28121	1.65%	0.190%
24	14.557	2118	2120	2123	rBV	46659	49129	2.89%	0.333%
25	14.786	2156	2159	2165	rBV2	70992	97188	5.71%	0.658%
26	14.874	2170	2174	2178	rVV	66804	78068	4.59%	0.529%
27	14.957	2185	2188	2192	rVB	44444	48816	2.87%	0.330%
28	15.221	2231	2233	2241	rVB	78702	94774	5.57%	0.642%
29	15.621	2298	2301	2303	rBV	49156	67104	3.94%	0.454%
30	15.651	2303	2306	2311	rVB	262129	318410	18.71%	2.156%
31	16.074	2374	2378	2382	rVB	50113	70342	4.13%	0.476%
32	16.604	2464	2468	2472	rVB2	25806	40349	2.37%	0.273%
33	17.227	2569	2574	2582	rVB7	19854	38499	2.26%	0.261%

LSC Area Percent Report

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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-24(0-10)

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-BF110818.M
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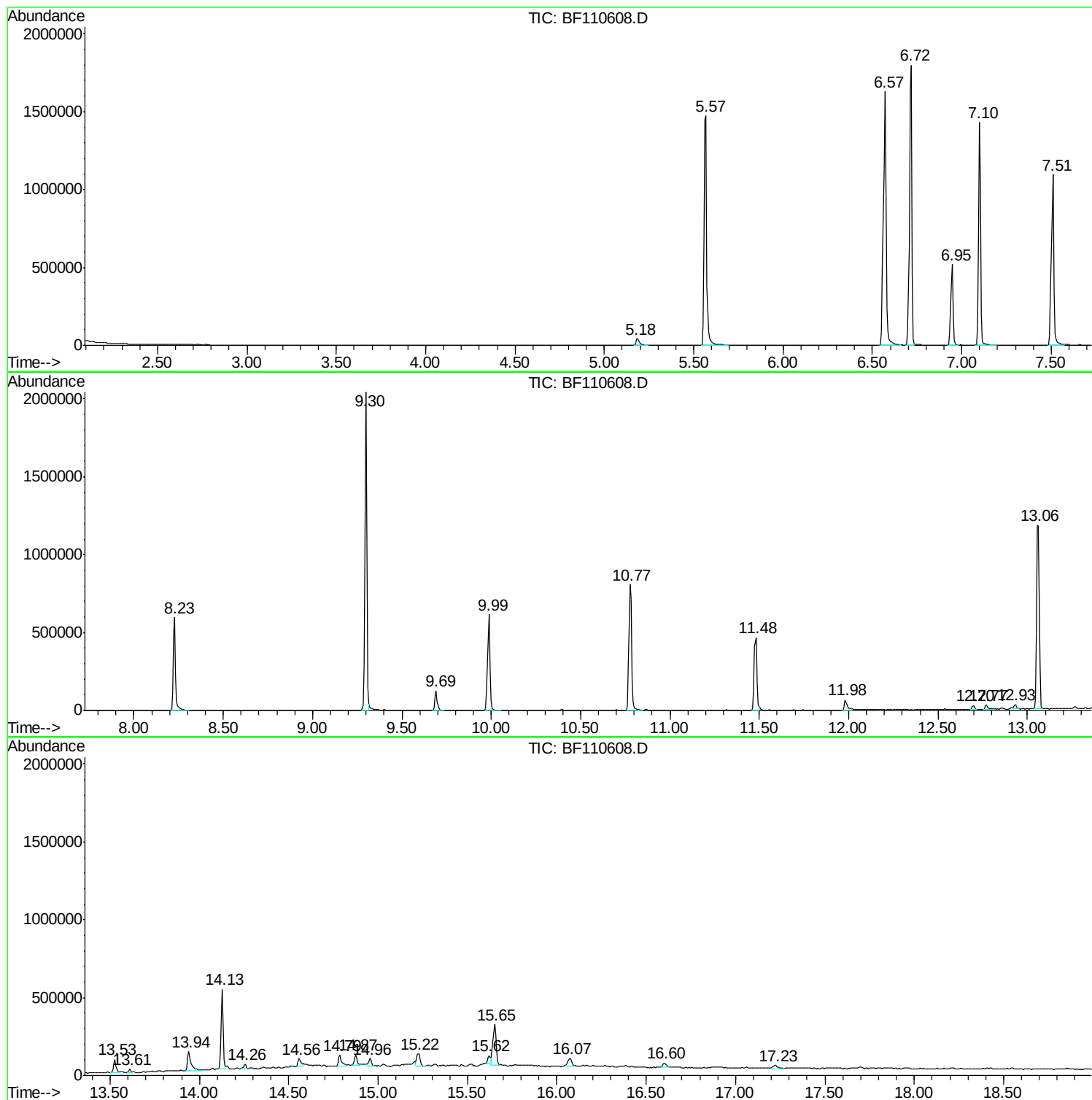
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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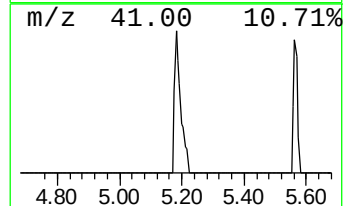
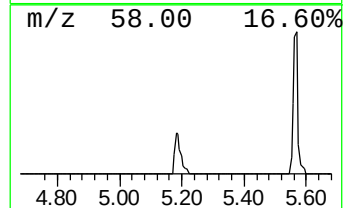
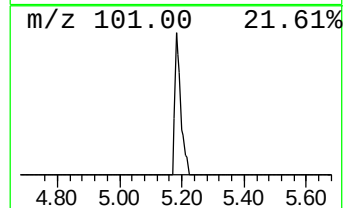
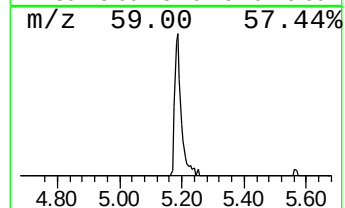
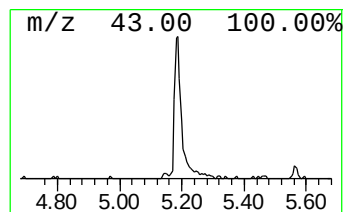
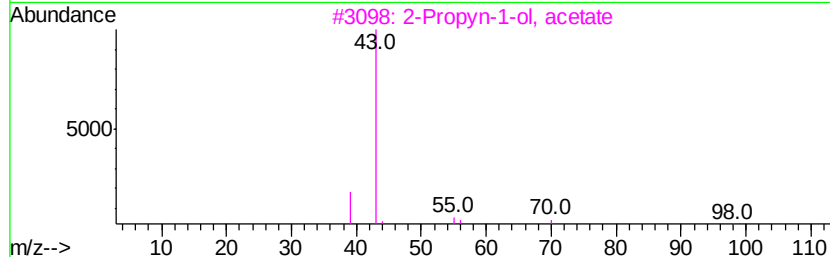
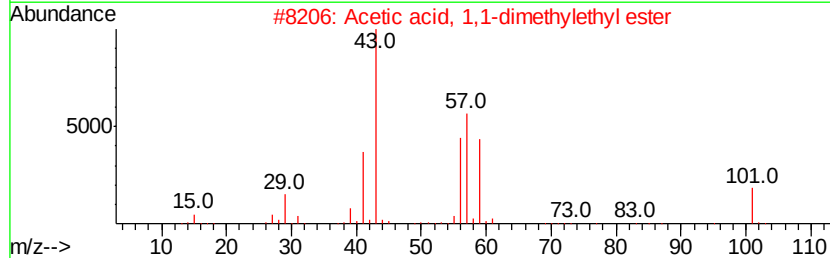
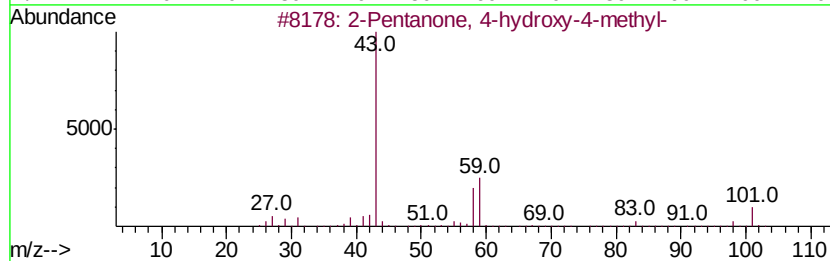
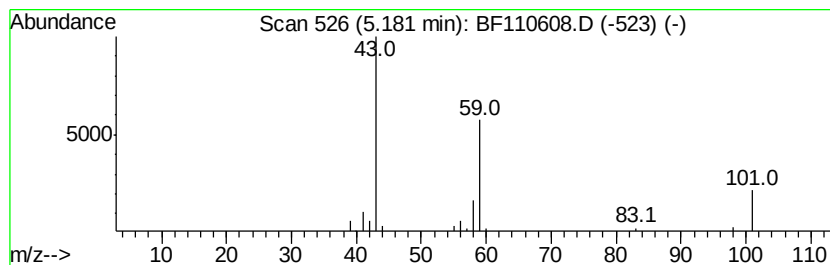
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.18	2.51 ng	55660	1,4-Dichlorobenzene-d4	6.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	40
3	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4	Acetone	58	C3H6O	000067-64-1	9
