

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
 Data File : BF111287.D
 Acq On : 11 Dec 2018 20:09
 Operator : JU/SJ
 Sample : J6157-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-3-TOTAL

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-BF120818.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.834	120	127	134	rVB	92533	150680	2.65%	0.332%
2	4.040	326	332	336	rBV	56861	72625	1.28%	0.160%
3	4.987	487	493	502	rVB2	281119	317816	5.59%	0.701%
4	5.410	560	565	577	rVB	1850127	1810294	31.83%	3.992%
5	6.422	733	737	745	rBV2	1278379	1646837	28.95%	3.632%
6	6.563	757	761	764	rBV	3626578	3018268	53.06%	6.656%
7	6.792	797	800	804	rBV	1549518	1360479	23.92%	3.000%
8	6.951	823	827	831	rBV	3878063	3269228	57.47%	7.210%
9	7.351	890	895	898	rBV	3025081	2820281	49.58%	6.219%
10	8.075	1014	1018	1022	rBV	1951934	1826875	32.12%	4.029%
11	9.157	1197	1202	1205	rBV	6321360	5688174	100.00%	12.544%
12	9.545	1265	1268	1271	rBV	1074273	802385	14.11%	1.769%
13	9.833	1313	1317	1321	rVB	2588599	2222495	39.07%	4.901%
14	10.033	1348	1351	1354	rBV	75286	71732	1.26%	0.158%
15	10.251	1384	1388	1390	rBV	124302	109139	1.92%	0.241%
16	10.616	1446	1450	1454	rBV	3101708	2817552	49.53%	6.213%
17	11.316	1565	1569	1573	rBV	2725944	2271973	39.94%	5.010%
18	11.710	1633	1636	1640	rVB2	215676	184020	3.24%	0.406%
19	11.857	1655	1661	1672	rBV	2664768	2712025	47.68%	5.981%
20	12.539	1773	1777	1779	rBV2	100338	117018	2.06%	0.258%
