

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120618\
 Data File : BF111138.D
 Acq On : 6 Dec 2018 15:08
 Operator : JU/SJ
 Sample : J6204-13
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HLSP-SB-7B-(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	505	rVB	563581	799935	5.76%	0.682%
2	5.422	562	567	571	rBV	11072575	12446244	89.70%	10.606%
3	6.439	733	740	744	rBV2	11495806	13875908	100.00%	11.824%
4	6.575	758	763	766	rBV	12461282	12778717	92.09%	10.889%
5	6.804	799	802	806	rVB	3360254	2707543	19.51%	2.307%
6	6.963	825	829	832	rBV	10864236	9622651	69.35%	8.200%
7	7.363	892	897	900	rBV	8088755	8537143	61.52%	7.275%
8	8.086	1016	1020	1023	rBV	4343047	3521522	25.38%	3.001%
9	9.169	1198	1204	1207	rBV	13378449	13269275	95.63%	11.307%
10	9.551	1266	1269	1273	rBV	823578	729269	5.26%	0.621%
11	9.839	1314	1318	1322	rVB2	4533898	3861813	27.83%	3.291%
12	10.627	1447	1452	1455	rBV	9302258	8404187	60.57%	7.162%
13	11.321	1566	1570	1573	rBV	4699499	3839225	27.67%	3.272%
14	11.857	1655	1661	1673	rBV	1450175	1486050	10.71%	1.266%
15	12.639	1791	1794	1807	rBV	511804	621166	4.48%	0.529%
16	12.915	1835	1841	1844	rBV	11882762	12364396	89.11%	10.536%
17	13.392	1914	1922	1926	rBV3	70263	150075	1.08%	0.128%
18	13.815	1990	1994	2002	rBV	862833	1045720	7.54%	0.891%
19	13.957	2014	2018	2021	rBV	3670472	3258832	23.49%	2.777%
20	14.451	2099	2102	2113	rBV	380334	488575	3.52%	0.416%
21	15.080	2206	2209	2212	rBV	202748	234186	1.69%	0.200%
22	15.398	2257	2263	2268	rBV	2069831	2488257	17.93%	2.120%