5	tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	9



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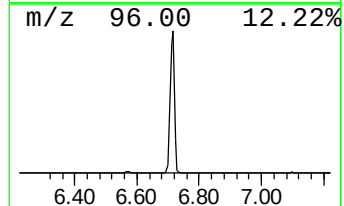
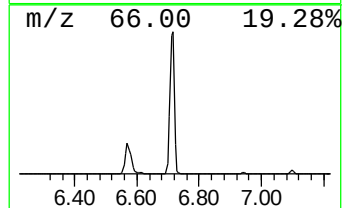
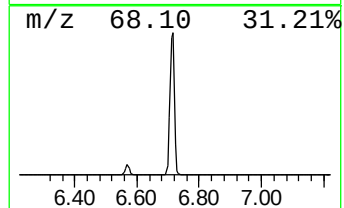
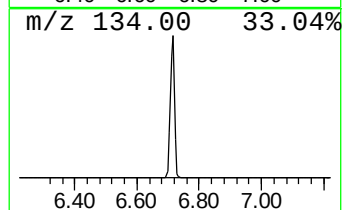
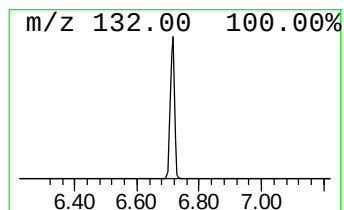
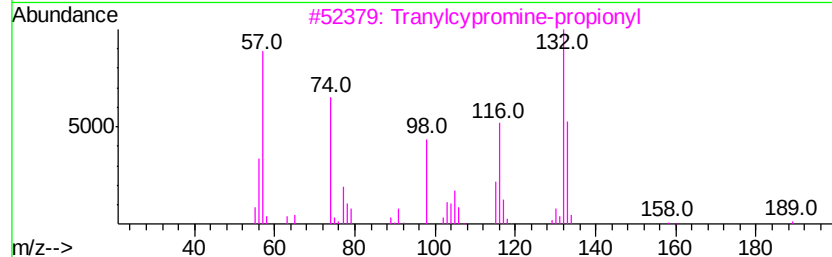
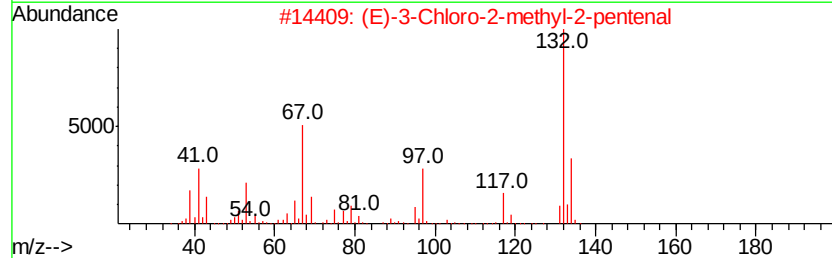
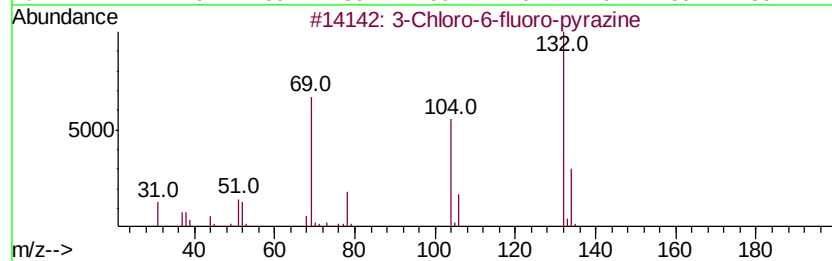
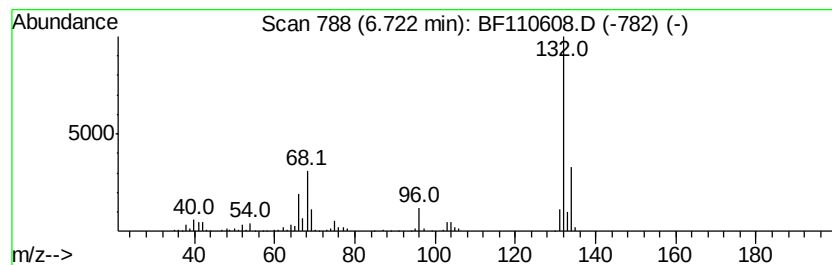
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	74.59 ng	1653250	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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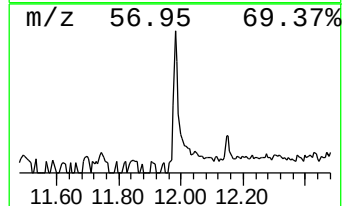
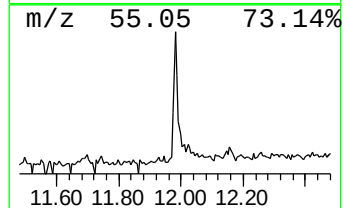
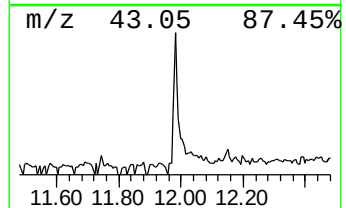
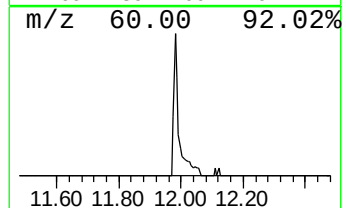
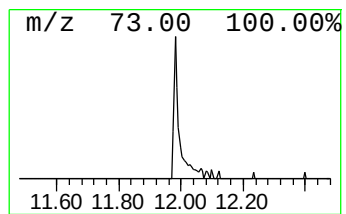
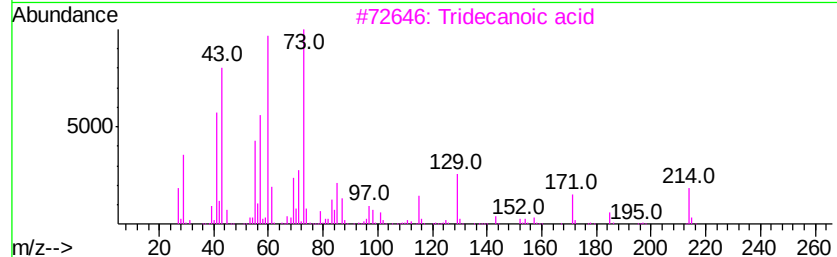
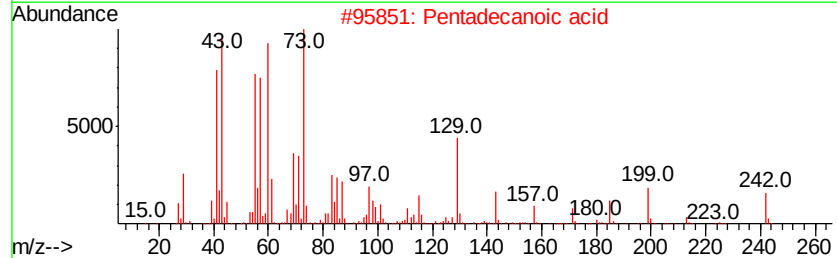
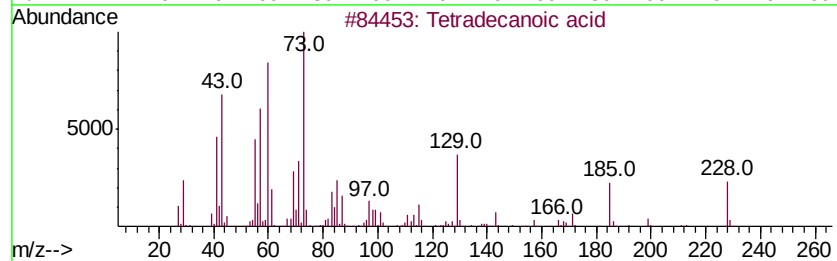
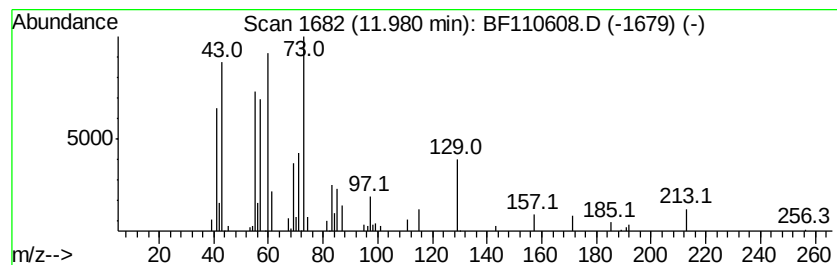
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	3.16 ng	68701	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	53
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49



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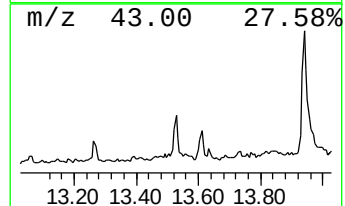
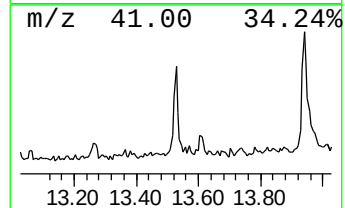
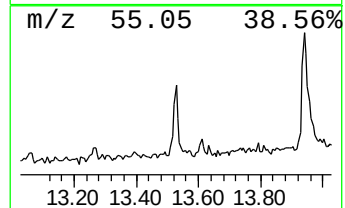
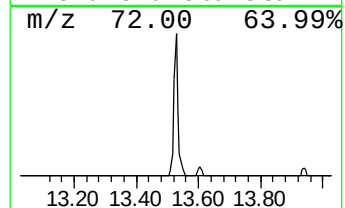
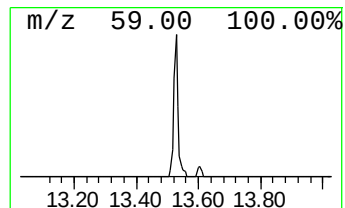
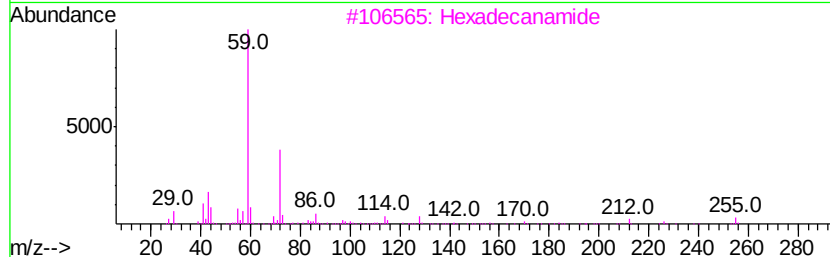
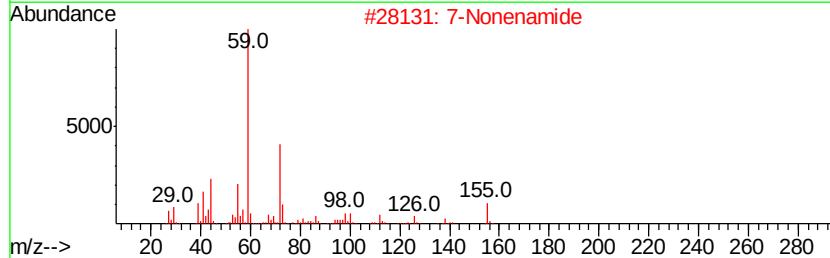
