

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120618\
 Data File : BF111136.D
 Acq On : 6 Dec 2018 14:13
 Operator : JU/SJ
 Sample : J6204-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HLSP-SB-1B-(2-6)

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-BF120518.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	5.022	490	499	506	rVB2	559191	841427	6.17%	0.653%
2	5.428	562	568	571	rBV	11895467	12259573	89.92%	9.511%
3	6.440	733	740	743	rBV2	12003419	13634233	100.00%	10.577%
4	6.575	758	763	767	rBV	12525283	12593754	92.37%	9.770%
5	6.804	799	802	806	rVB	3940781	3154439	23.14%	2.447%
6	6.963	825	829	832	rBV	10812927	9565755	70.16%	7.421%
7	7.363	892	897	900	rBV	8141047	8355196	61.28%	6.482%
8	8.086	1016	1020	1023	rBV	5049984	4093489	30.02%	3.176%
9	9.169	1198	1204	1207	rBV	13421362	13052158	95.73%	10.125%
10	9.557	1266	1270	1273	rBV	772199	686170	5.03%	0.532%
11	9.839	1312	1318	1322	rBV2	5003465	4502775	33.03%	3.493%
12	10.628	1447	1452	1455	rBV	8951606	8273484	60.68%	6.418%
13	11.322	1566	1570	1574	rBV	5172320	4406944	32.32%	3.419%
14	11.780	1644	1648	1651	rBV2	135473	148781	1.09%	0.115%
15	11.863	1657	1662	1677	rBV	4050194	3961917	29.06%	3.074%
16	12.563	1771	1781	1790	rBV3	190550	425323	3.12%	0.330%
17	12.645	1791	1795	1806	rVV2	1520103	1522203	11.16%	1.181%
18	12.916	1836	1841	1844	rBV	11720229	11958800	87.71%	9.277%
19	13.127	1874	1877	1880	rBV	156556	157566	1.16%	0.122%