23	15.456	2269	2273	2277	rVB	118790	157992	1.14%	0.135%
24	15.880	2341	2345	2349	rVB2	158683	224832	1.62%	0.192%
25	15.927	2349	2353	2362	rBV5	113746	209630	1.51%	0.179%
26	17.409	2600	2605	2616	rVB5	94067	227670	1.64%	0.194%

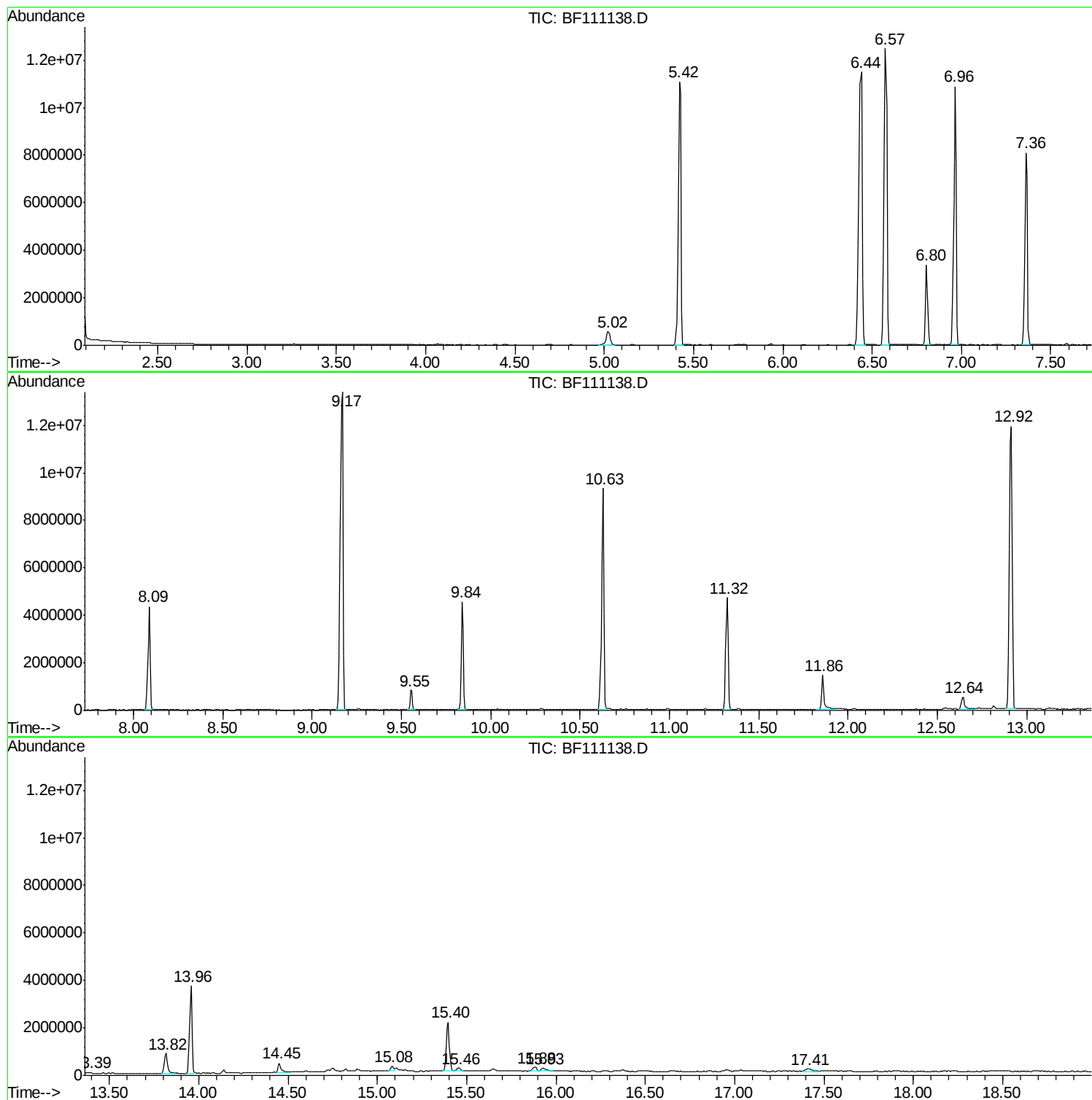
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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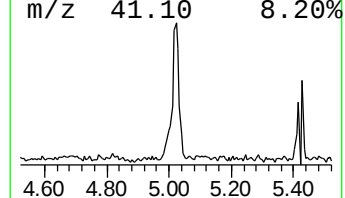
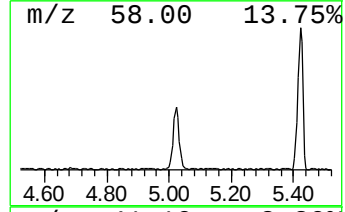
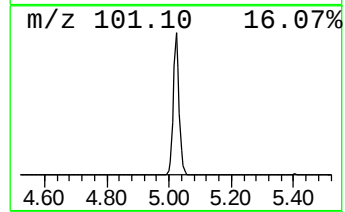
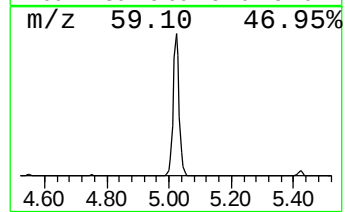
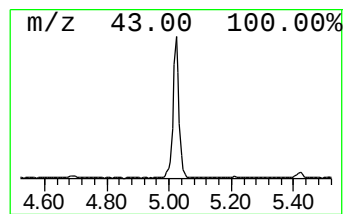
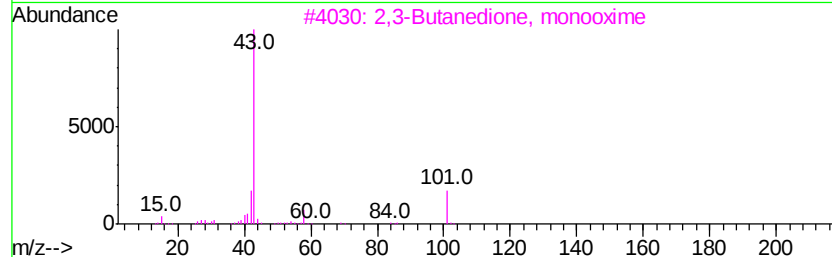
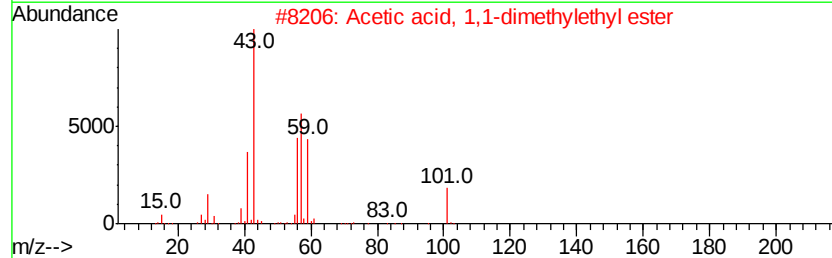
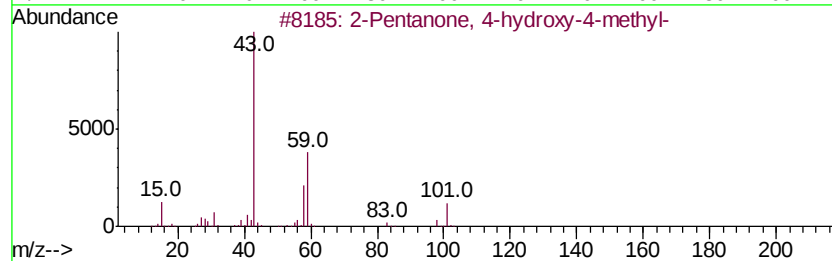
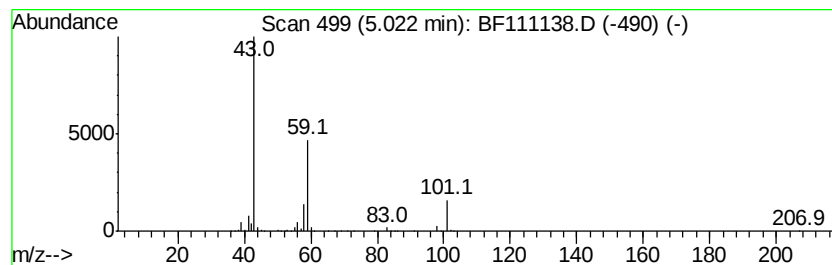