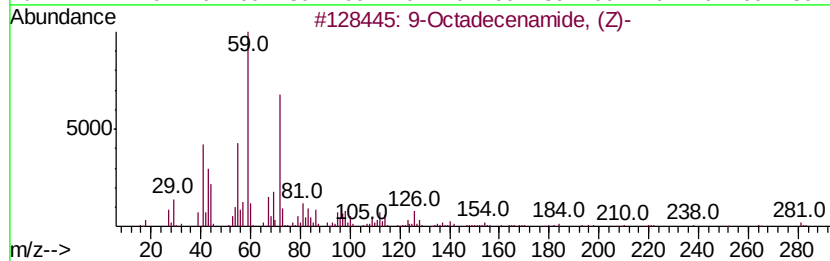
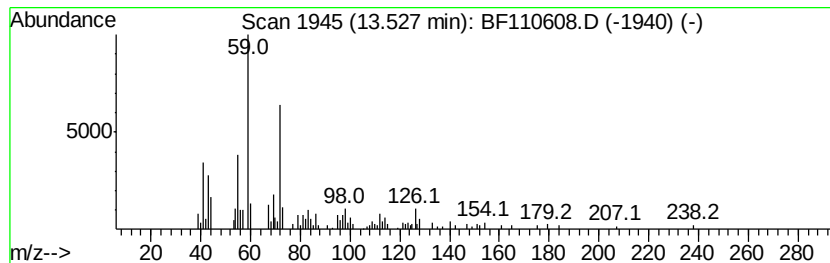
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	3.88 ng	87974	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		7-Nonenamide	155	C9H17NO	090949-53-4	72
3		Hexadecanamide	255	C16H33NO	000629-54-9	64
4		Dodecanamide	199	C12H25NO	001120-16-7	53
5		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50



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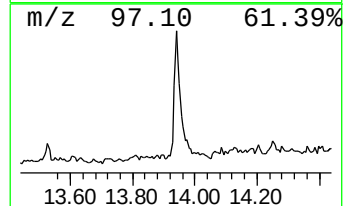
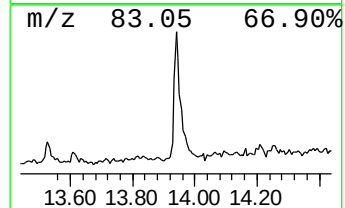
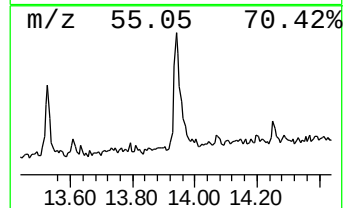
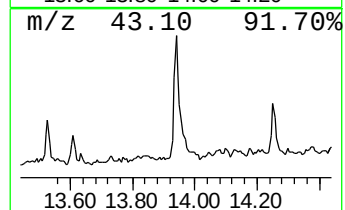
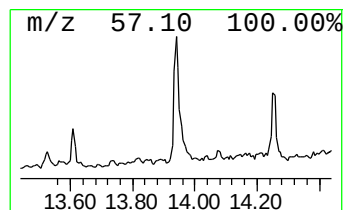
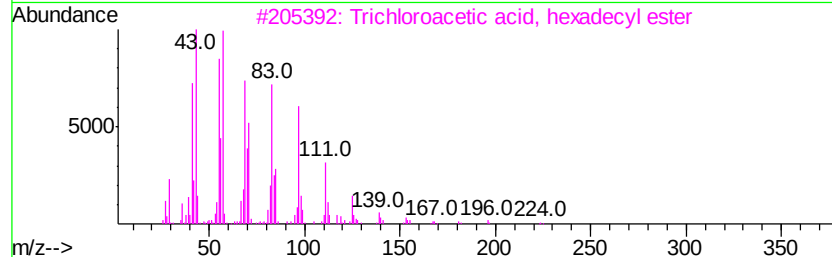
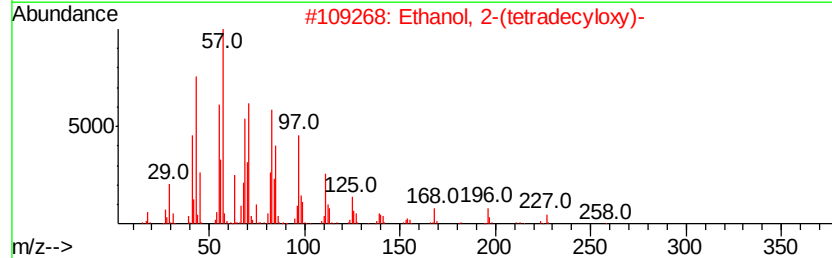
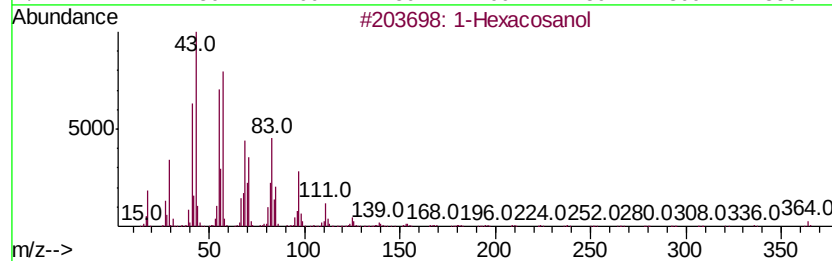
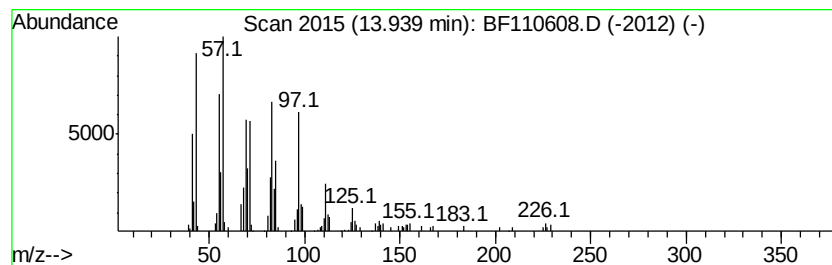
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Hexacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	8.25 ng	186968	Chrysene-d12	14.13
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexacosanol	382 C26H54O	000506-52-5	91
2	Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1	91
3	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	87
4	Octacosyl trifluoroacetate	506 C30H57F3O2	1000351-74-9	87
5	n-Tetracosanol-1	354 C24H50O	000506-51-4	87



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B-24(0-10)

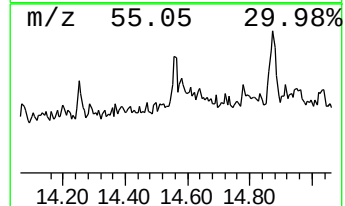
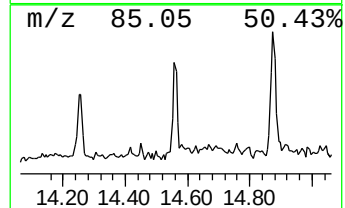
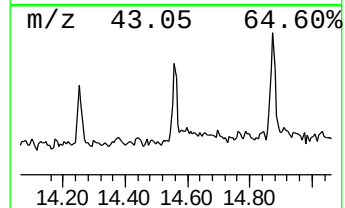
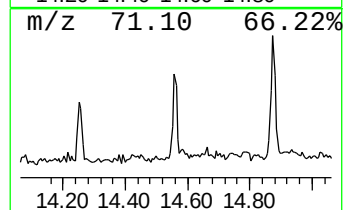
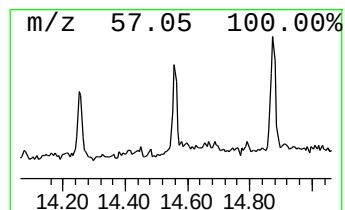
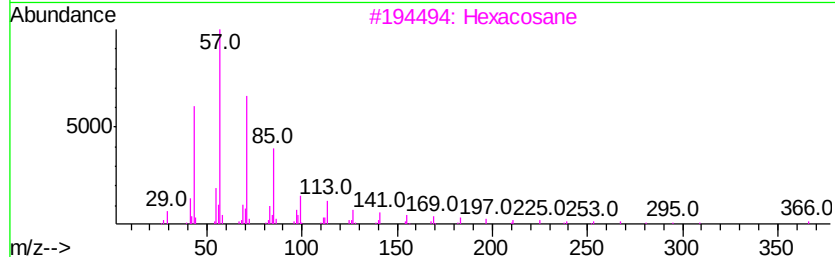