20	13.392	1915	1922	1929	rBV4	85806	179740	1.32%	0.139%
21	13.816	1990	1994	2004	rBV	3409773	3663540	26.87%	2.842%
22	13.957	2014	2018	2022	rBV	4650569	4054474	29.74%	3.145%
23	14.139	2046	2049	2052	rBV	205987	199697	1.46%	0.155%
24	14.451	2098	2102	2114	rBV	496947	612572	4.49%	0.475%
25	14.745	2149	2152	2155	rBV	227531	217755	1.60%	0.169%
26	14.821	2161	2165	2169	rVB	956640	898466	6.59%	0.697%
27	15.080	2205	2209	2211	rBV	350208	415016	3.04%	0.322%
28	15.392	2257	2262	2267	rVV	2432048	2813803	20.64%	2.183%
29	15.451	2268	2272	2276	rVB	227521	262647	1.93%	0.204%
30	15.874	2340	2344	2348	rBV	263877	368863	2.71%	0.286%
31	15.921	2348	2352	2361	rVV	460489	801021	5.88%	0.621%
32	16.368	2424	2428	2434	rVB	107827	168416	1.24%	0.131%
33	17.033	2535	2541	2551	rBV4	156926	421022	3.09%	0.327%
34	17.404	2600	2604	2612	rVB10	103777	233009	1.71%	0.181%

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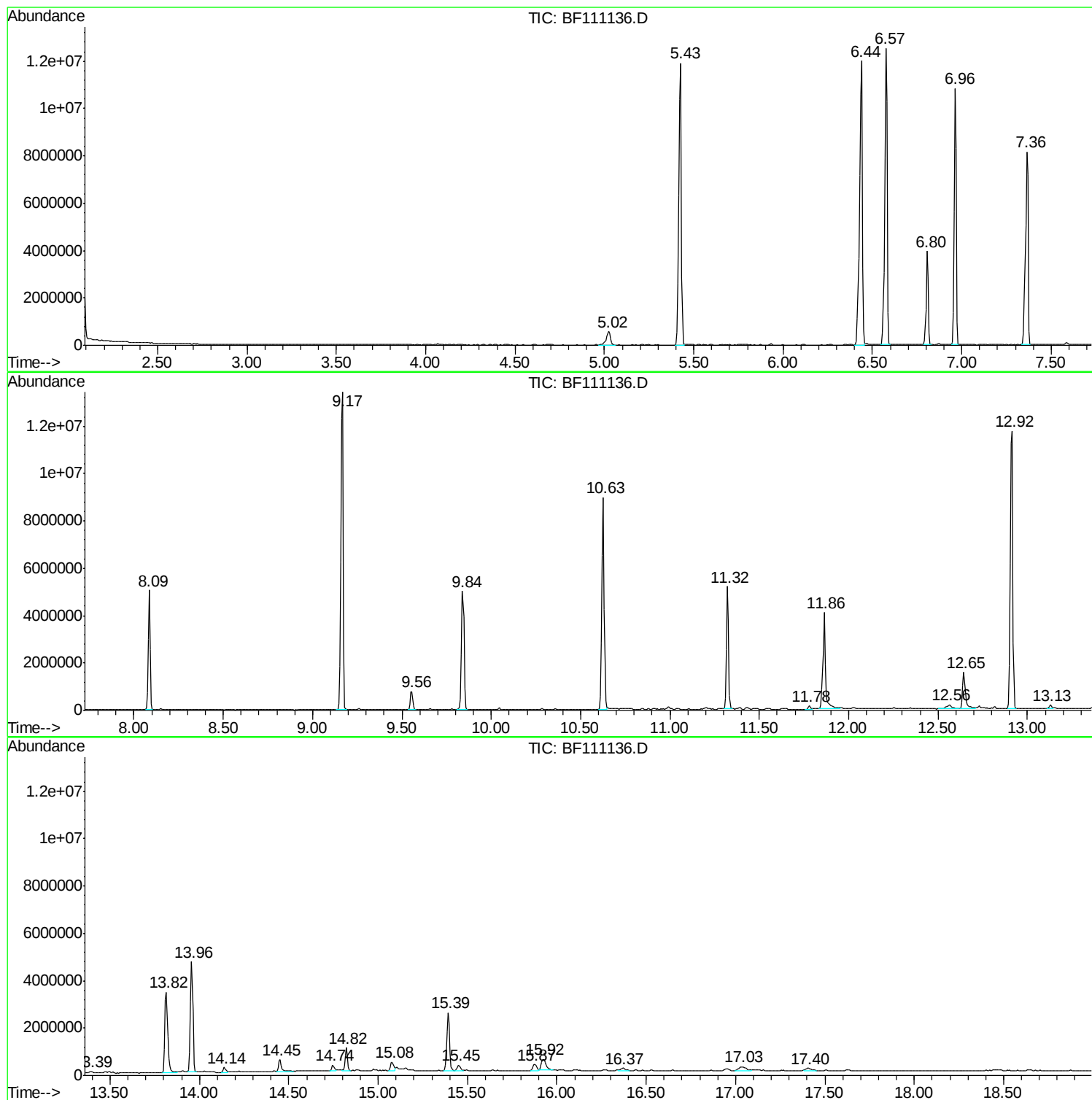
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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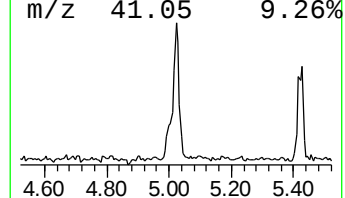
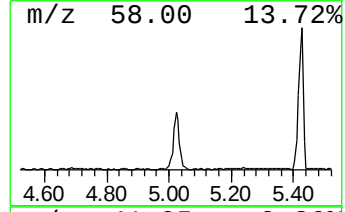
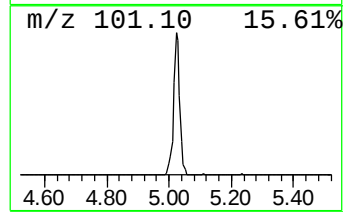
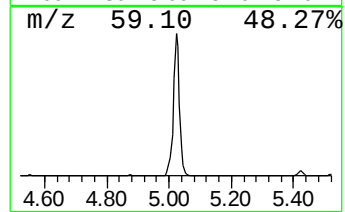
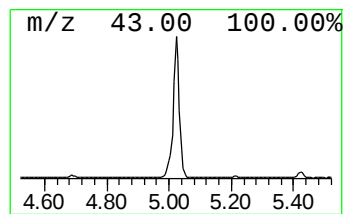
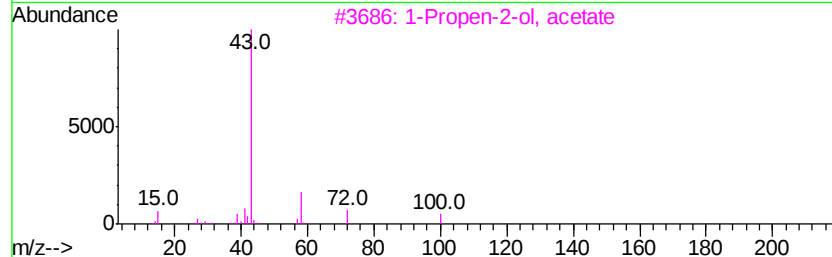
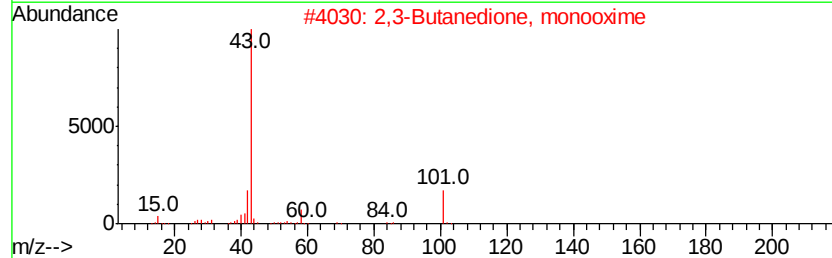
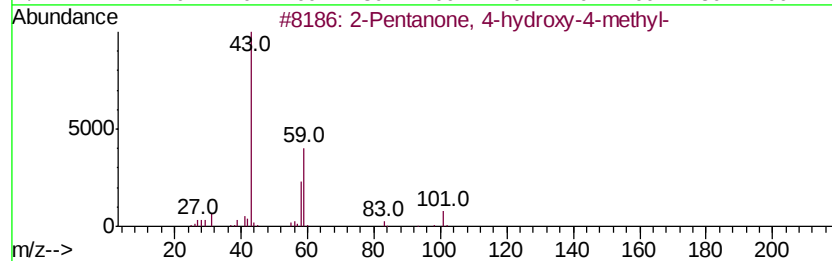
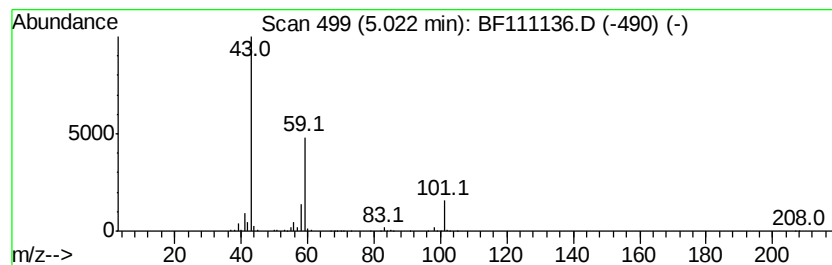