21	12.639	1790	1794	1807	rBV	1856311	1781366	31.32%	3.928%
22	12.904	1835	1839	1842	rBV	4756370	4167214	73.26%	9.190%
23	13.810	1989	1993	2001	rBV2	609850	837357	14.72%	1.847%
24	13.951	2013	2017	2021	rBV	1988966	1961590	34.49%	4.326%
25	14.133	2045	2048	2054	rBV	74612	85201	1.50%	0.188%
26	14.445	2098	2101	2108	rBV2	120924	136809	2.41%	0.302%
27	14.751	2150	2153	2156	rBV	160000	141315	2.48%	0.312%
28	15.080	2206	2209	2213	rBV	198612	192700	3.39%	0.425%
29	15.404	2258	2264	2268	rBV	1272457	1552305	27.29%	3.423%
30	15.451	2269	2272	2279	rVB	192014	249131	4.38%	0.549%
31	15.880	2340	2345	2349	rBV	177670	261568	4.60%	0.577%
32	15.933	2351	2354	2362	rVB9	73655	161433	2.84%	0.356%
33	16.374	2425	2429	2437	rVB2	121084	212075	3.73%	0.468%
34	16.609	2466	2469	2479	rVB6	70250	139131	2.45%	0.307%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.945	2523	2526	2536	rvB4	84019	176907	3.11%	0.390%
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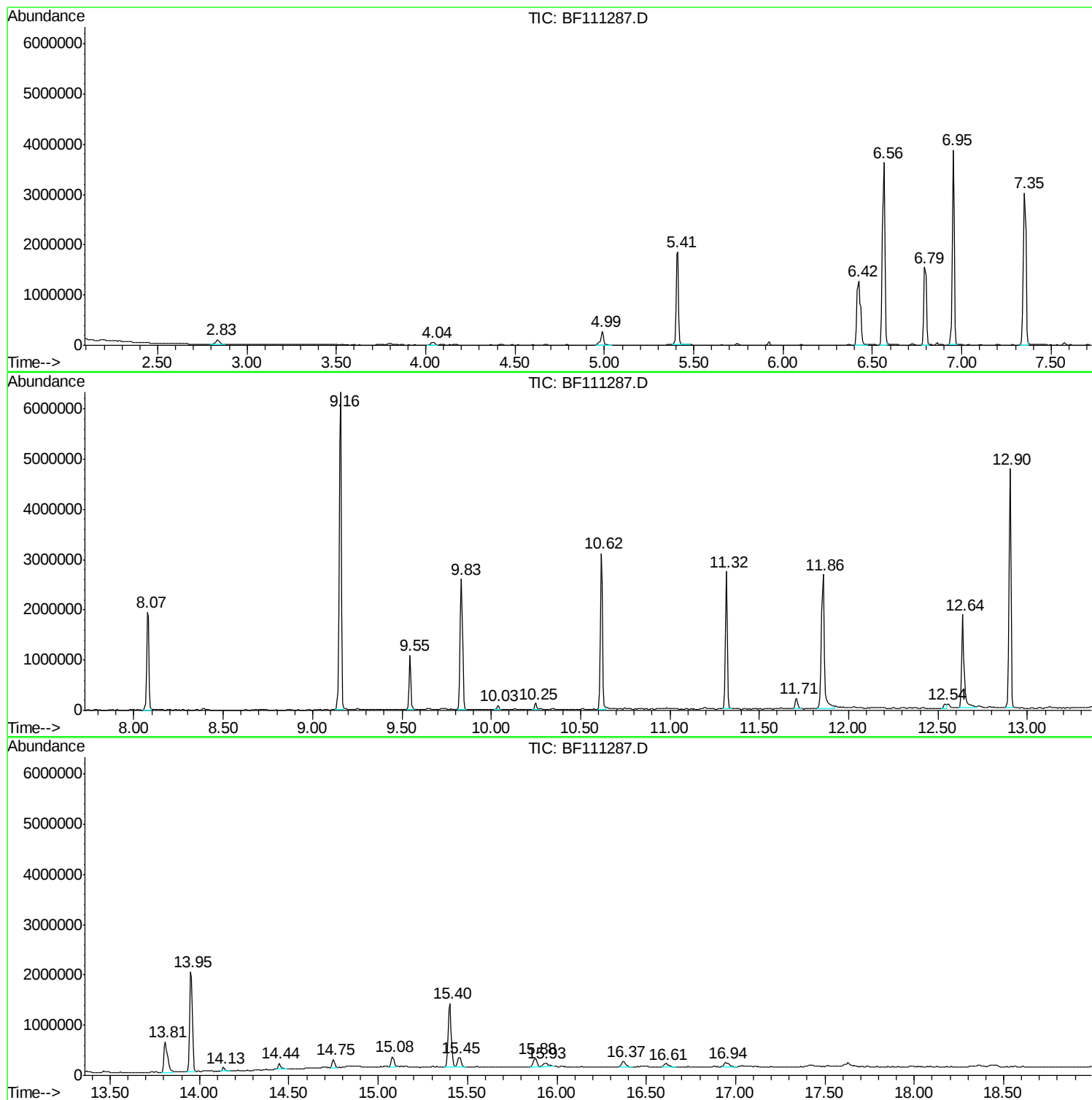
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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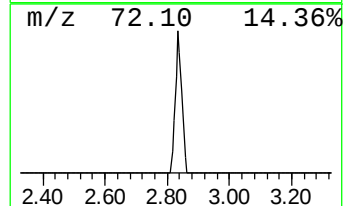
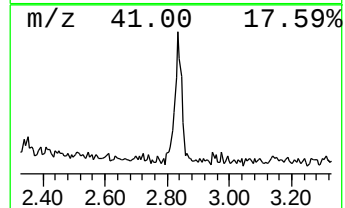
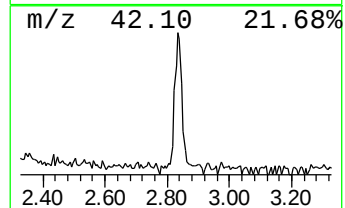
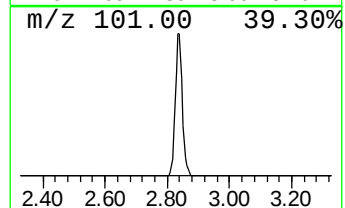
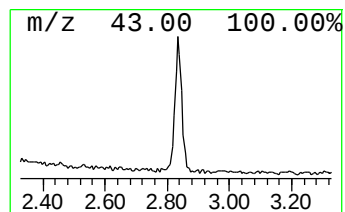
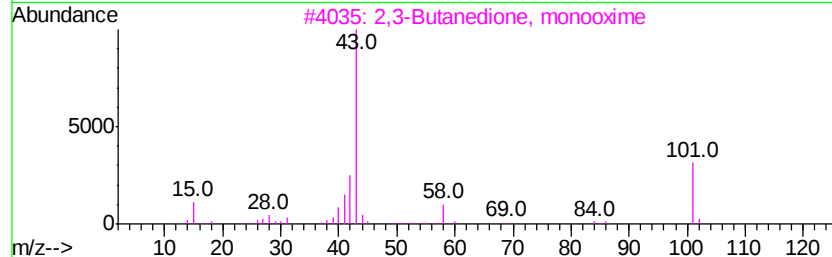
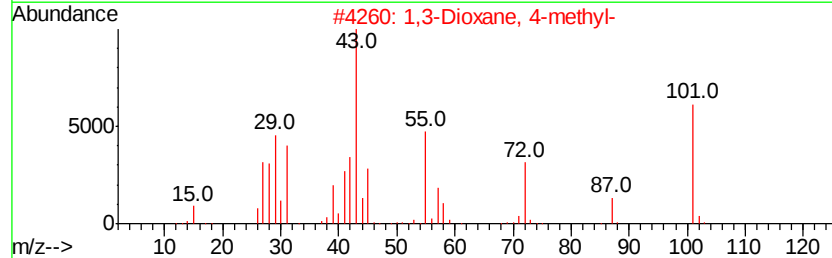
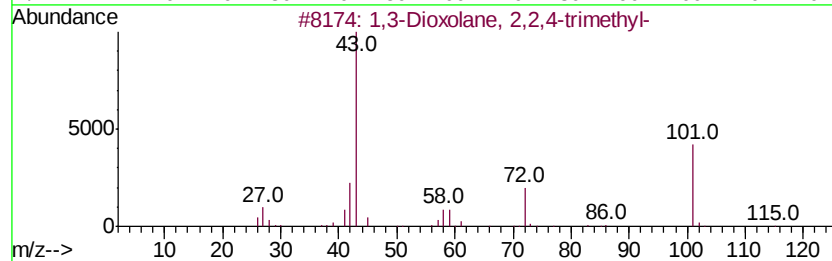