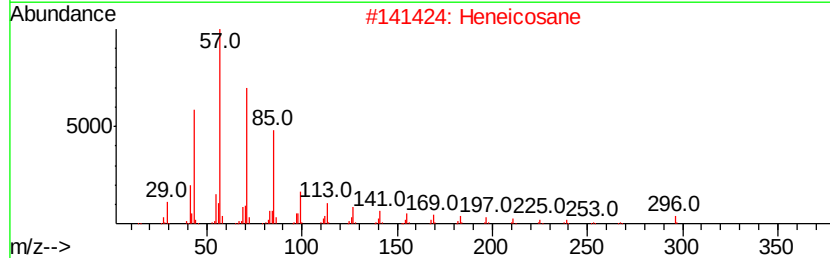
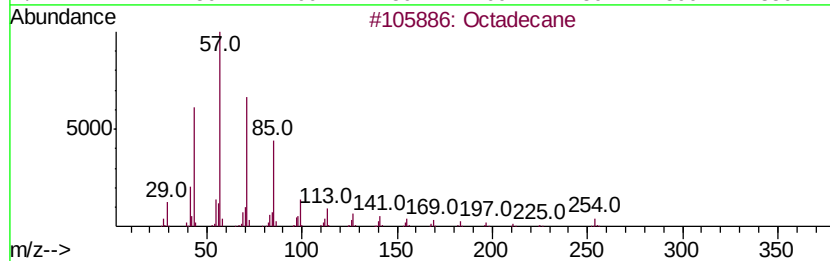
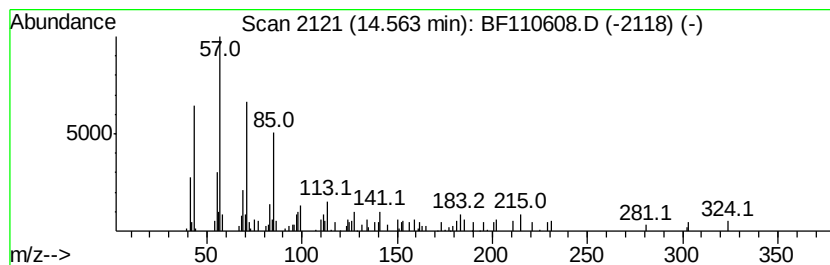
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.17 ng	49129	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	80
2		Heneicosane	296	C21H44	000629-94-7	74
3		Hexacosane	366	C26H54	000630-01-3	74
4		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	72
5		Pentacosane	352	C25H52	000629-99-2	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110818\
Data File : BF110608.D
Acq On : 9 Nov 2018 1:50
Operator : JU/SJ
Sample : J5859-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

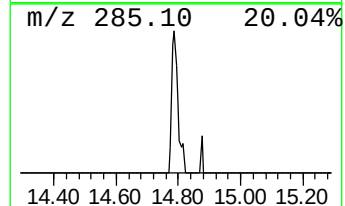
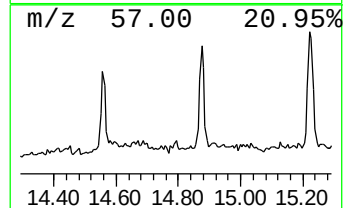
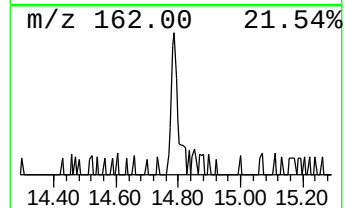
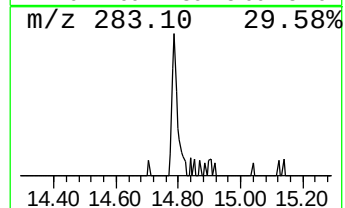
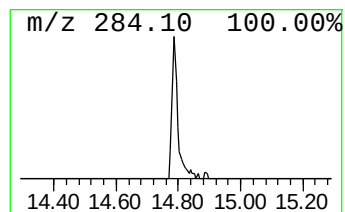
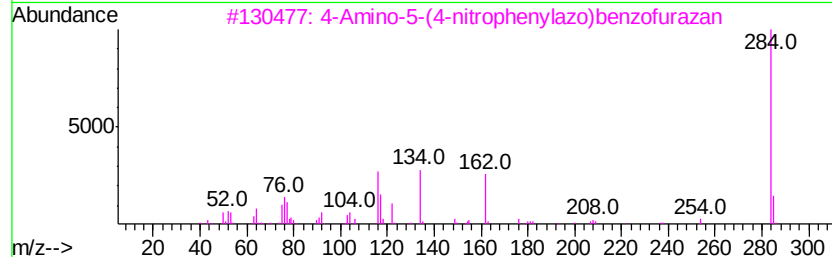
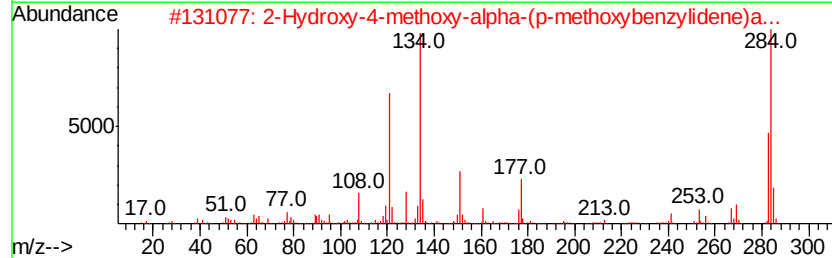
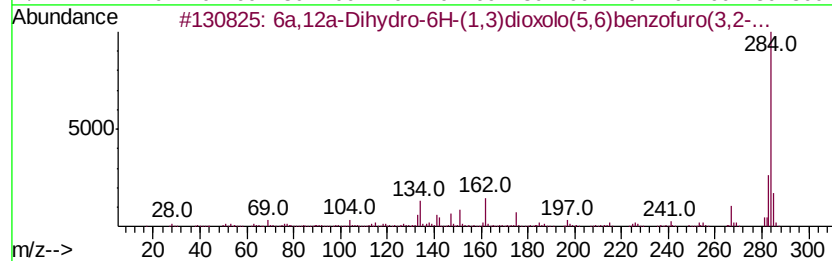
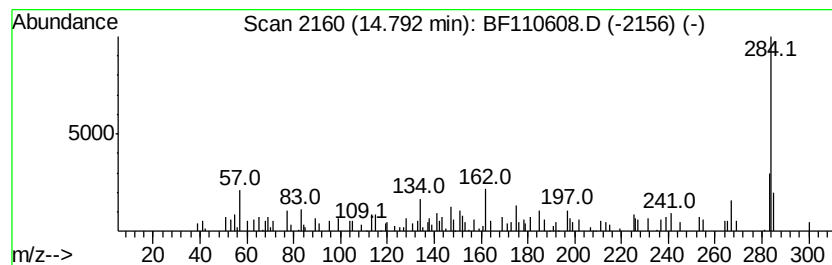
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.79	4.29 ng	97188	Chrysene-d12	14.13		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6a,12a-Dihydro-6H-(1,3)dioxolo(5...	284	C16H12O5	022091-18-5	91	
2	2-Hydroxy-4-methoxy-alpha-(p-met...	284	C17H16O4	002198-19-8	64	
3	4-Amino-5-(4-nitrophenylazo)benz...	284	C12H8N6O3	166766-07-0	58	
4	2-(9-Acridinyl)-4-methylbenzenea...	284	C20H16N2	035586-77-7	58	
5	Coumaran-5-ol-3-one, 2-[4-hydrox...	284	C16H12O5	1000129-33-1	58	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110818\