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	5.33 ng	841427	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Butane	58	C4H10	000106-97-8	9



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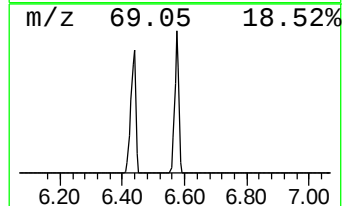
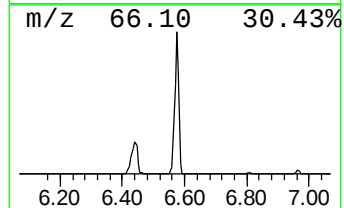
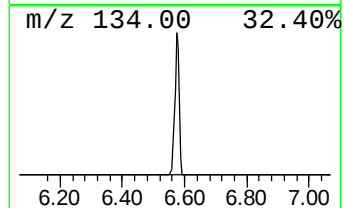
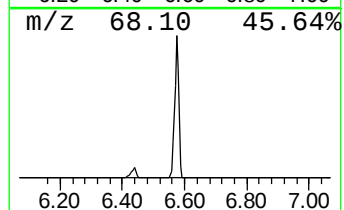
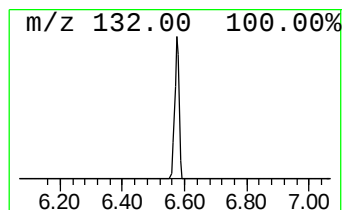
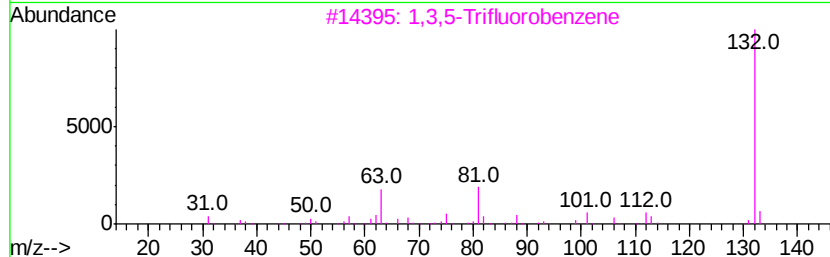
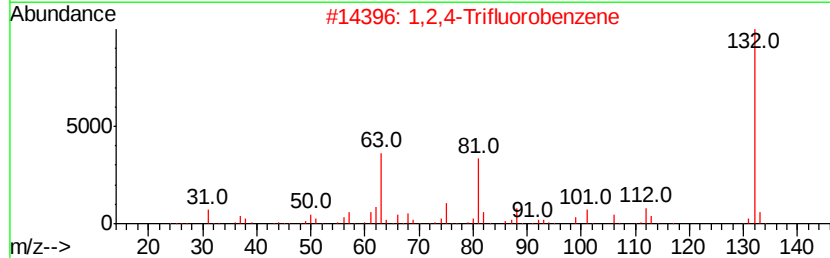
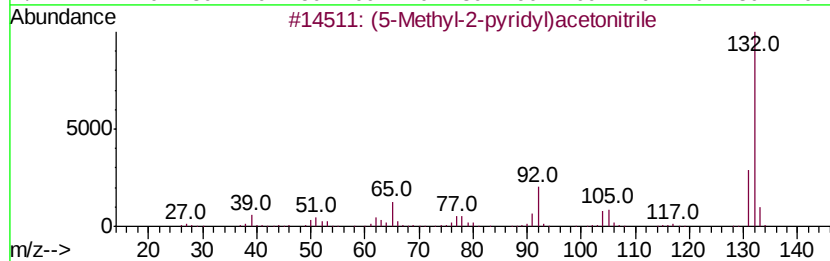
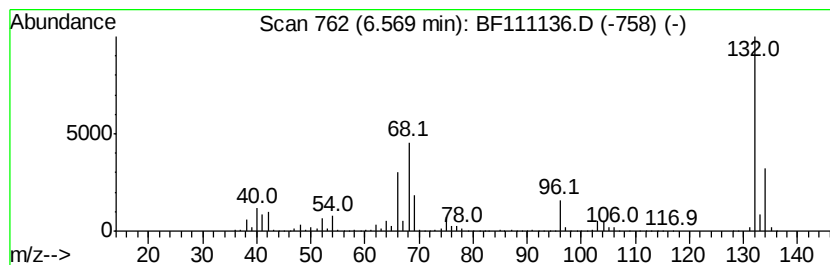
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	79.85 ng	12593800	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
2		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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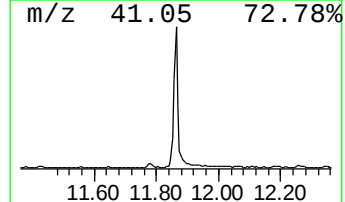
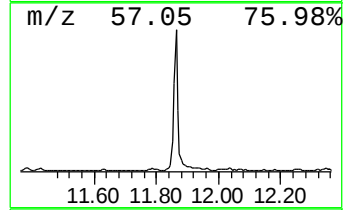
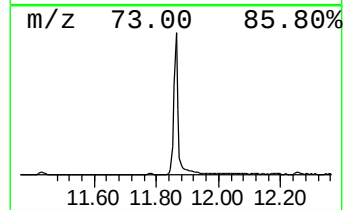
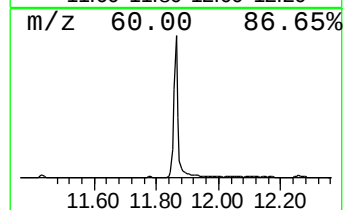
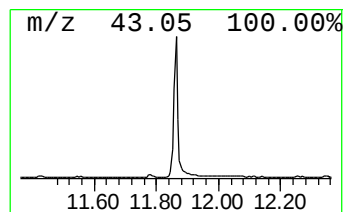
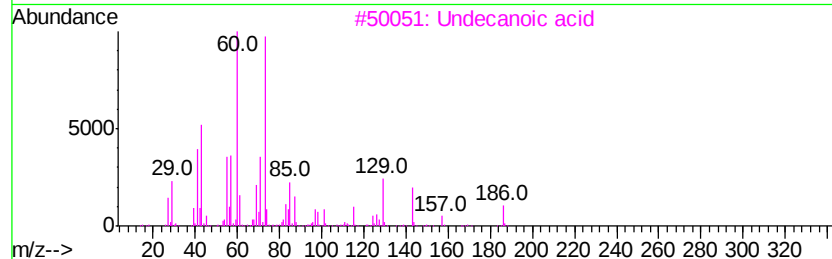
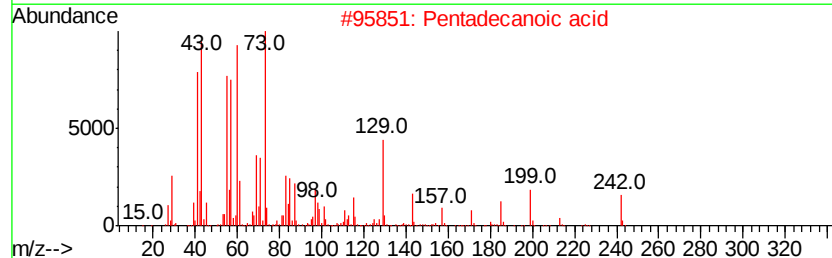
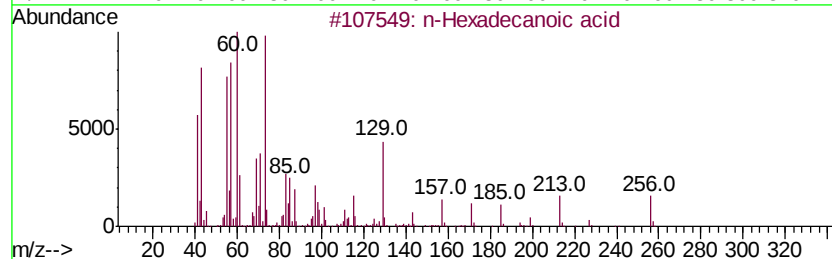
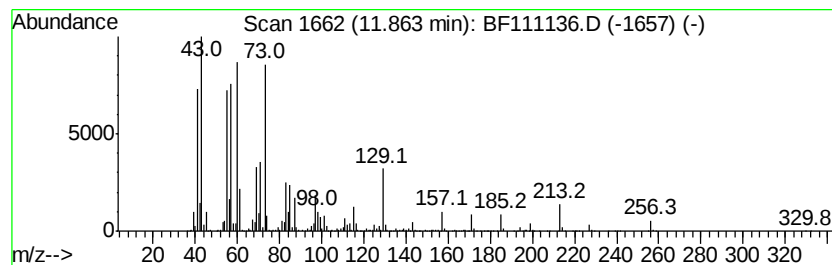
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	17.98 ng	3961920	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Undecanoic acid	186	C11H22O2	000112-37-8	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5		Tridecanoic acid	214	C13H26O2	000638-53-9	80