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	5.91 ng	799935	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	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7



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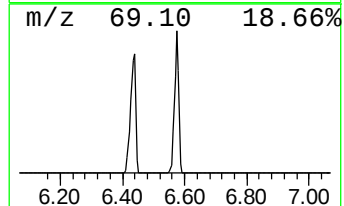
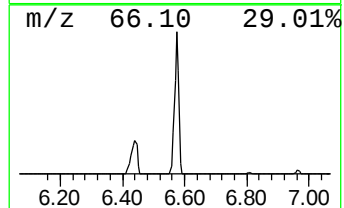
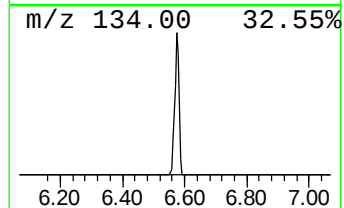
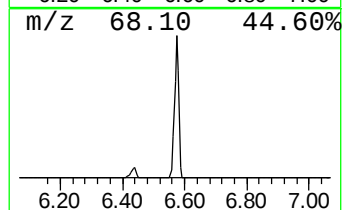
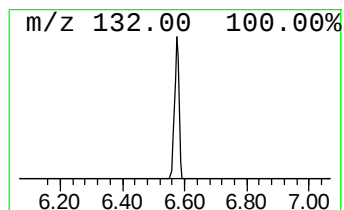
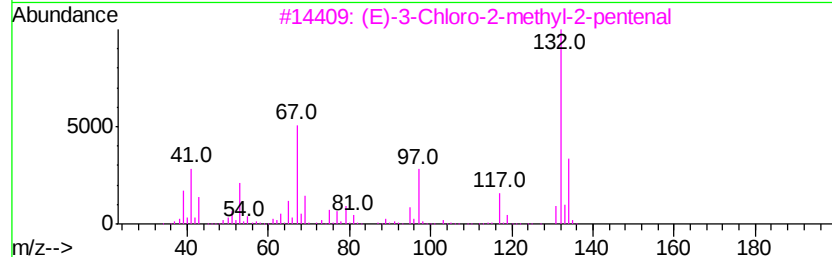
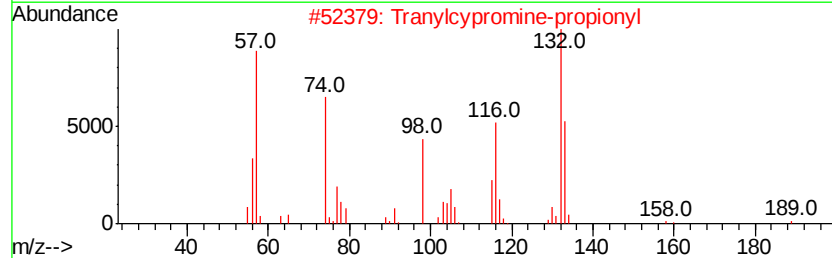
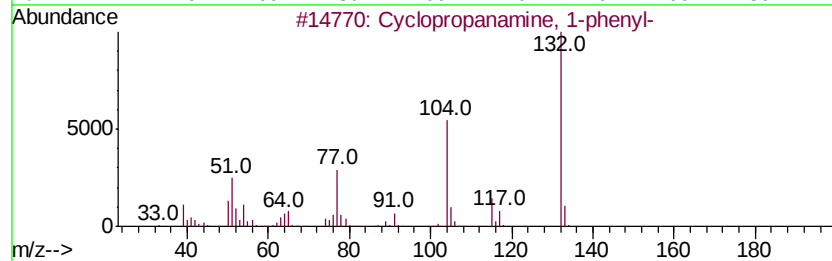
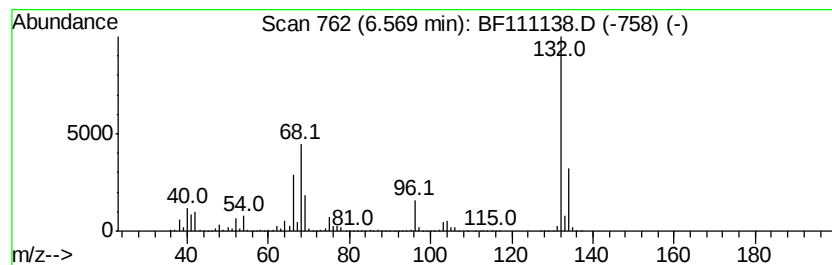
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	94.39 ng	12778700	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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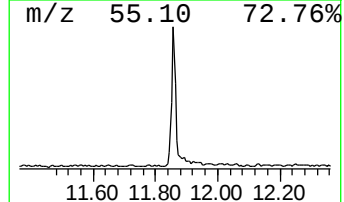