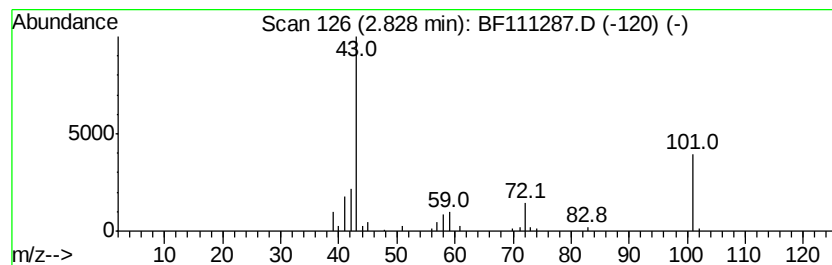
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	2.22 ng	150680	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	59
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9



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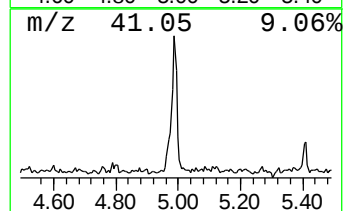
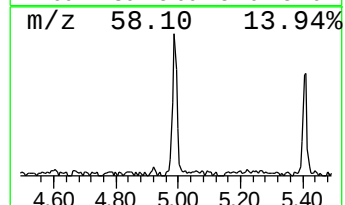
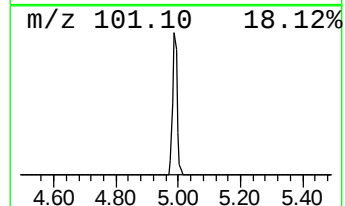
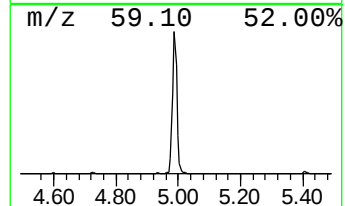
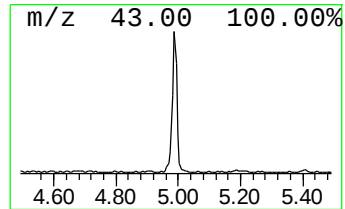
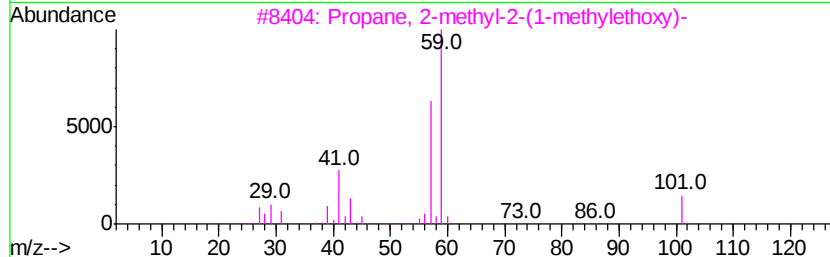
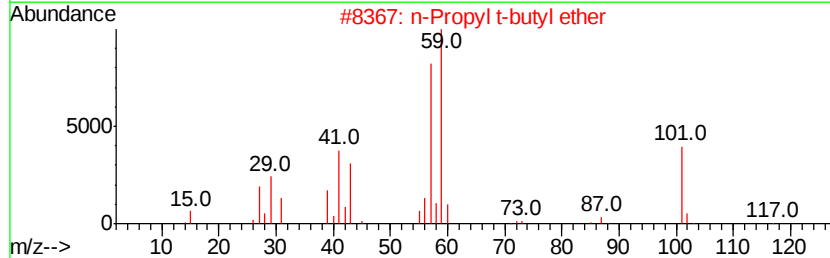
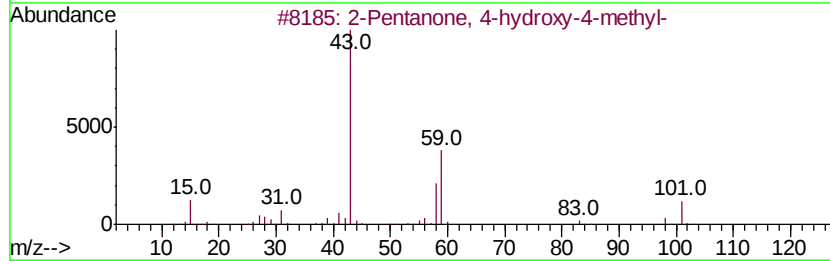
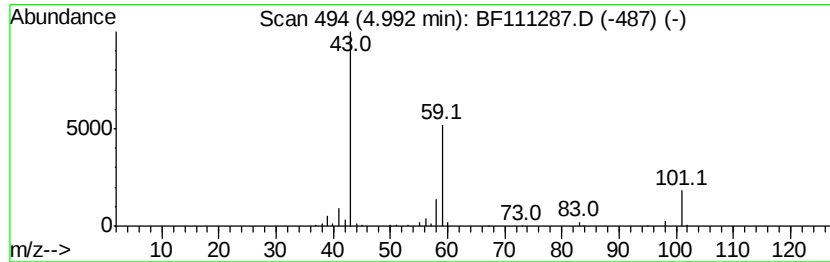
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	4.67 ng	317816	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	33
4		Acetic acid, 1,1-dimethylethyl ester	116	C6H12O2	000540-88-5	28
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25



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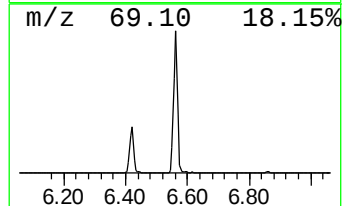
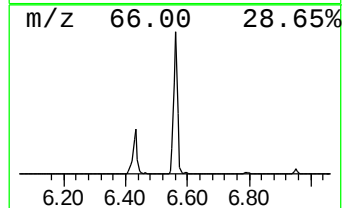
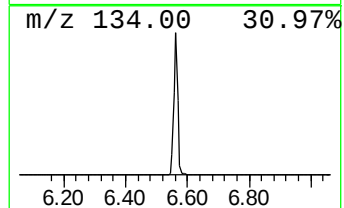
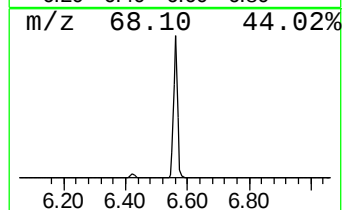
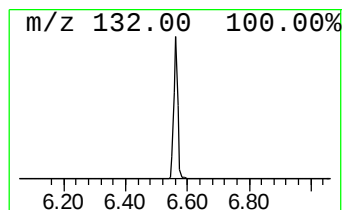
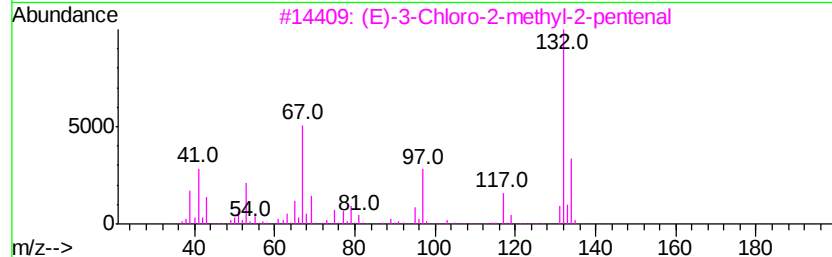
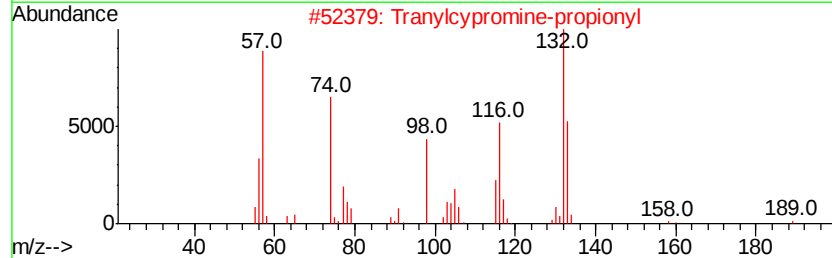
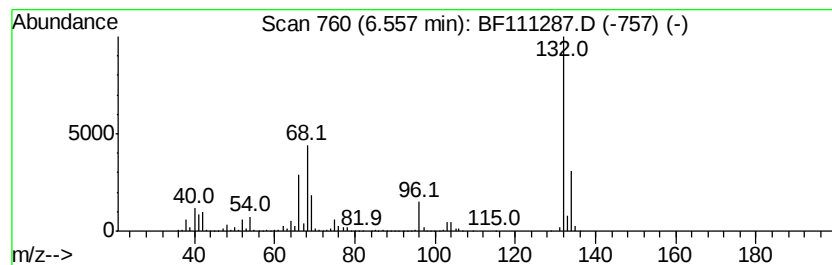
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	44.37 ng	3018270	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Xenon	132	Xe	007440-63-3	9