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Misc :
ALS Vial : 8 Sample Multiplier: 1

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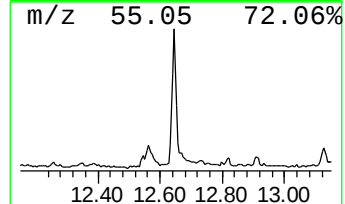
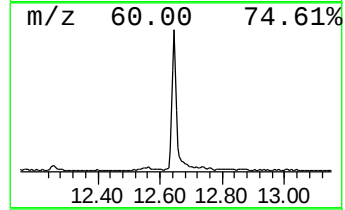
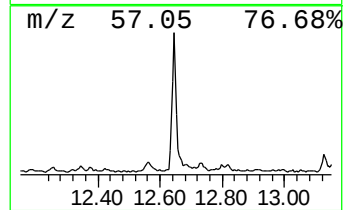
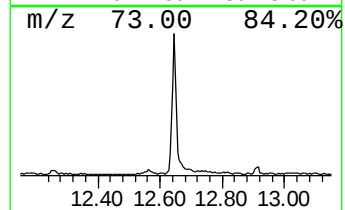
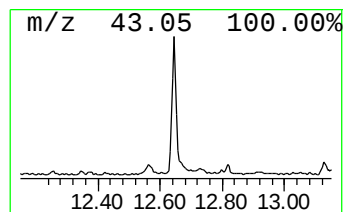
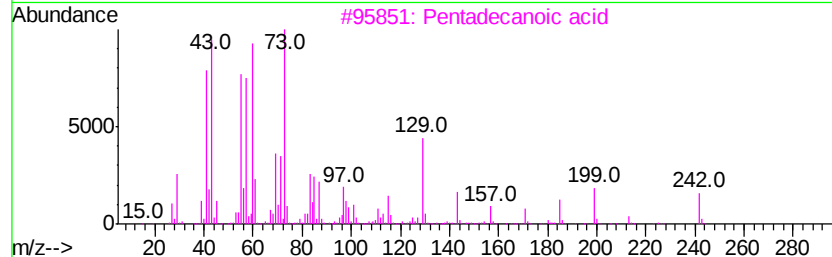
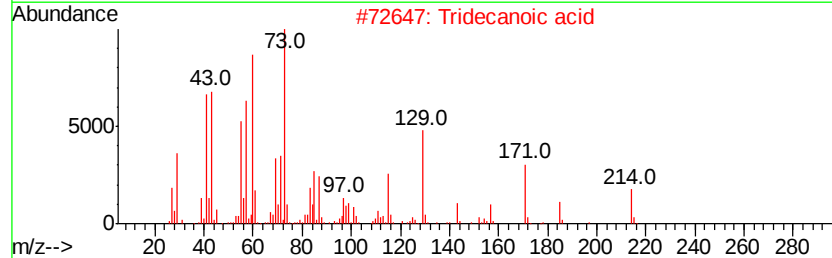
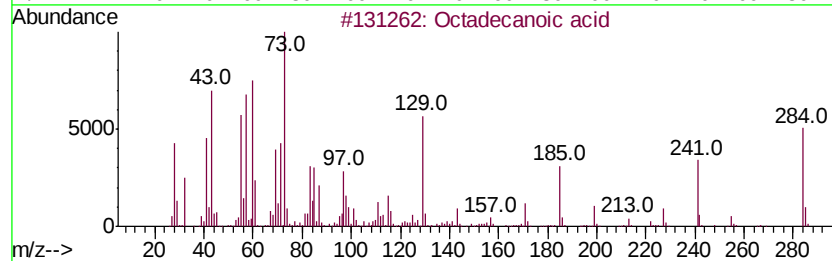
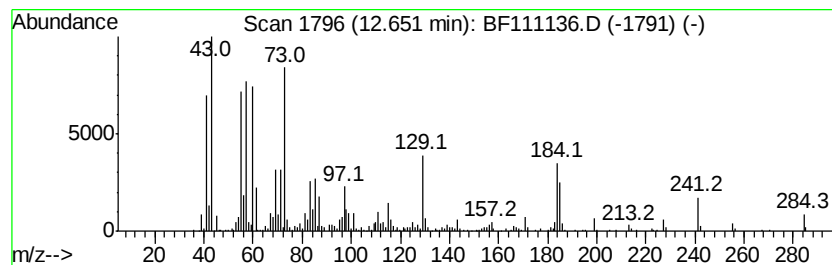
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	7.51 ng	1522200	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



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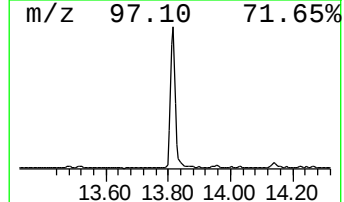
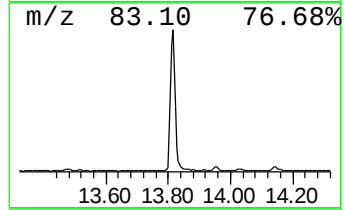
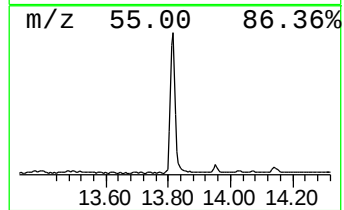
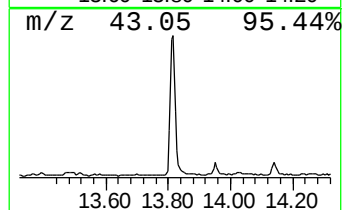
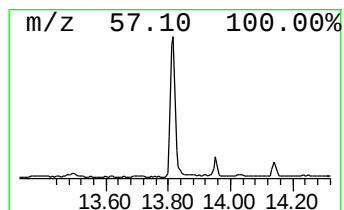
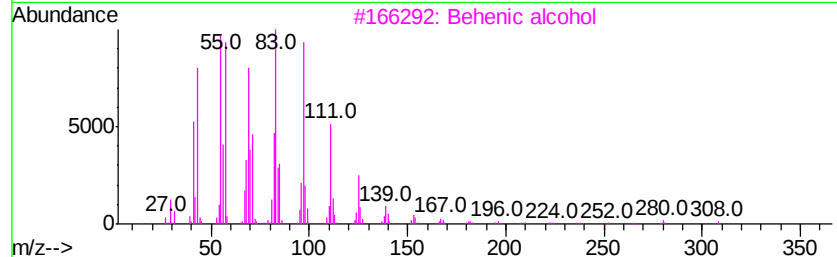
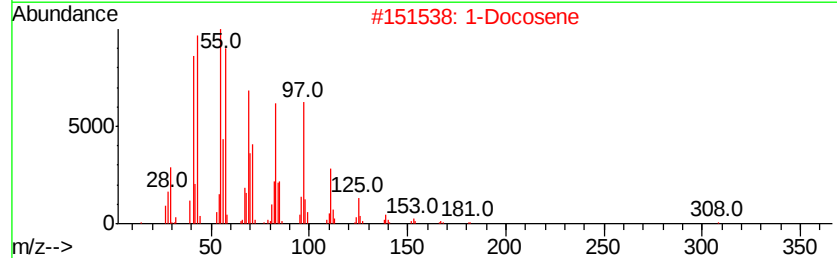
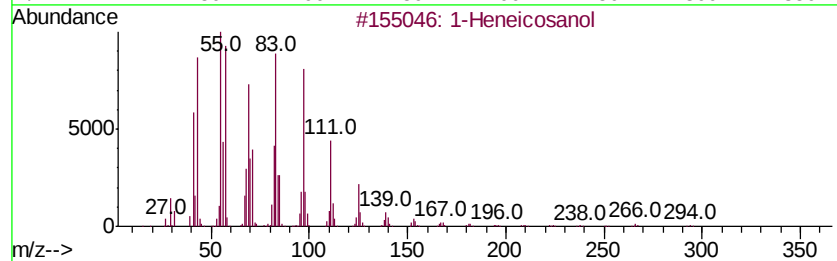
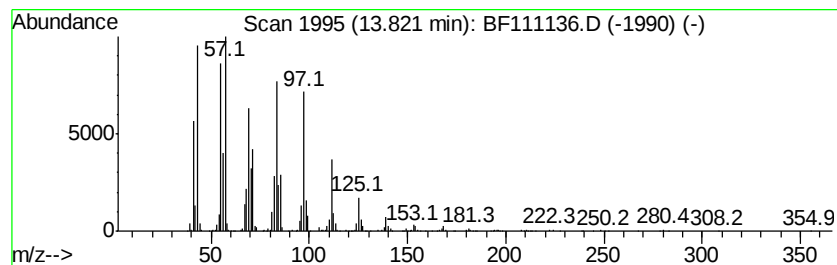
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	18.07 ng	3663540	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		1-Docosene	308	C22H44	001599-67-3	94
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111136.D
Acq On : 6 Dec 2018 14:13
Operator : JU/SJ
Sample : J6204-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HLSP-SB-1B-(2-6)