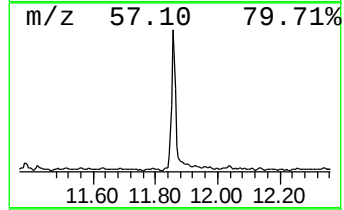
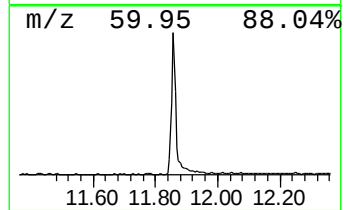
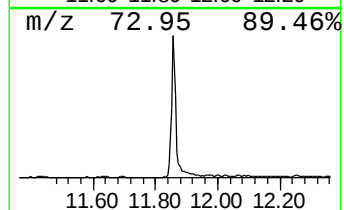
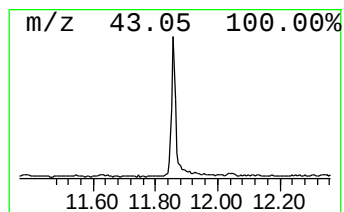
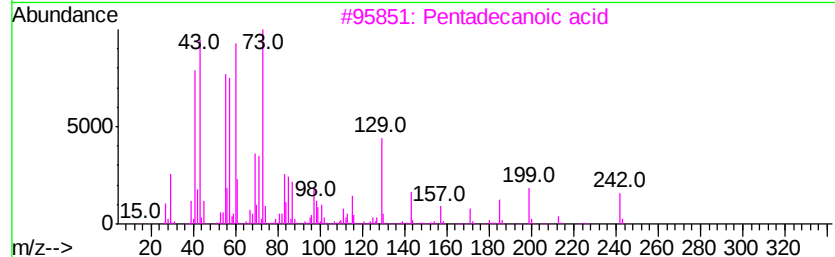
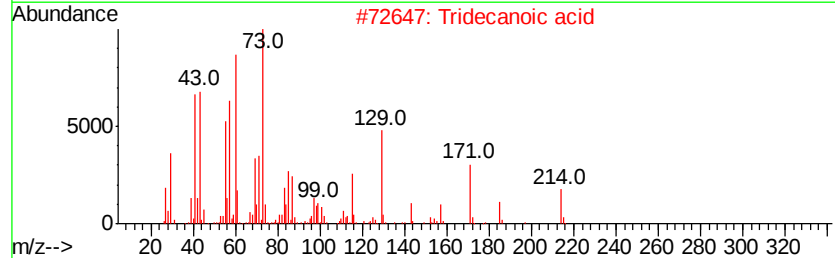
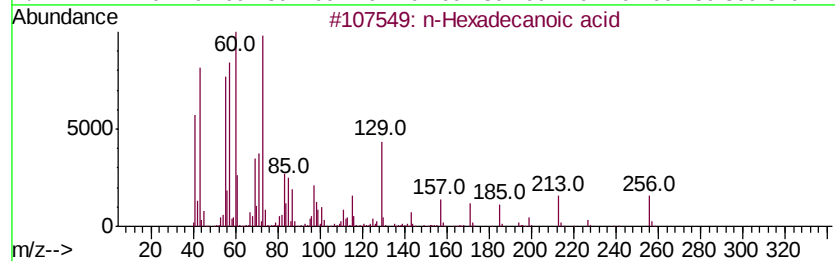
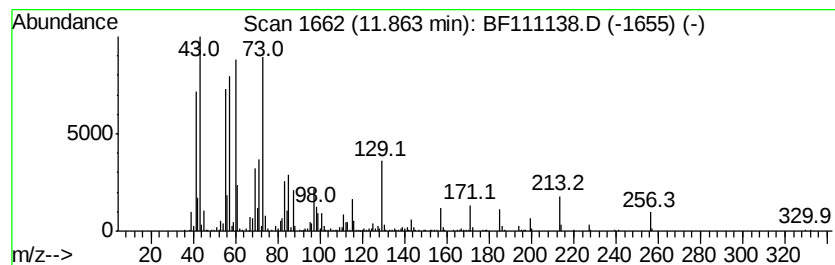
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	7.74 ng	1486050	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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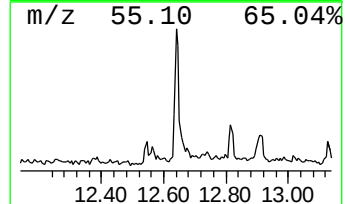
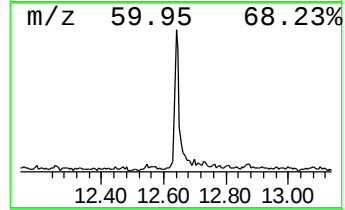
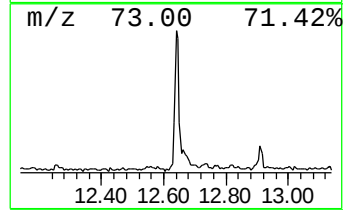
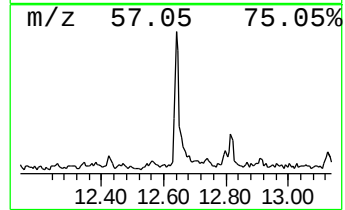
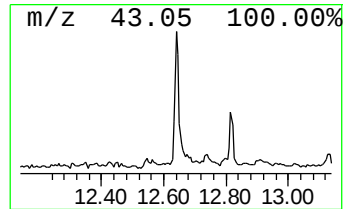