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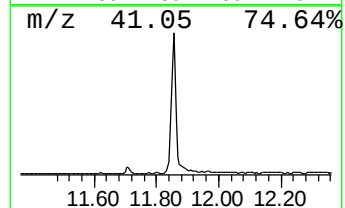
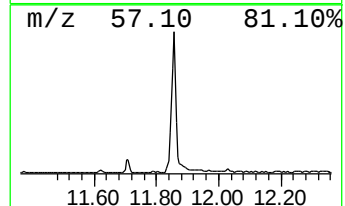
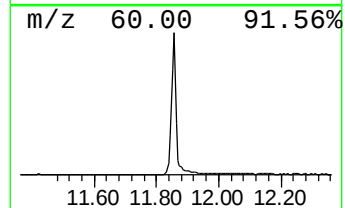
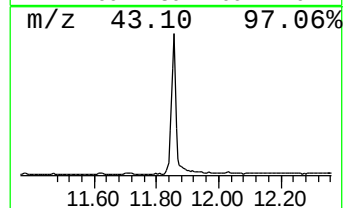
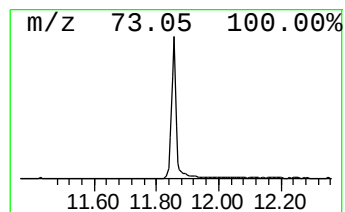
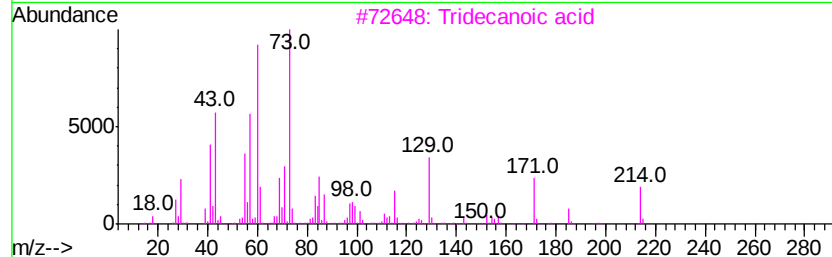
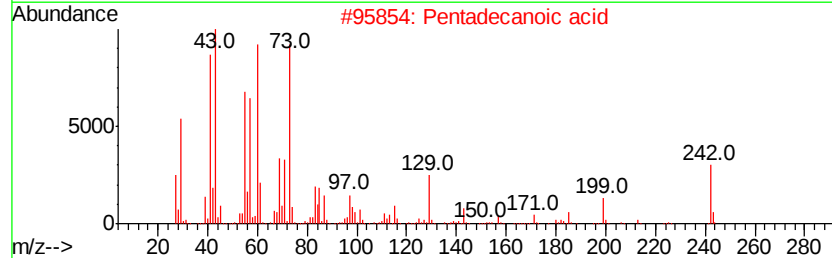
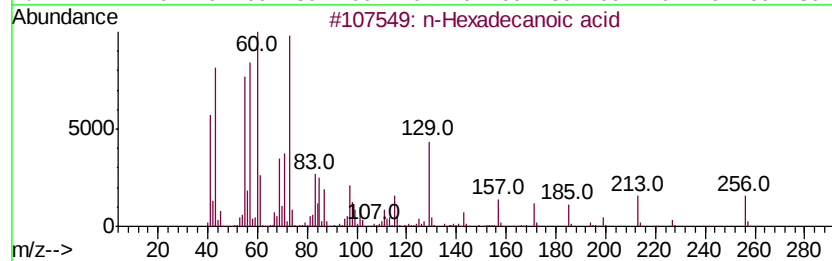
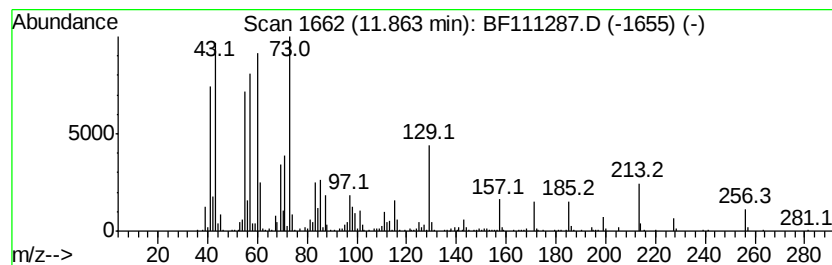
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	23.87 ng	2712030	Phenanthrene-d10	11.32

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	86
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	58



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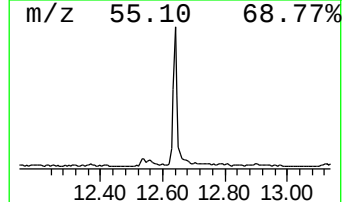
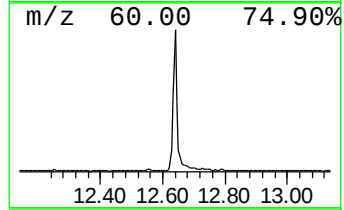
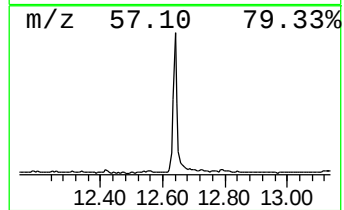
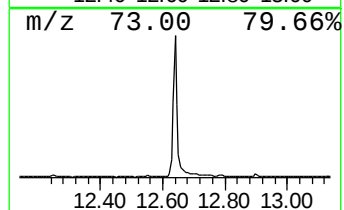
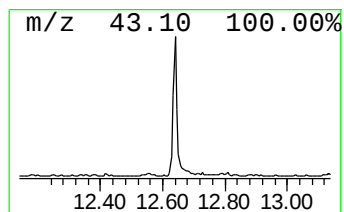
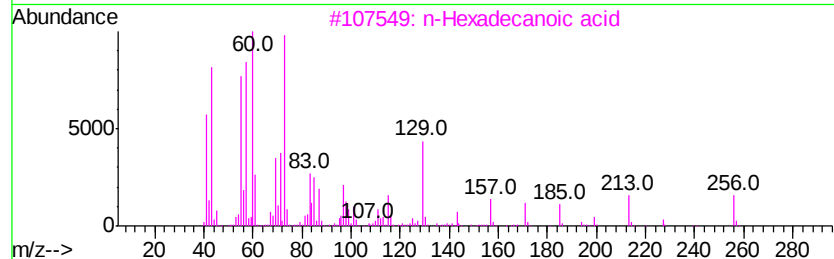
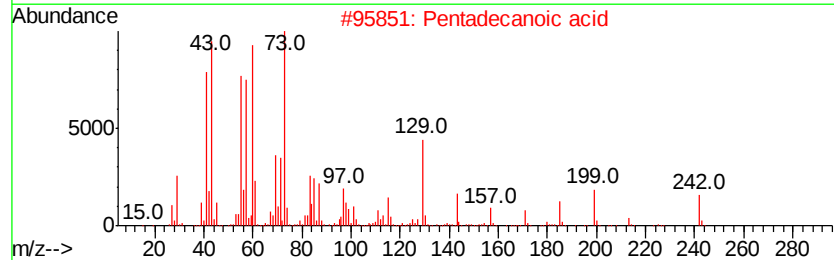
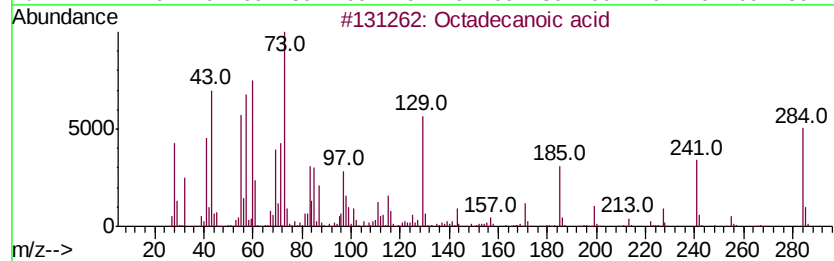
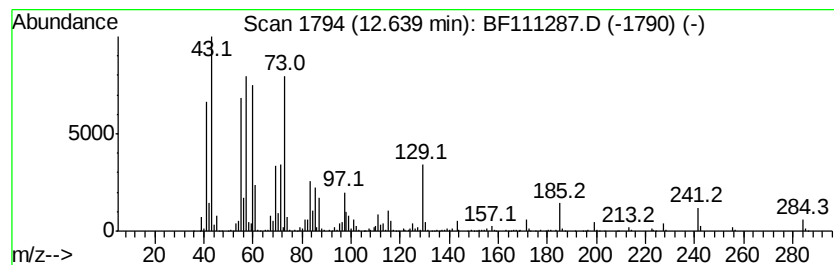
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	18.16 ng	1781370	Chrysene-d12	13.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4			Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111287.D
Acq On : 11 Dec 2018 20:09
Operator : JU/SJ
Sample : J6157-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMPOSITE-3-TOTAL