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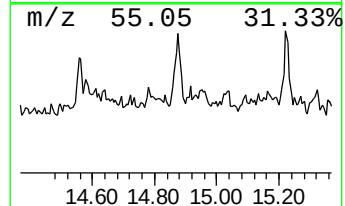
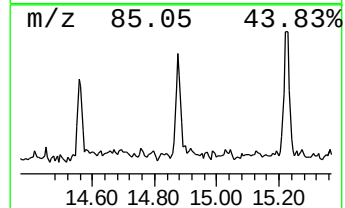
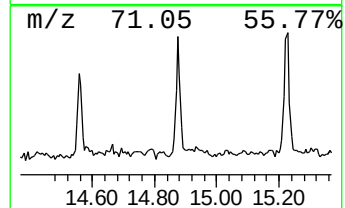
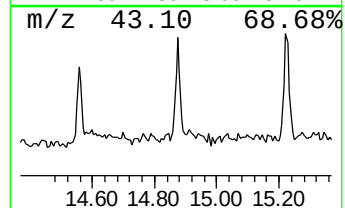
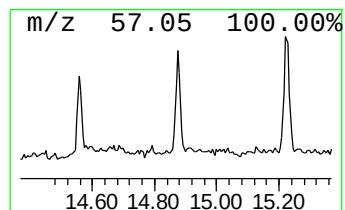
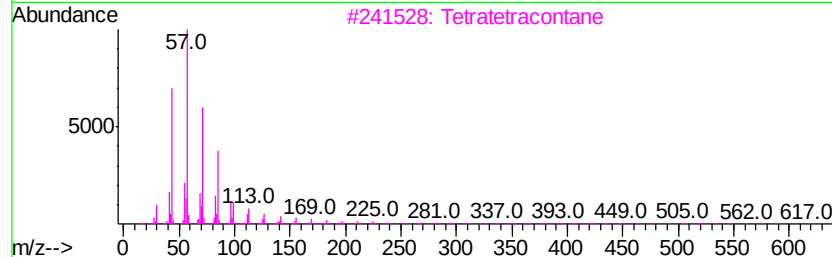
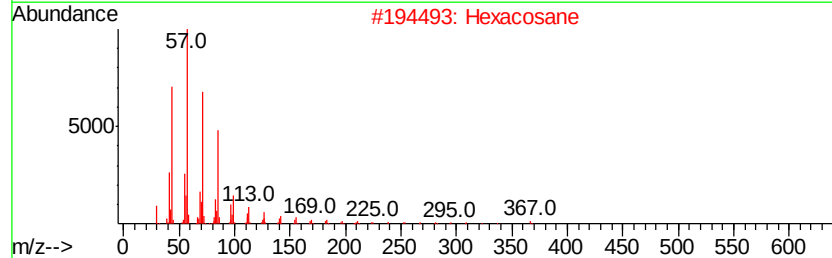
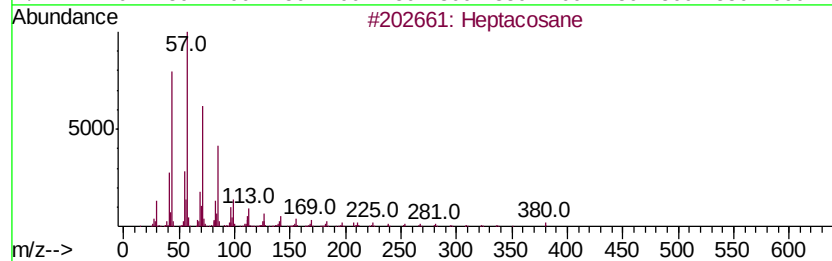
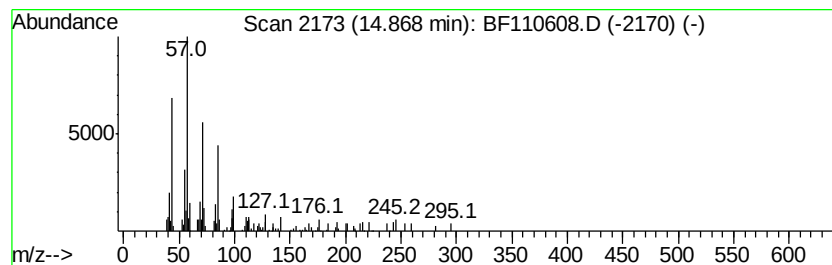
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.44 ng	78068	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	90
2	Hexacosane		366	C26H54	000630-01-3	87
3	Tetratetracontane		619	C44H90	007098-22-8	87
4	Octacosane		394	C28H58	000630-02-4	87
5	triacontane		422	C30H62	000638-68-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110818\
Data File : BF110608.D
Acq On : 9 Nov 2018 1:50
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ALS Vial : 26 Sample Multiplier: 1

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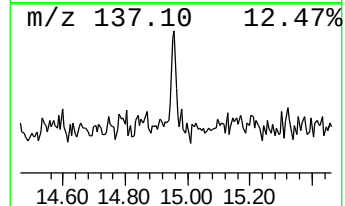
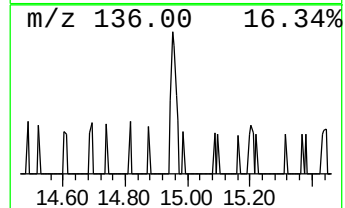
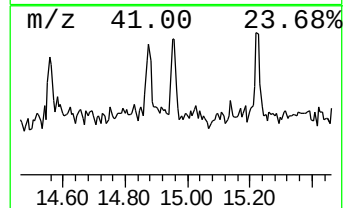
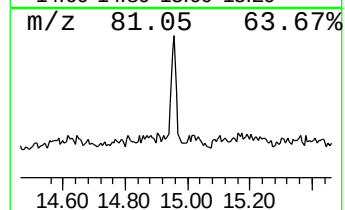
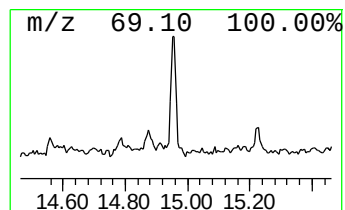
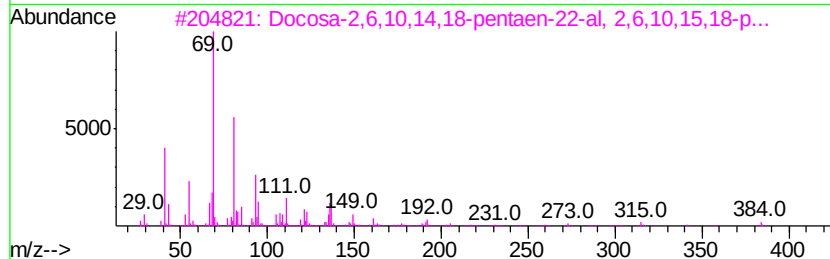
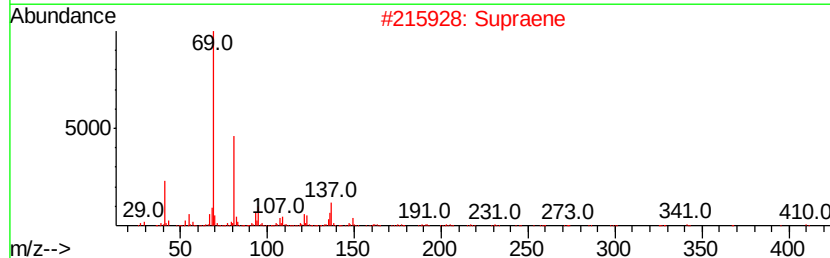
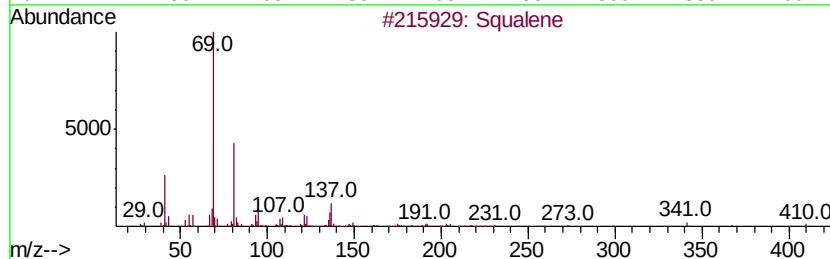
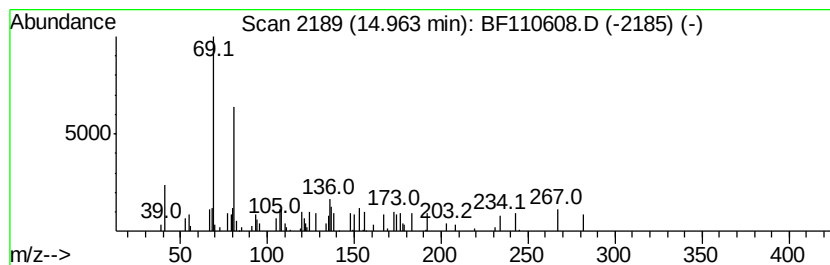
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.07 ng	48816	Perylene-d12	15.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	83
2		Supraene	410	C30H50	007683-64-9	72
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
4		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	50