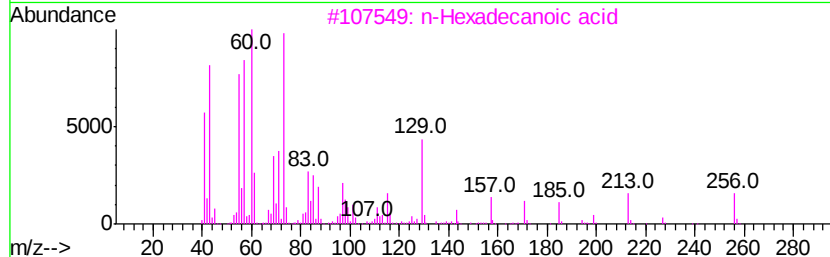
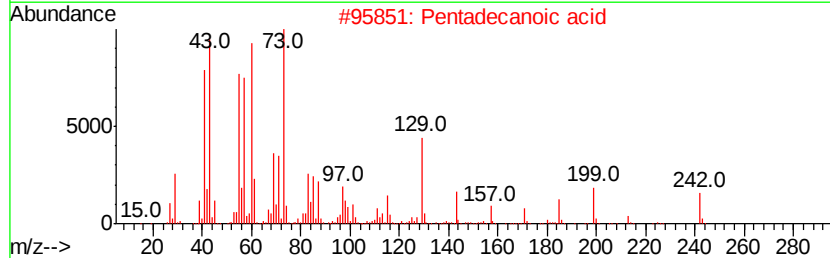
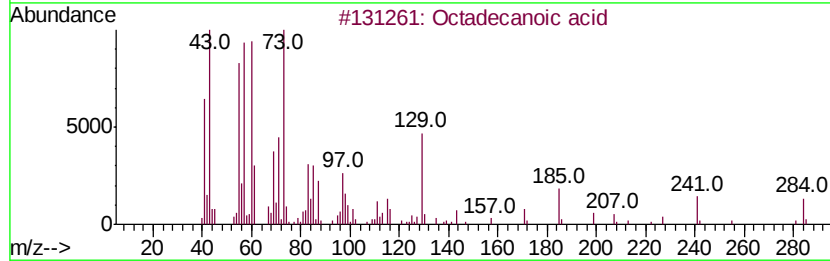
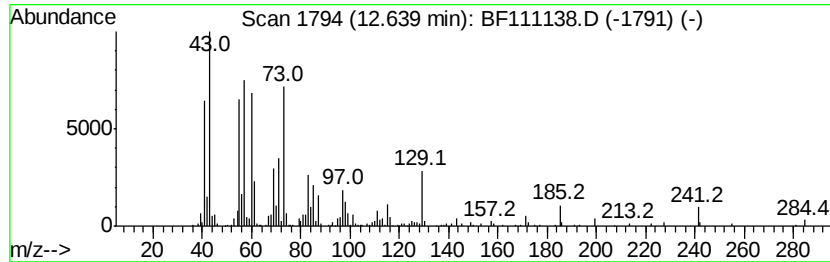
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	3.24 ng	621166	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4		n-Decanoic acid	172	C10H20O2	000334-48-5	53
5		N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25



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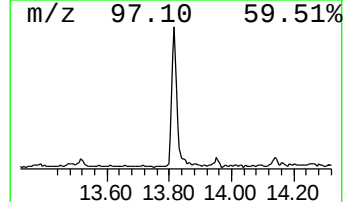
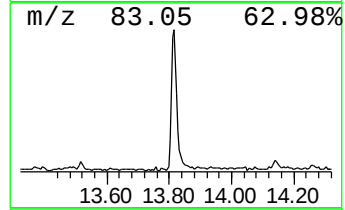
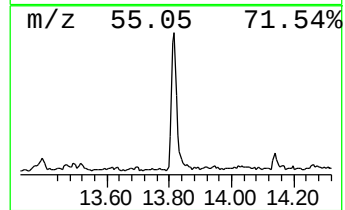
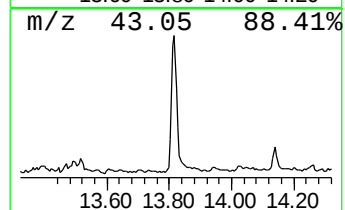
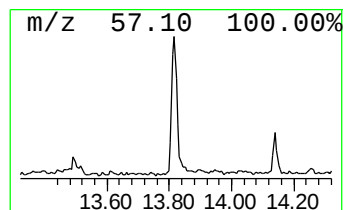
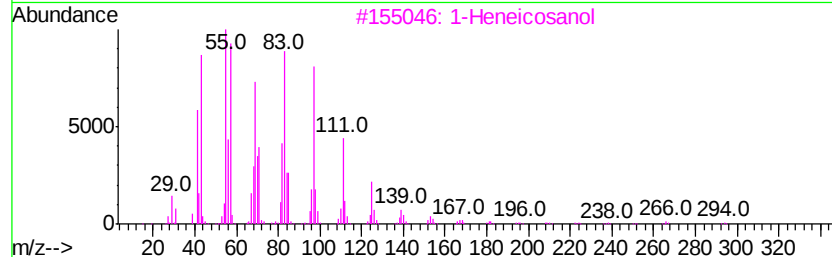
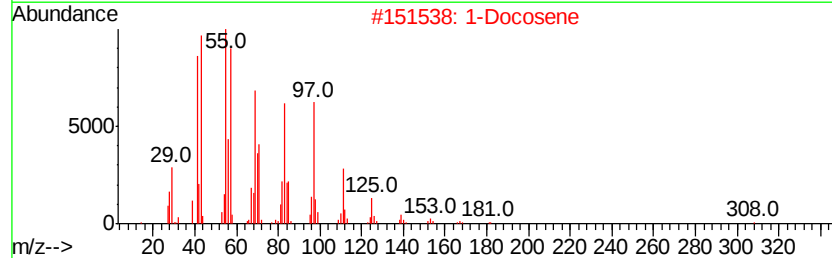
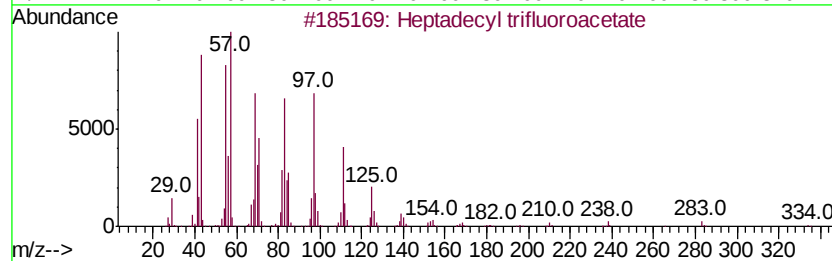