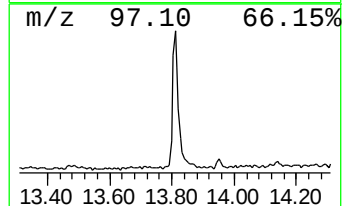
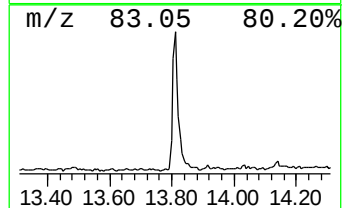
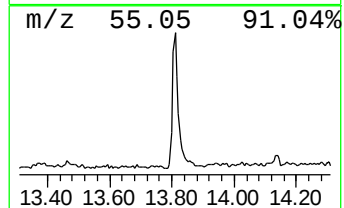
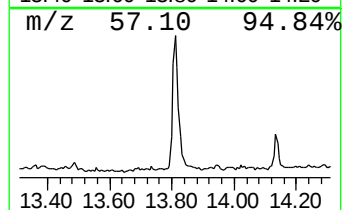
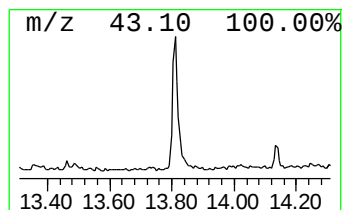
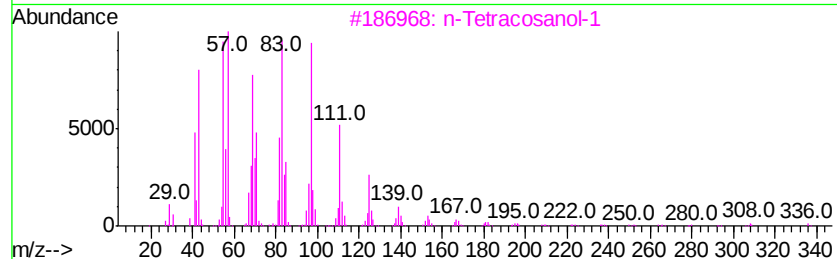
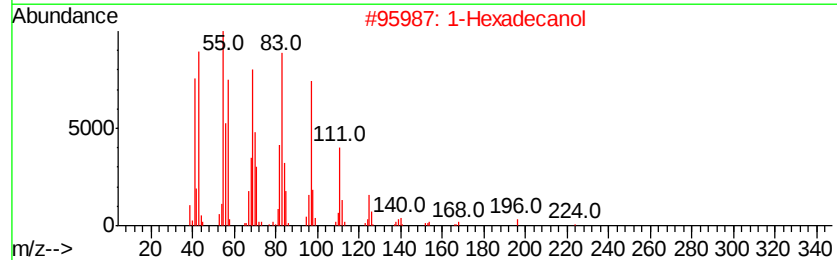
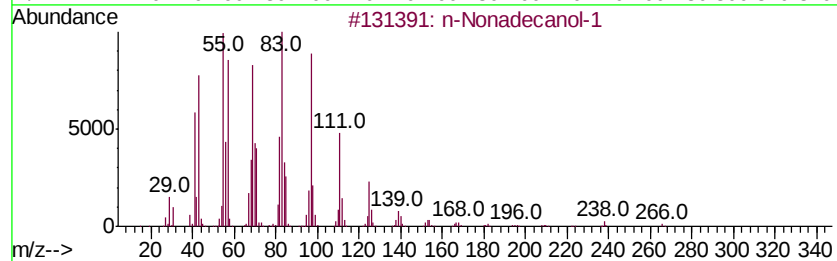
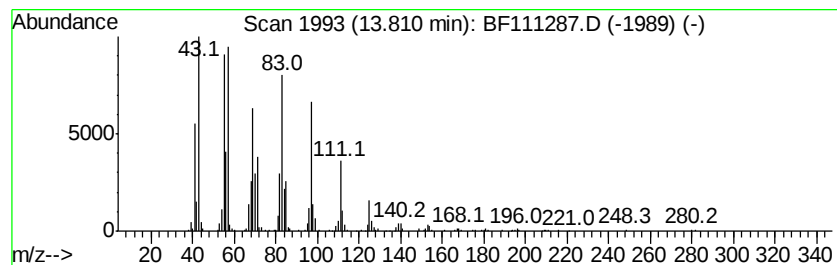
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	8.54 ng	837357	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2		1-Hexadecanol	242	C16H34O	036653-82-4	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		n-Heptadecanol-1	256	C17H36O	001454-85-9	91
5		1-Octadecanol	270	C18H38O	000112-92-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
 Data File : BF111287.D
 Acq On : 11 Dec 2018 20:09
 Operator : JU/SJ
 Sample : J6157-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-3-TOTAL

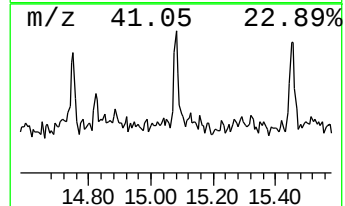
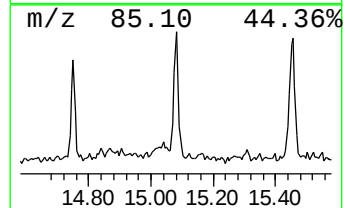
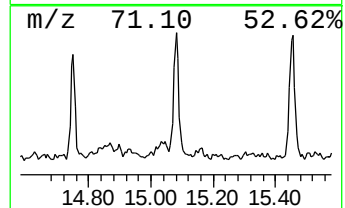
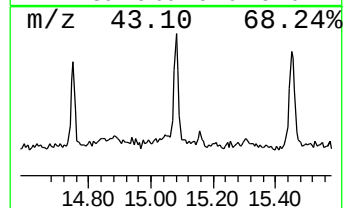
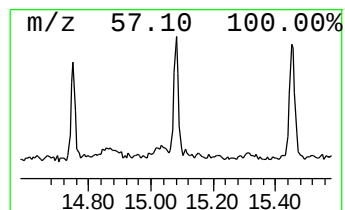
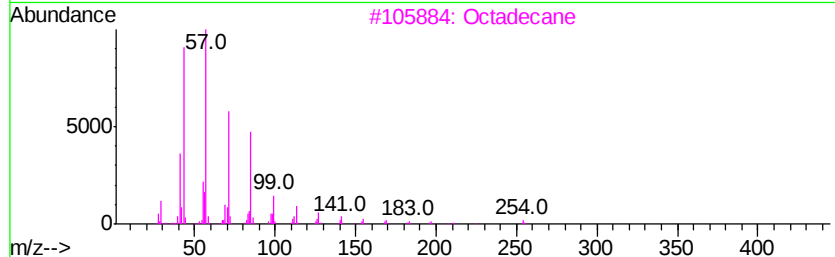
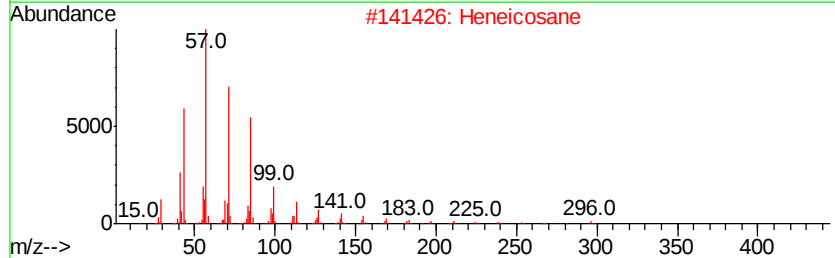
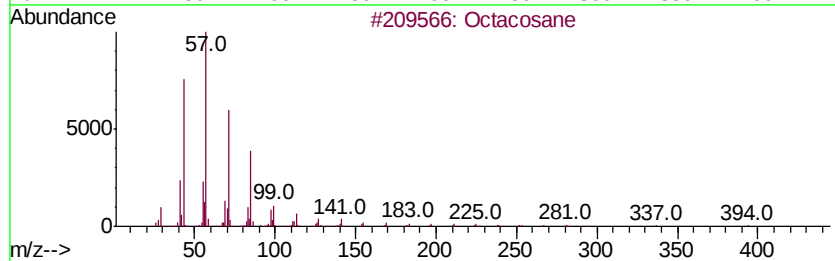
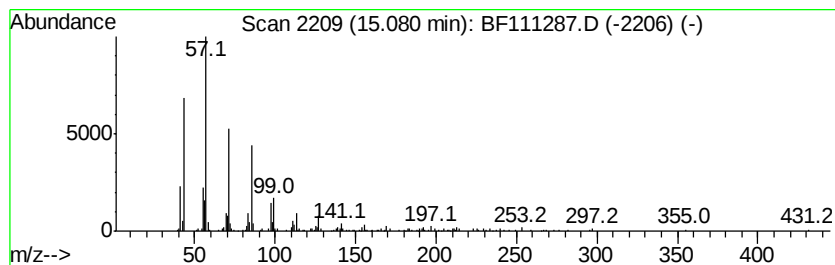
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	2.48 ng	192700	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Octadecane	254	C18H38	000593-45-3	87
4		Hexacosane	366	C26H54	000630-01-3	86