5		3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	50



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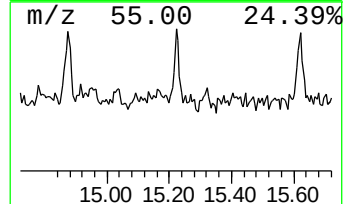
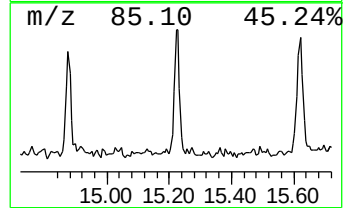
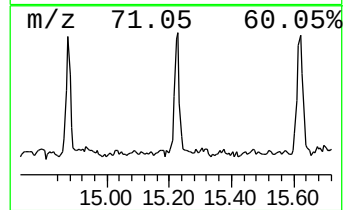
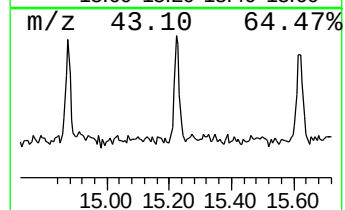
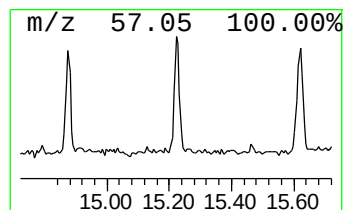
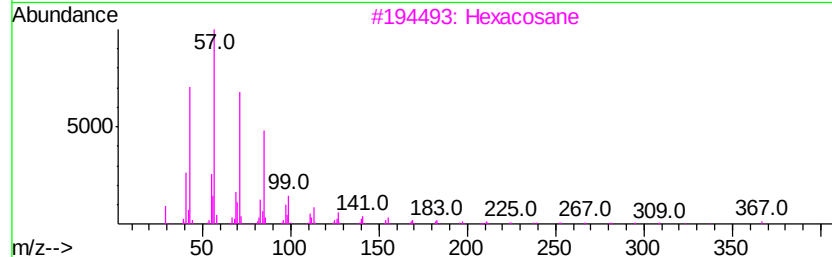
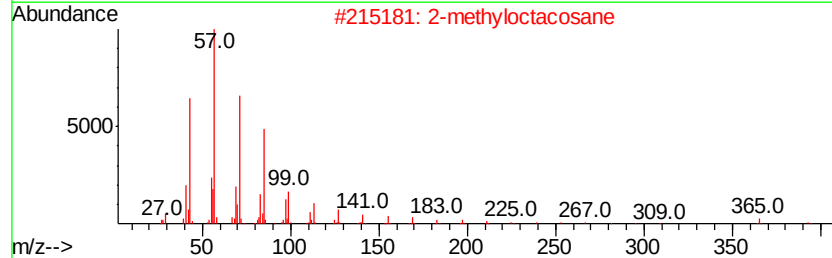
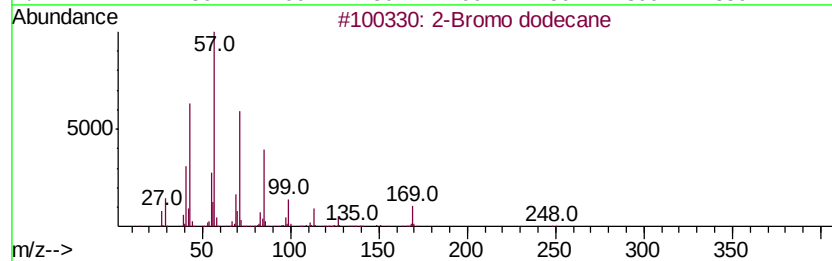
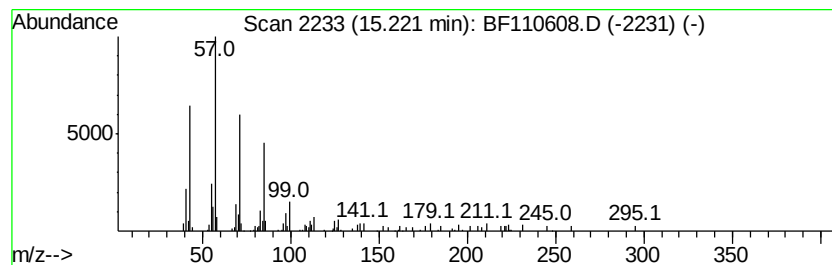
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-Bromo dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.22	5.95 ng	94774	Perylene-d12		15.65
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	83
2	2-methyloctacosane	408	C29H60	1000376-72-8	83
3	Hexacosane	366	C26H54	000630-01-3	83
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5	Tetracosane	338	C24H50	000646-31-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110818\
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Acq On : 9 Nov 2018 1:50
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Misc :
ALS Vial : 26 Sample Multiplier: 1

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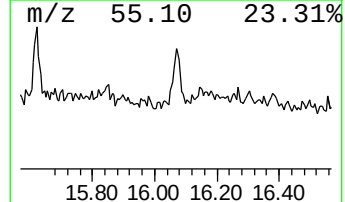
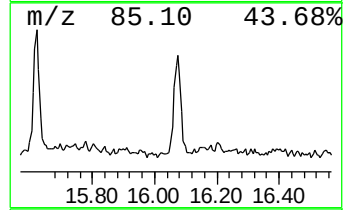
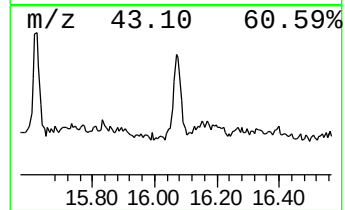
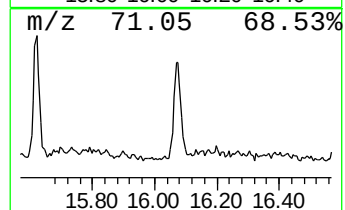
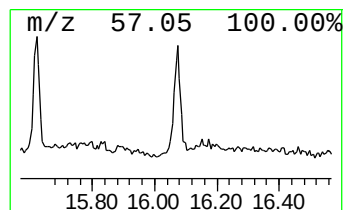
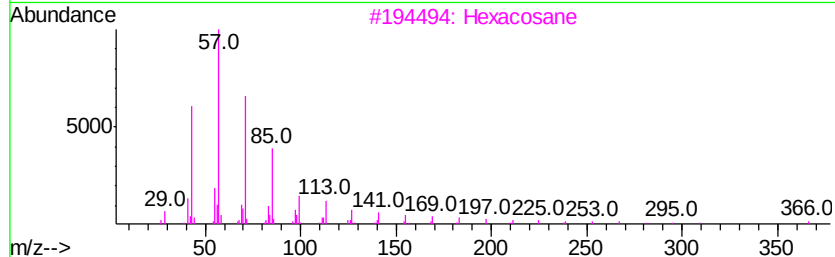
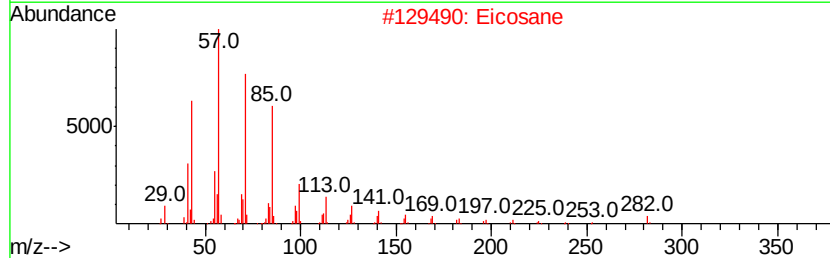
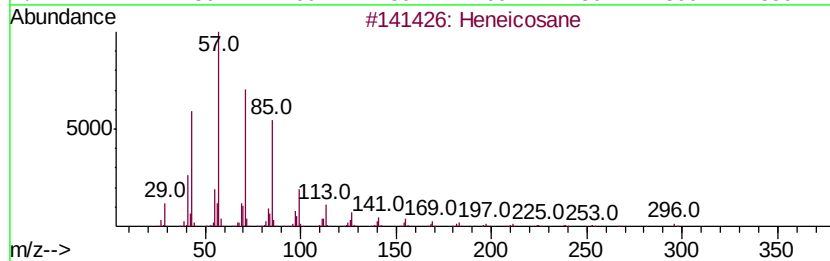
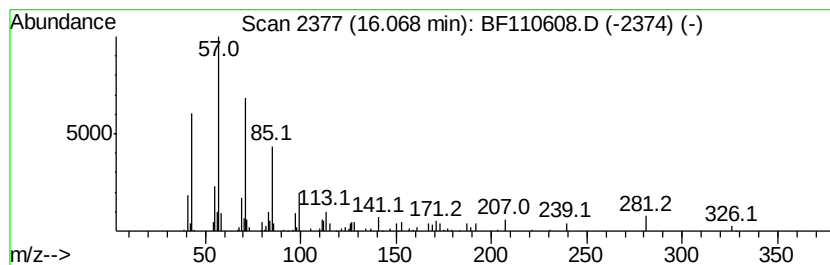