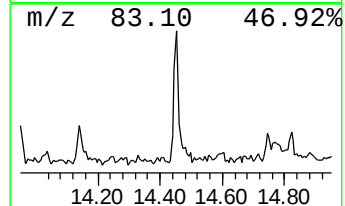
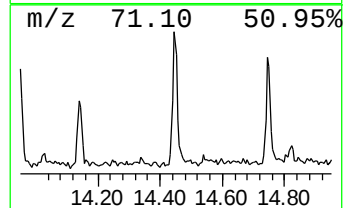
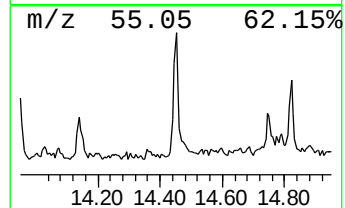
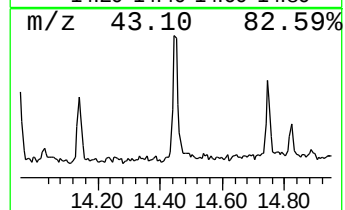
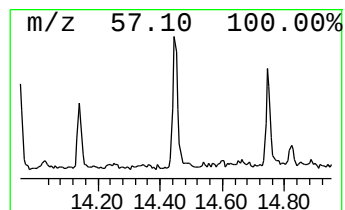
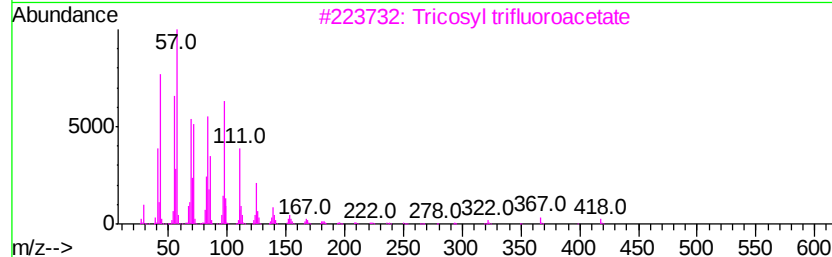
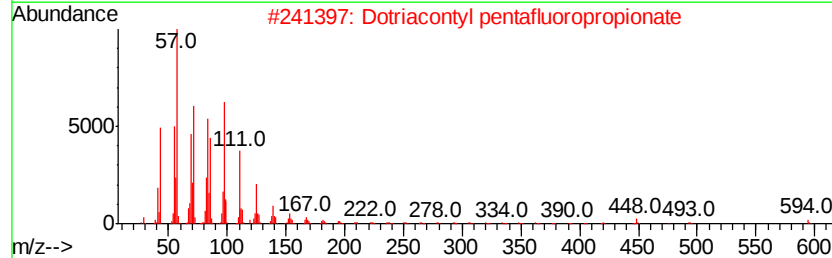
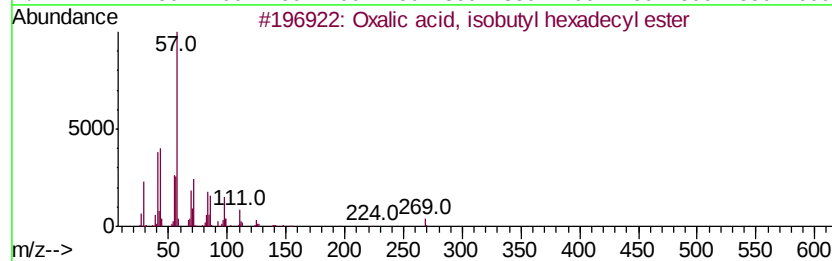
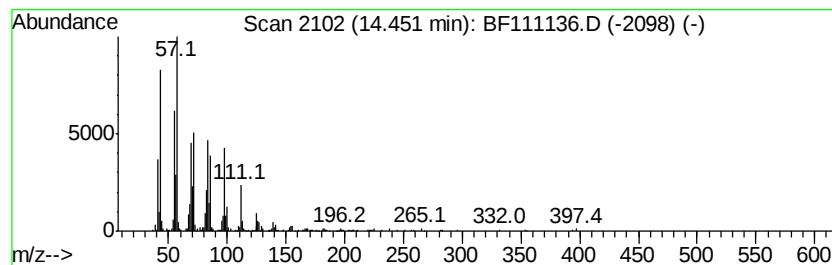
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxalic acid, isobutyl hexad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	3.02 ng	612572	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	91
3		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
4		Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	87
5		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
 Data File : BF111136.D
 Acq On : 6 Dec 2018 14:13
 Operator : JU/SJ
 Sample : J6204-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

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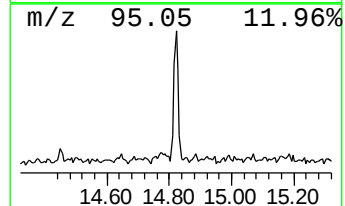
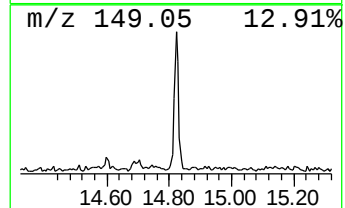
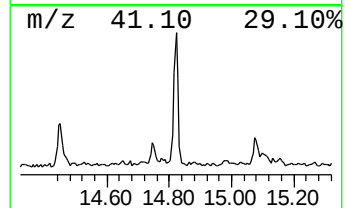
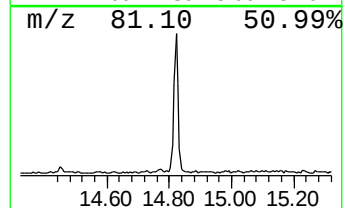
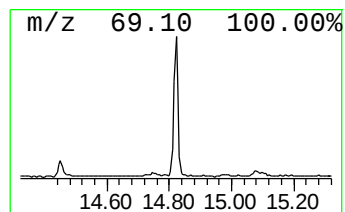
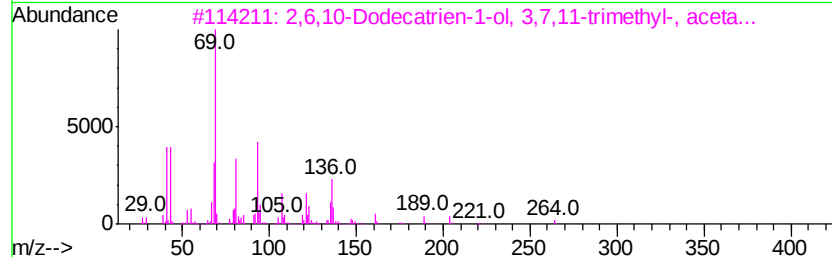
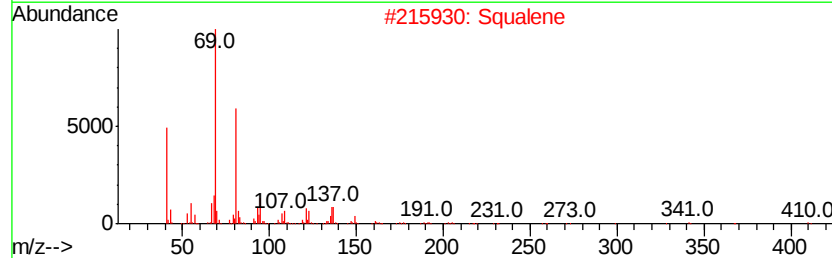
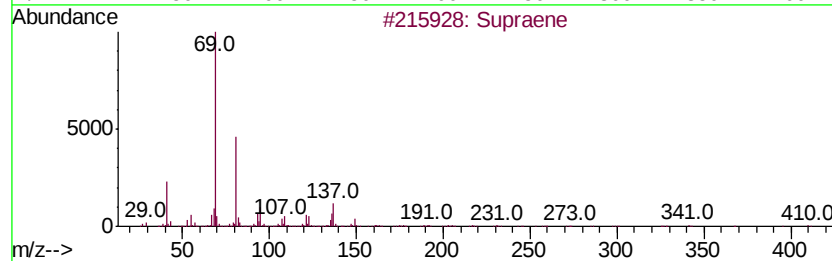
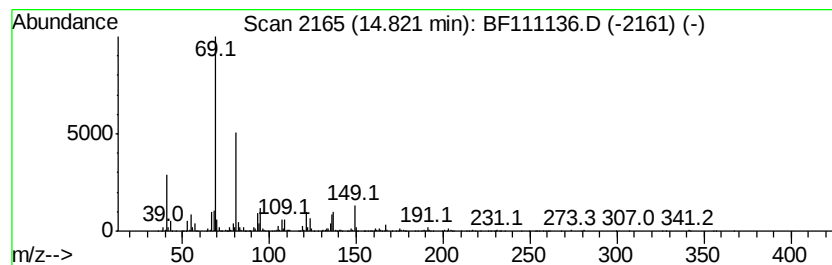
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	6.39 ng	898466	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	90