5		Triacontane	422	C30H62	000638-68-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111287.D
Acq On : 11 Dec 2018 20:09
Operator : JU/SJ
Sample : J6157-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-3-TOTAL

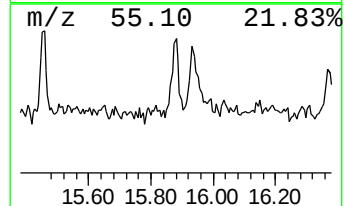
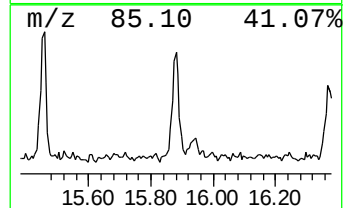
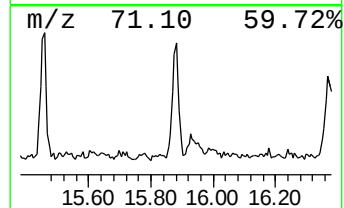
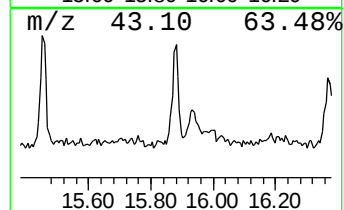
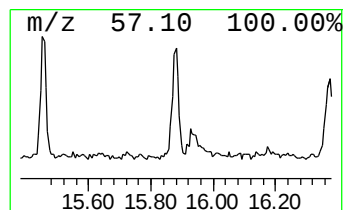
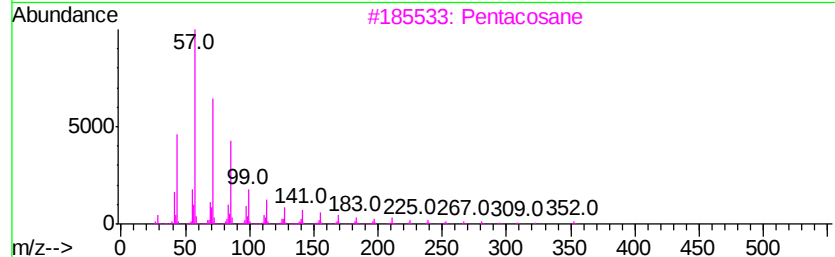
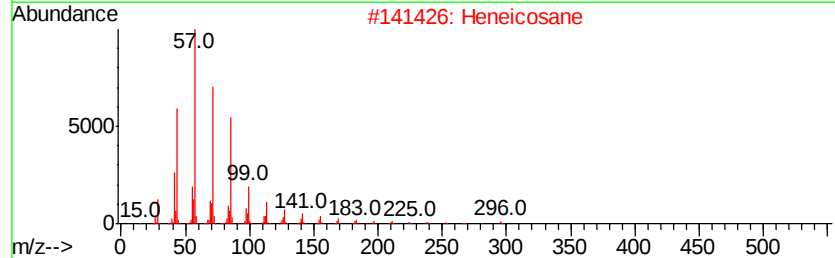
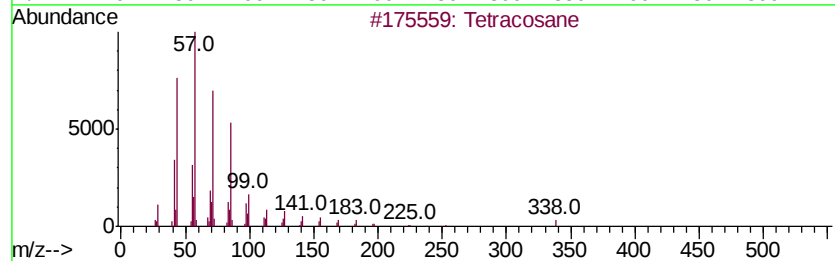
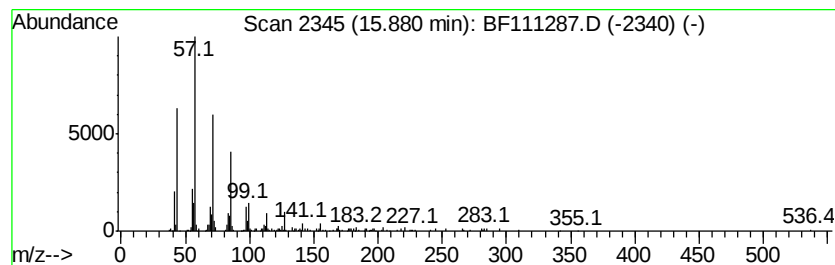
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	3.37 ng	261568	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111287.D
Acq On : 11 Dec 2018 20:09
Operator : JU/SJ
Sample : J6157-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

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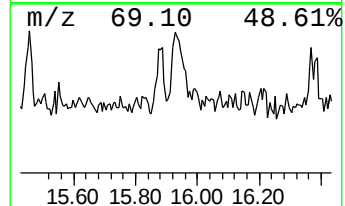
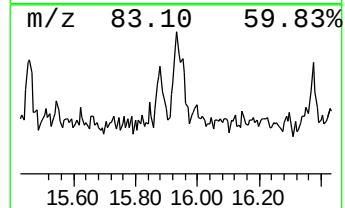
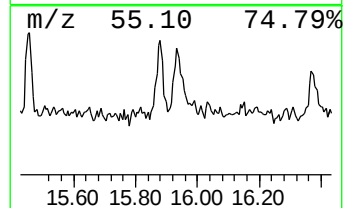
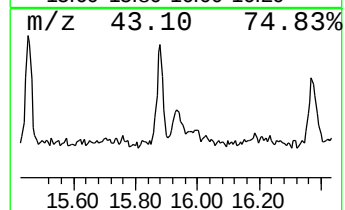
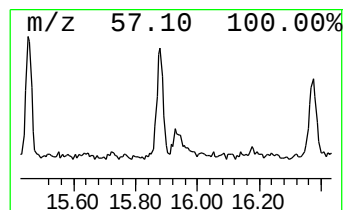
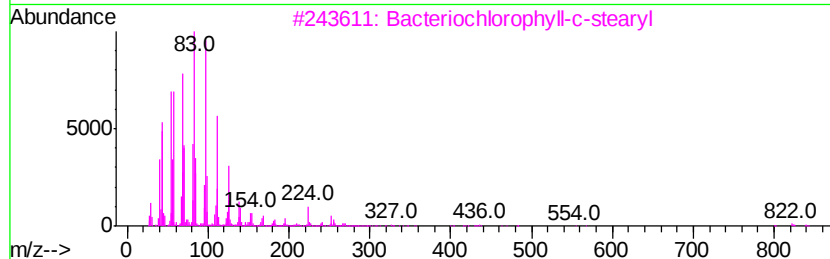
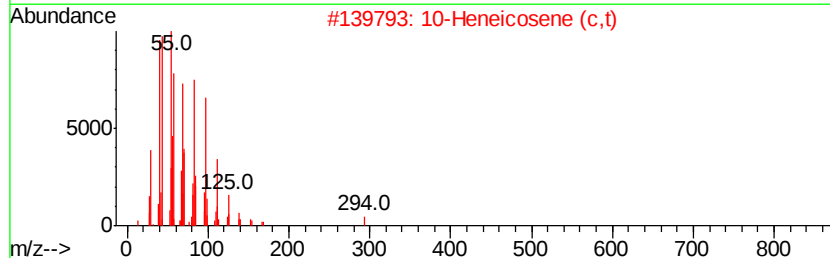
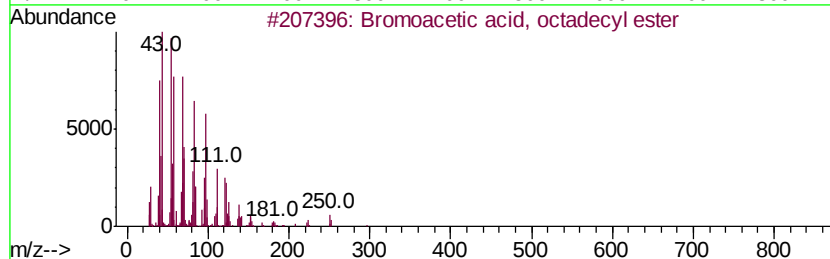
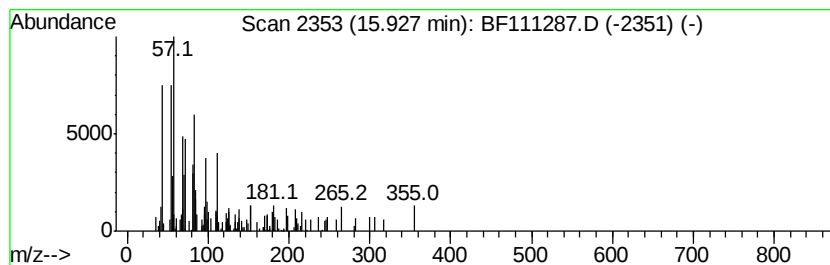
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Bromoacetic acid, octadecyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.08 ng	161433	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	74