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	4.42 ng	70342	Perylene-d12	15.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	83
2		Eicosane	282	C20H42	000112-95-8	81
3		Hexacosane	366	C26H54	000630-01-3	80
4		Octadecane	254	C18H38	000593-45-3	80
5		Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110818\
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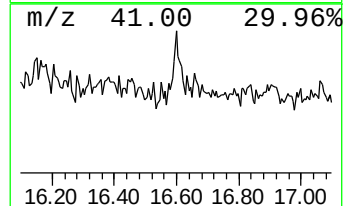
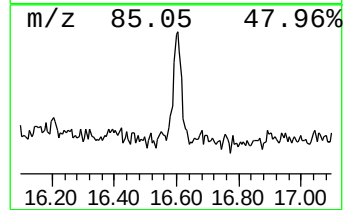
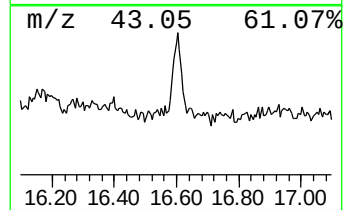
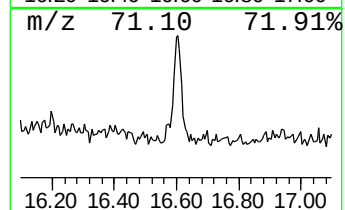
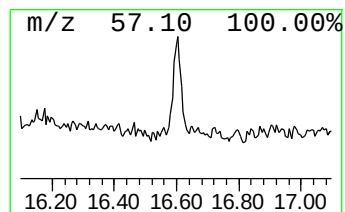
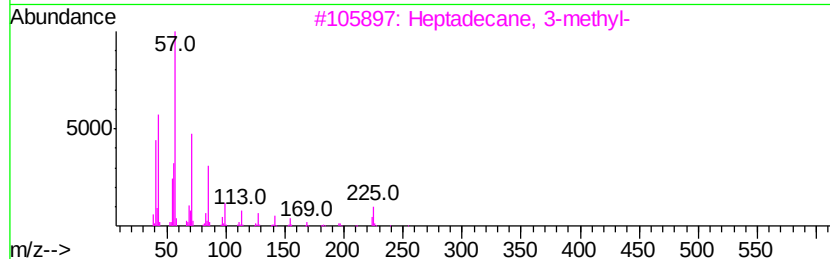
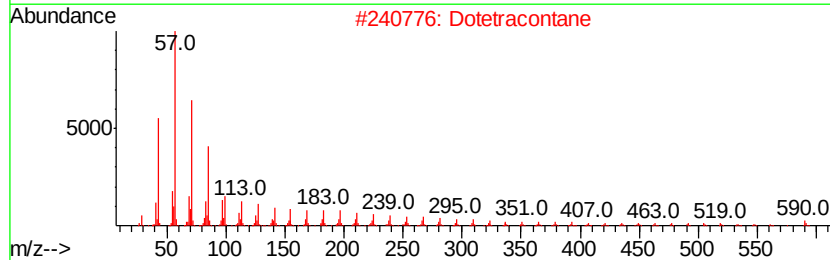
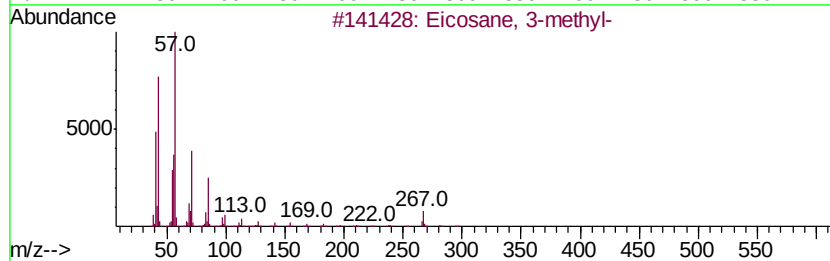
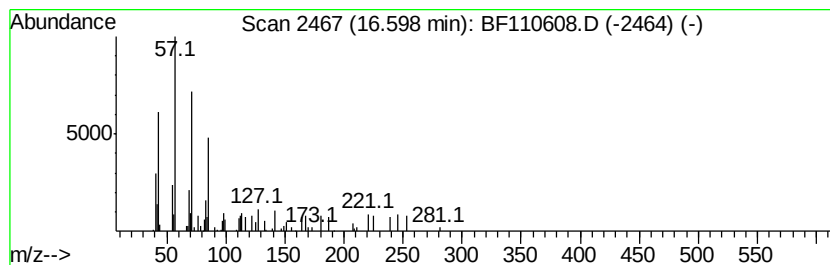
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Eicosane, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	2.53 ng	40349	Perylene-d12	15.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 3-methyl-	296	C21H44	006418-46-8	72
2			Dotetracontane	591	C42H86	007098-20-6	72
3			Heptadecane, 3-methyl-	254	C18H38	006418-44-6	64
4			Octacosane	394	C28H58	000630-02-4	64
5			Octadecane, 2-methyl-	268	C19H40	001560-88-9	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110818\
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Acq On : 9 Nov 2018 1:50
Operator : JU/SJ
Sample : J5859-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-24(0-10)

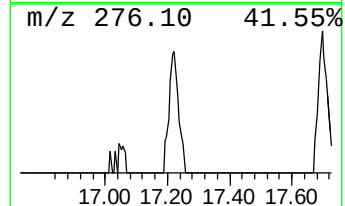
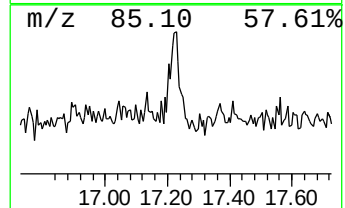
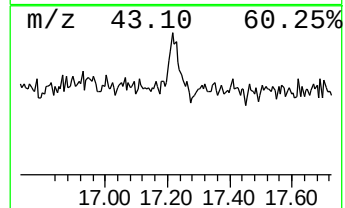
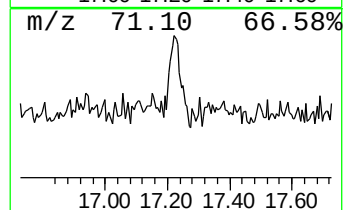
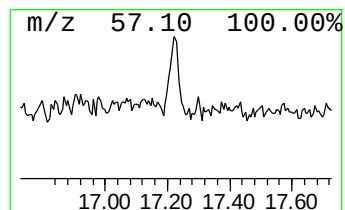