2		Squalene	410	C30H50	000111-02-4	90
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
4		1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	47
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111136.D
Acq On : 6 Dec 2018 14:13
Operator : JU/SJ
Sample : J6204-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

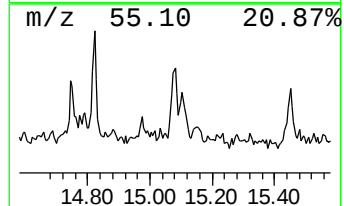
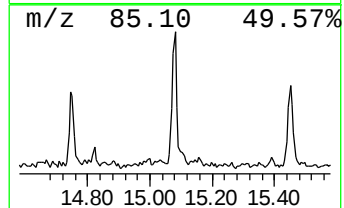
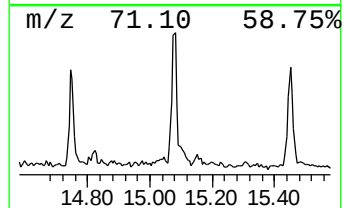
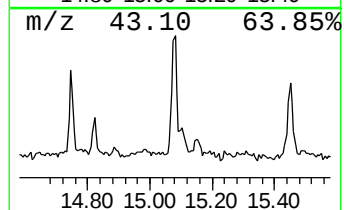
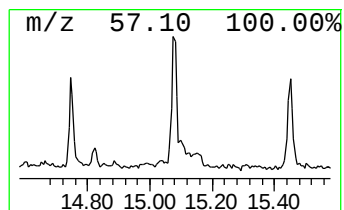
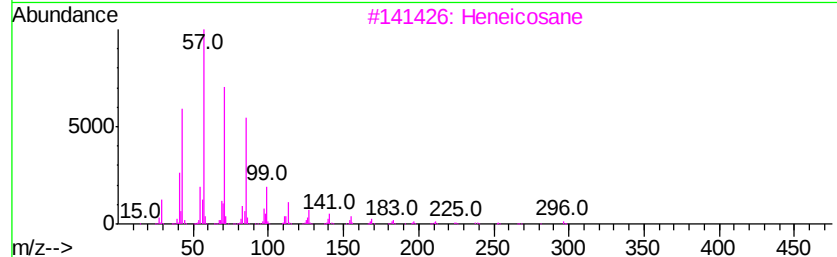
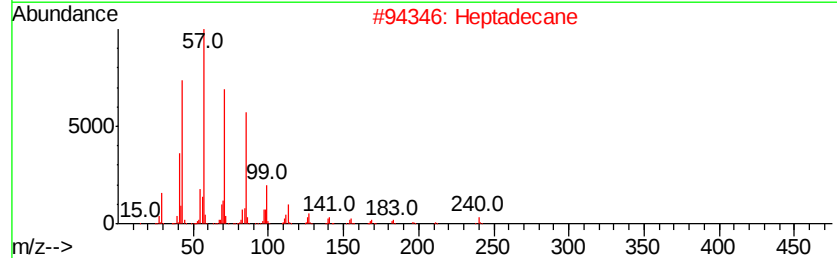
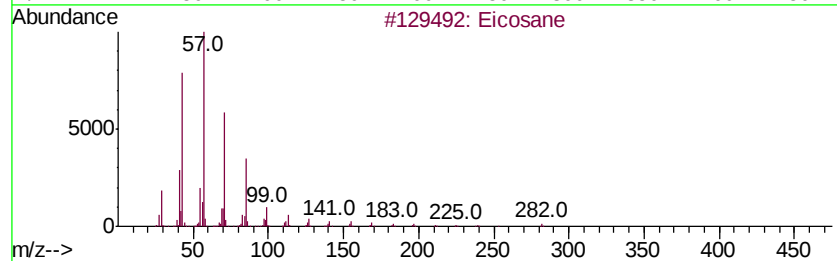
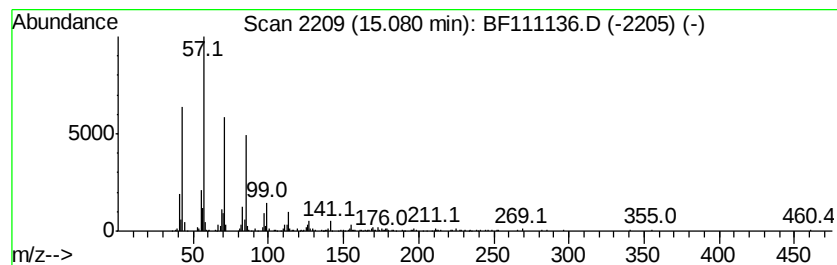
Instrument :
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ClientSampleId :
HLSP-SB-1B-(2-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	2.95 ng	415016	Perylene-d12	15.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	94
2	Heptadecane	240 C17H36	000629-78-7	91
3	Heneicosane	296 C21H44	000629-94-7	91
4	Tetracosane	338 C24H50	000646-31-1	91
5	Octadecane	254 C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111136.D
Acq On : 6 Dec 2018 14:13
Operator : JU/SJ
Sample : J6204-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HLSP-SB-1B-(2-6)

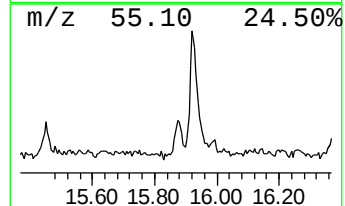
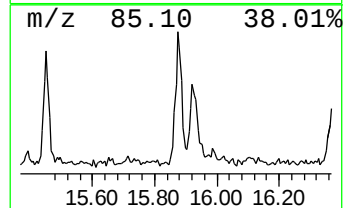
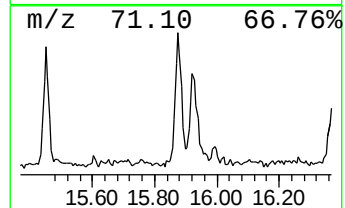
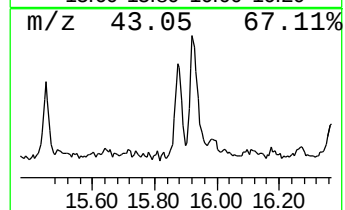