2		10-Heneicosene (c,t)	294	C21H42	095008-11-0	64
3		Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	62
4		Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	62
5		Disparlure	282	C19H38O	029804-22-6	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111287.D
Acq On : 11 Dec 2018 20:09
Operator : JU/SJ
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMPOSITE-3-TOTAL

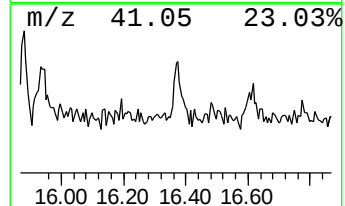
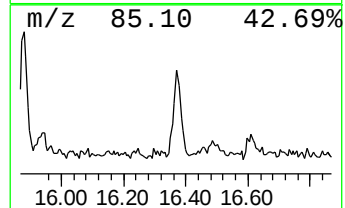
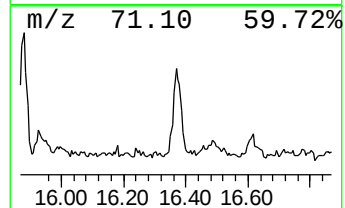
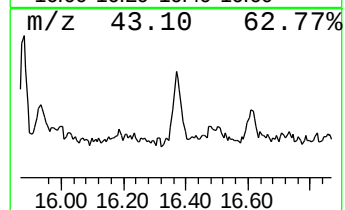
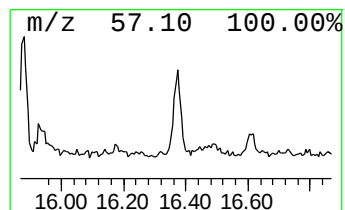
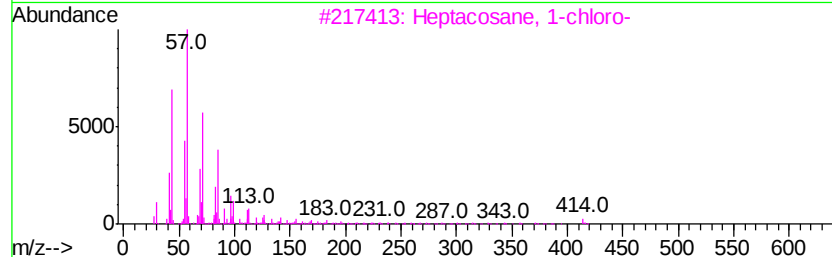
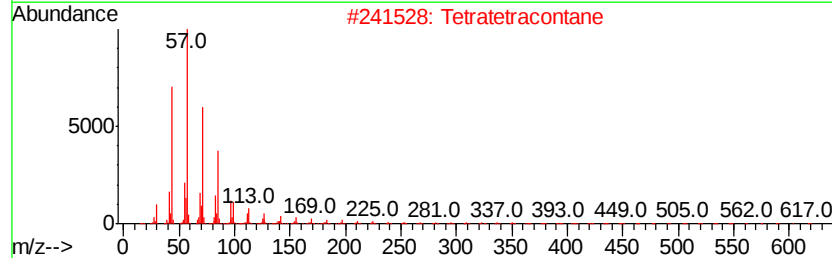
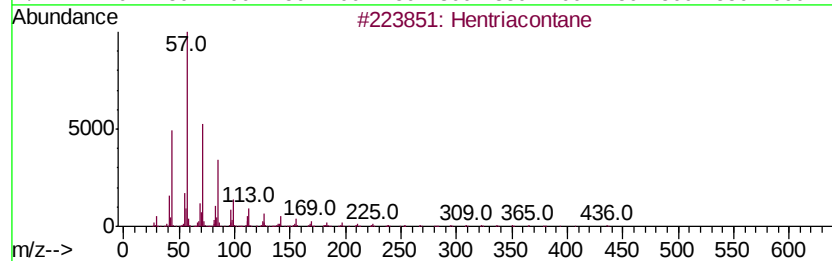
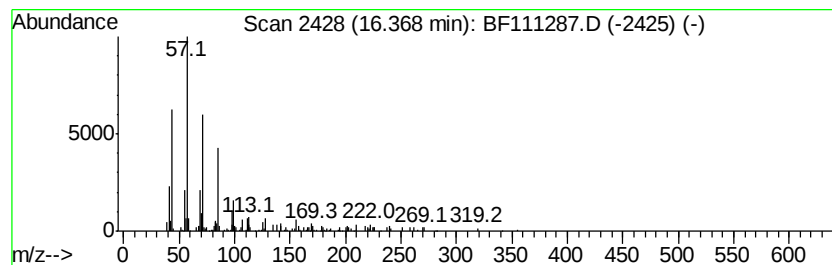
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	2.73 ng	212075	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	87
2		Tetratetracontane	619	C44H90	007098-22-8	86
3		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86
4		Pentacosane	352	C25H52	000629-99-2	86
5		Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111287.D
Acq On : 11 Dec 2018 20:09
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ClientSampleId :
COMPOSITE-3-TOTAL

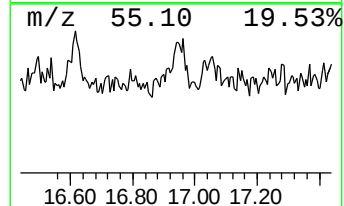
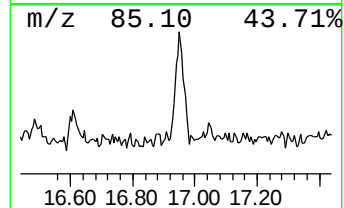
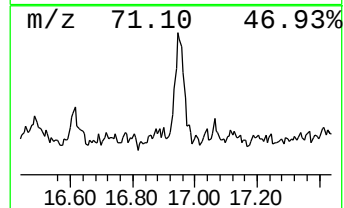
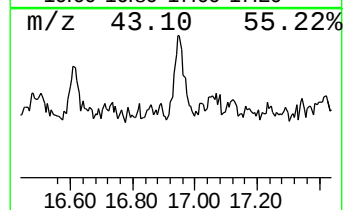