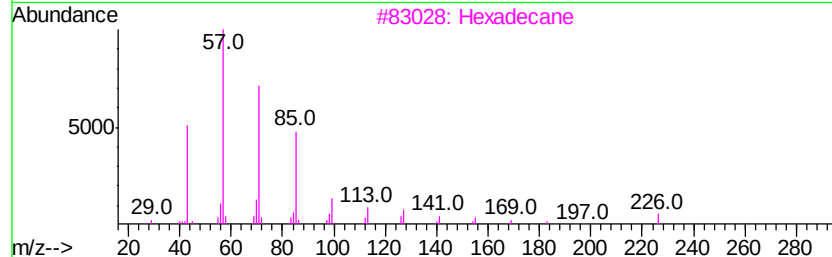
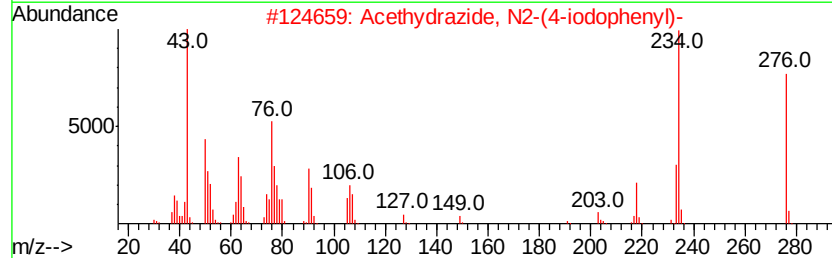
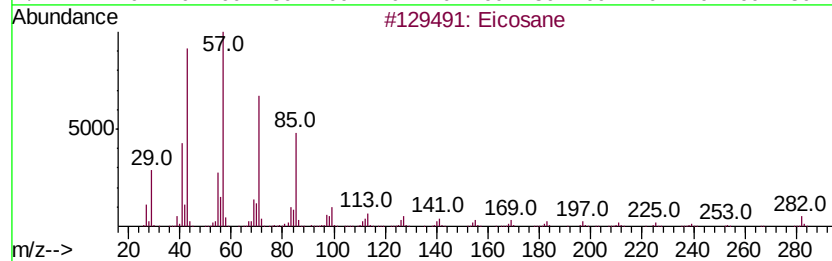
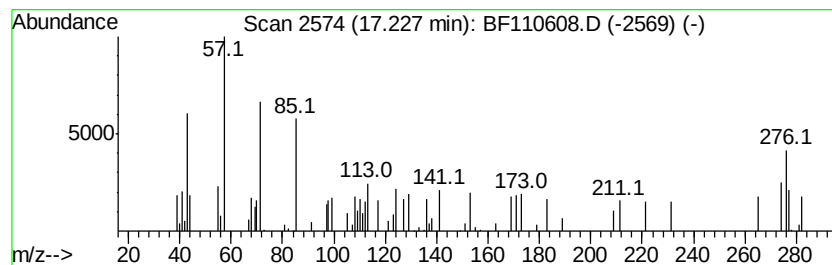
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.23 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.23	2.42 ng	38499	Perylene-d12	15.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	15
2		Acethydrazide, N2-(4-iodophenyl)-	276	C8H9IN2O	014579-96-5	11
3		Hexadecane	226	C16H34	000544-76-3	10
4		Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	10
5		7-Octadecanone	268	C18H36O	018277-00-4	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110818\
 Data File : BF110608.D
 Acq On : 9 Nov 2018 1:50
 Operator : JU/SJ
 Sample : J5859-05
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-24(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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...	5.18	2.5	ng	55660	1	6.95	443269	20.0
unknown6.72	6.72	74.6	ng	1653250	1	6.95	443269	20.0
Tetradecanoic acid	11.98	3.2	ng	68701	4	11.48	435279	20.0
9-Octadecenamide, ...	13.53	3.9	ng	87974	5	14.13	453511	20.0
1-Hexacosanol	13.94	8.3	ng	186968	5	14.13	453511	20.0
Octadecane	14.56	2.2	ng	49129	5	14.13	453511	20.0
6a,12a-Dihydro-6H...	14.79	4.3	ng	97188	5	14.13	453511	20.0
Heptacosane	14.87	3.4	ng	78068	5	14.13	453511	20.0
Squalene	14.96	3.1	ng	48816	6	15.65	318410	20.0
2-Bromo dodecane	15.22	6.0	ng	94774	6	15.65	318410	20.0
Heneicosane	16.07	4.4	ng	70342	6	15.65	318410	20.0
Eicosane, 3-methyl-	16.60	2.5	ng	40349	6	15.65	318410	20.0
unknown17.23	17.23	2.4	ng	38499	6	15.65	318410	20.0