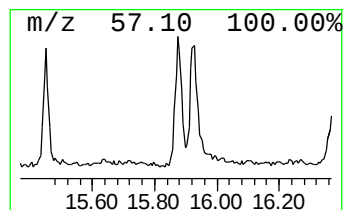
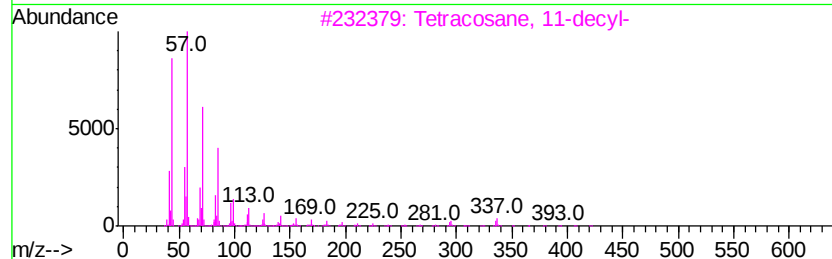
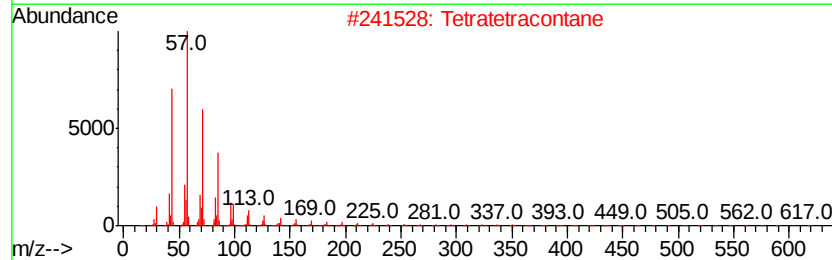
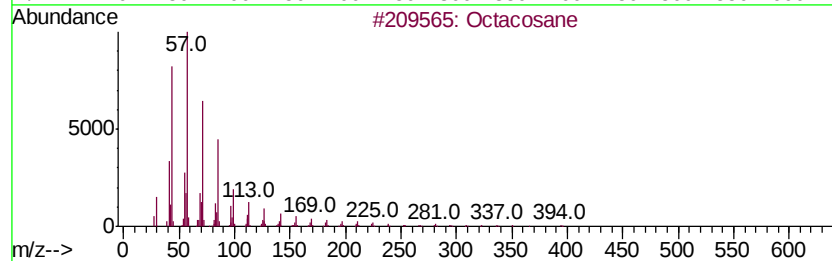
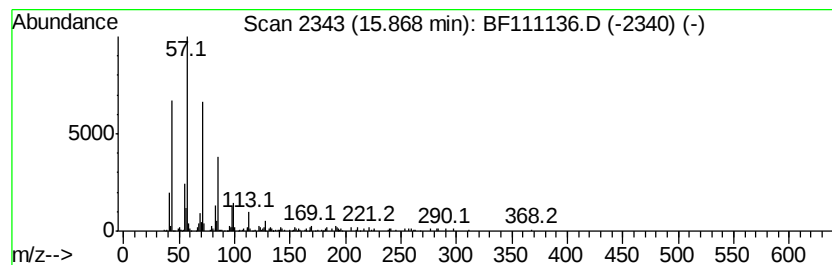
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.62 ng	368863	Perylene-d12	15.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111136.D
Acq On : 6 Dec 2018 14:13
Operator : JU/SJ
Sample : J6204-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

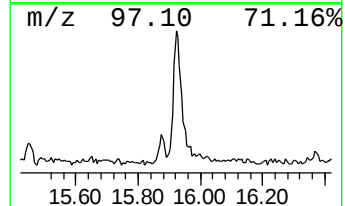
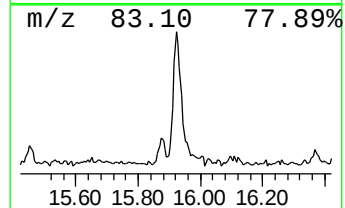
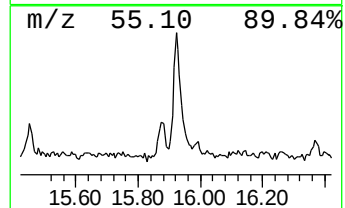
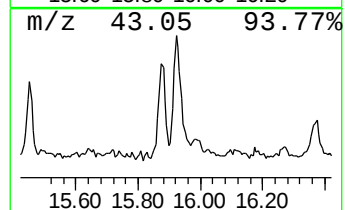
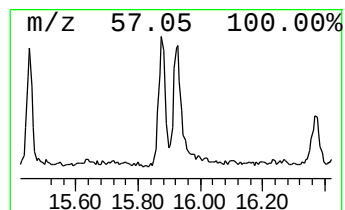
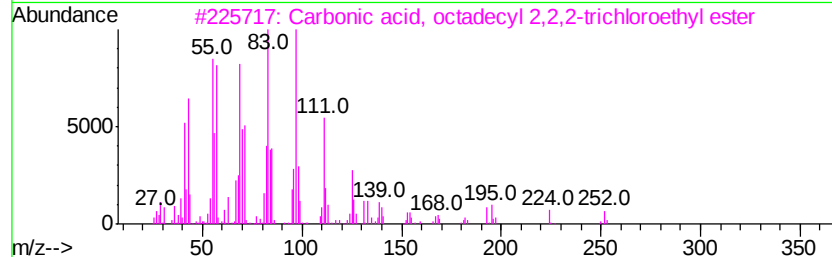
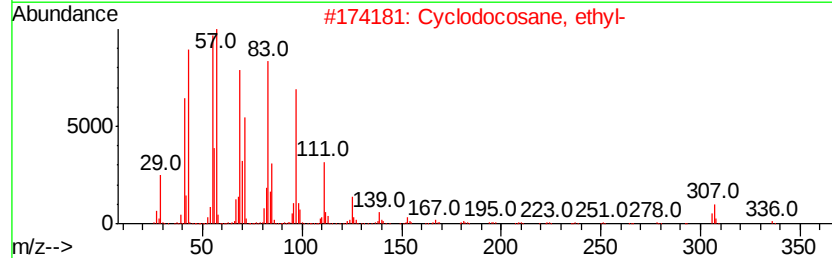
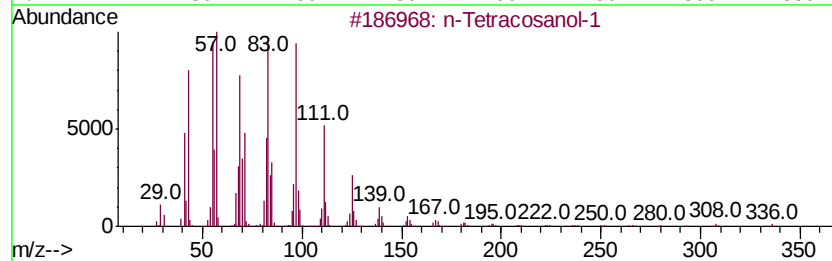
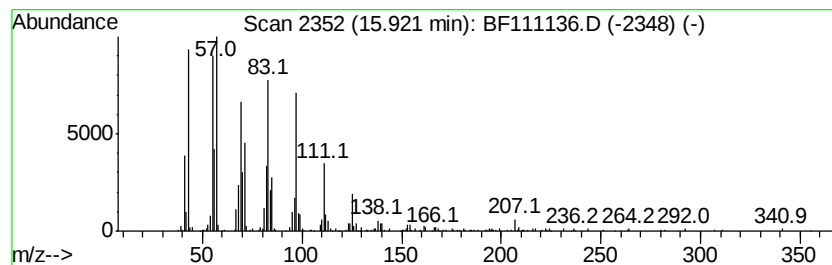
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ClientSampleId :
HLSP-SB-1B-(2-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.92	5.69 ng	801021	Perylene-d12	15.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91
3	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111136.D
Acq On : 6 Dec 2018 14:13
Operator : JU/SJ
Sample : J6204-04
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ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
HLSP-SB-1B-(2-6)

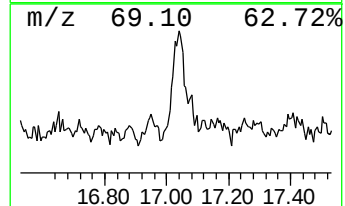
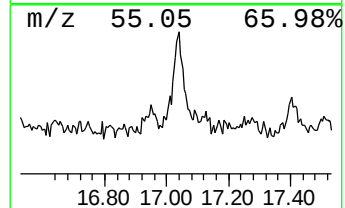
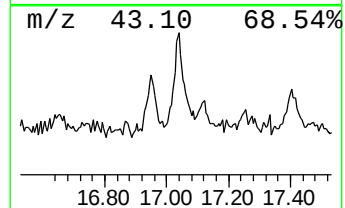