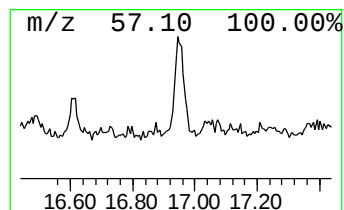
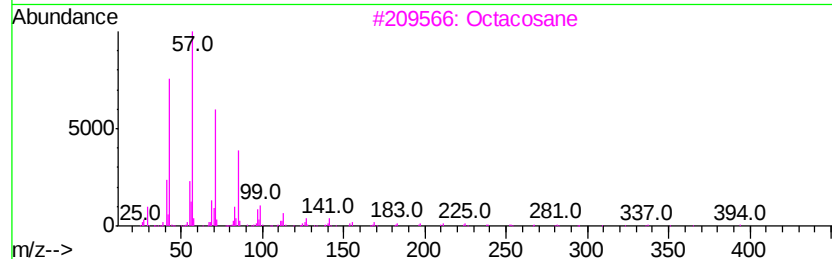
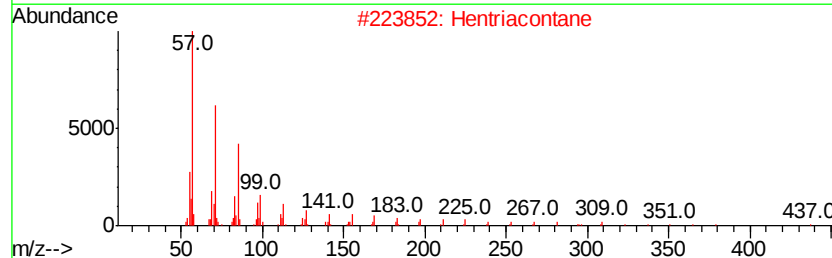
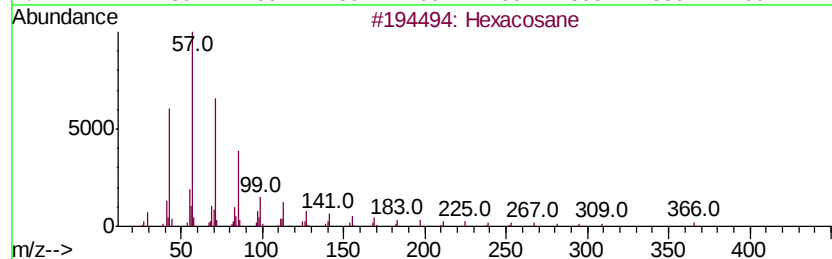
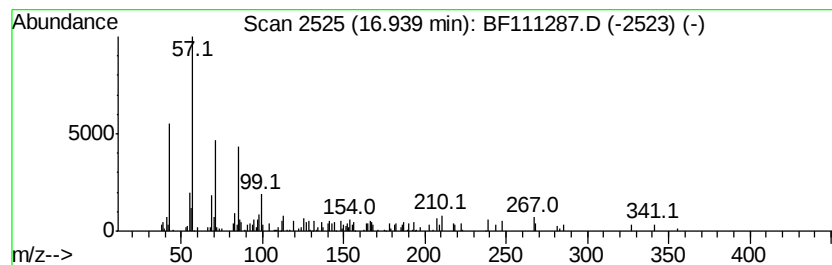
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.94	2.28 ng	176907	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	83
2		Hentriacontane	437	C31H64	000630-04-6	83
3		Octacosane	394	C28H58	000630-02-4	83
4		2-methyltetracosane	352	C25H52	1000376-72-6	83
5		Heneicosane	296	C21H44	000629-94-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
Data File : BF111287.D
Acq On : 11 Dec 2018 20:09
Operator : JU/SJ
Sample : J6157-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMPOSITE-3-TOTAL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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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2-Pentanone, 4-hy...	4.99	4.7	ng	317816	1	6.79	1360480	20.0
unknown6.56	6.56	44.4	ng	3018270	1	6.79	1360480	20.0
n-Hexadecanoic acid	11.86	23.9	ng	2712030	4	11.32	2271970	20.0
Octadecanoic acid	12.64	18.2	ng	1781370	5	13.95	1961590	20.0
n-Nonadecanol-1	13.81	8.5	ng	837357	5	13.95	1961590	20.0
Octacosane	15.08	2.5	ng	192700	6	15.40	1552310	20.0
Tetracosane	15.88	3.4	ng	261568	6	15.40	1552310	20.0
Bromoacetic acid,...	15.93	2.1	ng	161433	6	15.40	1552310	20.0
Hentriacontane	16.37	2.7	ng	212075	6	15.40	1552310	20.0
Hexacosane	16.94	2.3	ng	176907	6	15.40	1552310	20.0