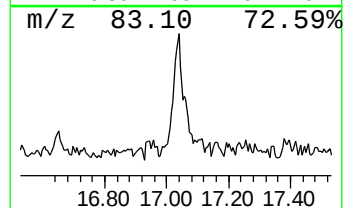
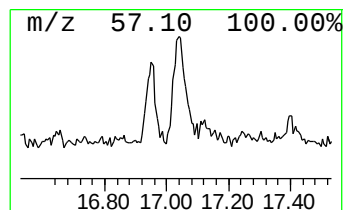
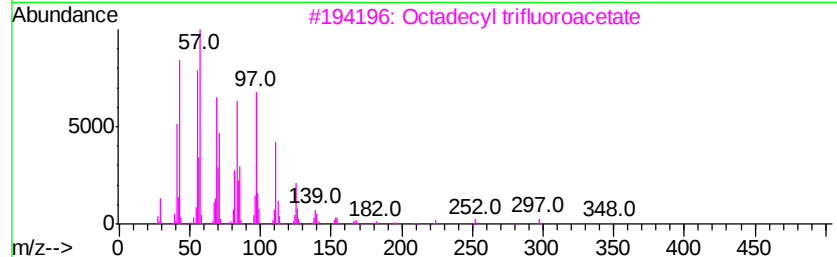
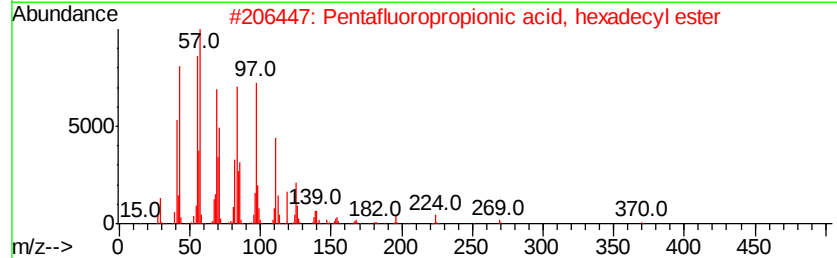
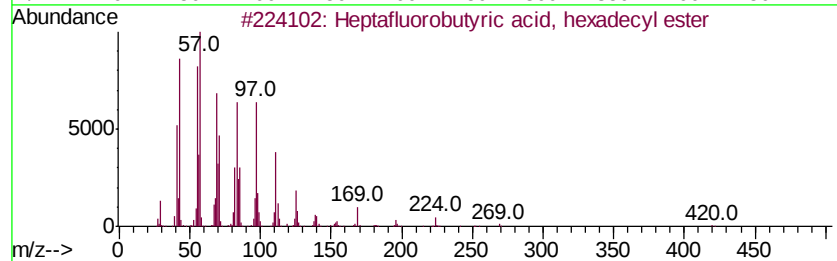
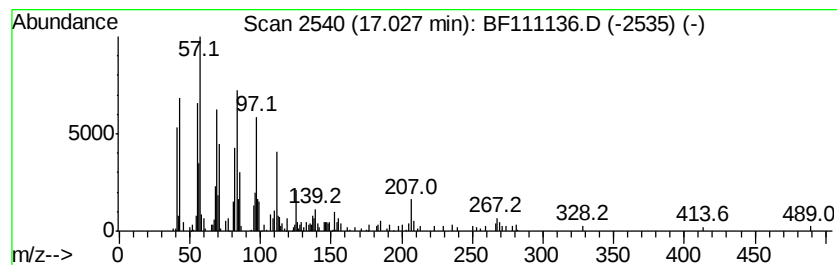
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptafluorobutyric acid, he... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.03	2.99 ng	421022	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
2		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
5		Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120618\
 Data File : BF111136.D
 Acq On : 6 Dec 2018 14:13
 Operator : JU/SJ
 Sample : J6204-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HLSP-SB-1B-(2-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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...	5.02	5.3	ng	841427	1	6.80	3154440	20.0
unknown6.57	6.57	79.8	ng	12593800	1	6.80	3154440	20.0
n-Hexadecanoic acid	11.86	18.0	ng	3961920	4	11.32	4406940	20.0
Octadecanoic acid	12.65	7.5	ng	1522200	5	13.96	4054470	20.0
1-Heneicosanol	13.82	18.1	ng	3663540	5	13.96	4054470	20.0
Oxalic acid, isob...	14.45	3.0	ng	612572	5	13.96	4054470	20.0
Supraene	14.82	6.4	ng	898466	6	15.39	2813800	20.0
Eicosane	15.08	3.0	ng	415016	6	15.39	2813800	20.0
Octacosane	15.87	2.6	ng	368863	6	15.39	2813800	20.0
n-Tetracosanol-1	15.92	5.7	ng	801021	6	15.39	2813800	20.0
Heptafluorobutyri...	17.03	3.0	ng	421022	6	15.39	2813800	20.0