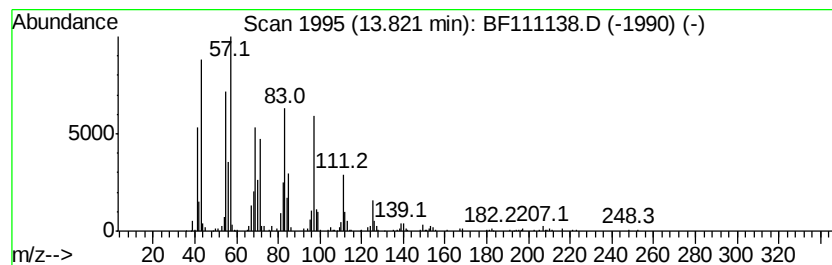
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	6.42 ng	1045720	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2		1-Docosene	308	C22H44	001599-67-3	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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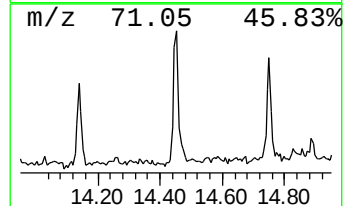
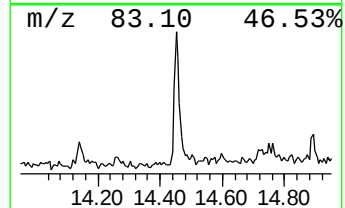
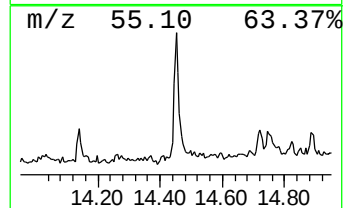
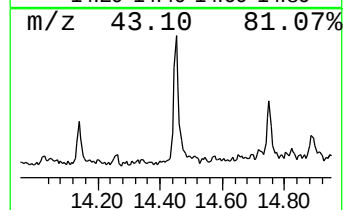
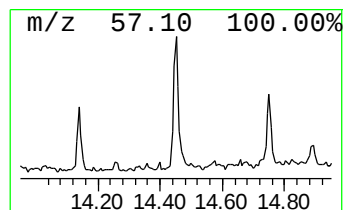
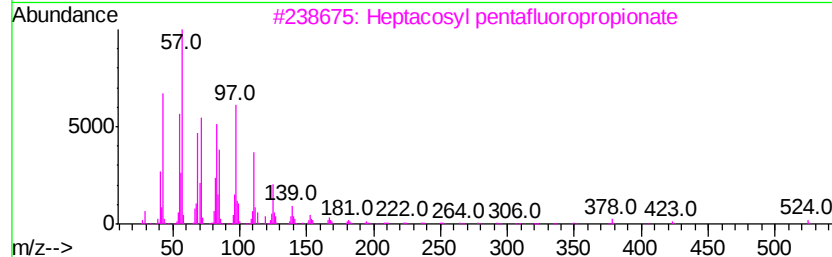
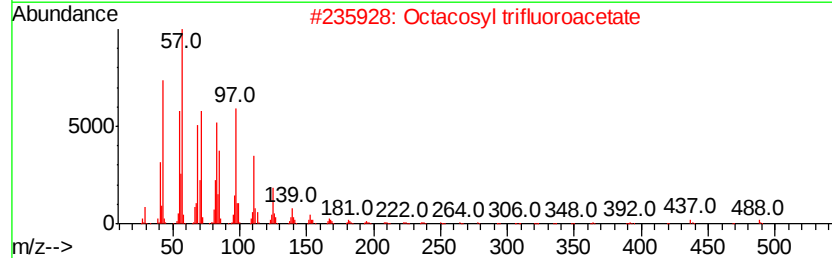
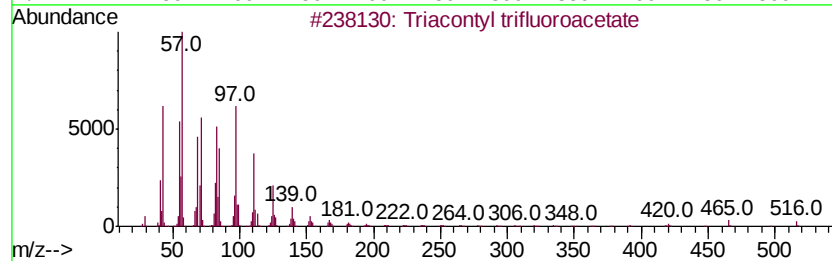
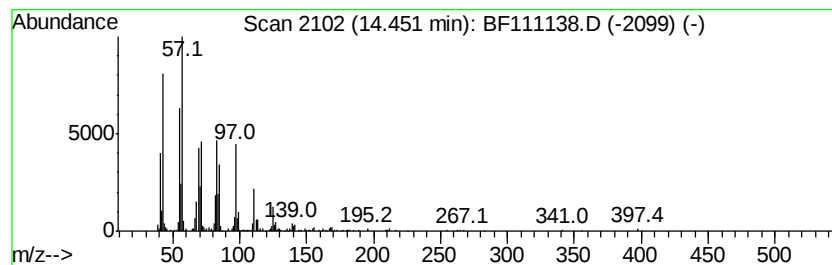
Instrument :
BNA_F
ClientSampleId :
HLSP-SB-7B-(2-6)

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 7 Triacontyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.45	3.00 ng	488575	Chrysene-d12	13.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	91
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	90
4	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	90
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120618\
Data File : BF111138.D
Acq On : 6 Dec 2018 15:08
Operator : JU/SJ
Sample : J6204-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HLSP-SB-7B-(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	5.9 ng		799935	1	6.80	2707540	20.0
unknown6.57	6.57	94.4 ng		12778700	1	6.80	2707540	20.0
n-Hexadecanoic acid	11.86	7.7 ng		1486050	4	11.32	3839230	20.0
Octadecanoic acid	12.64	3.2 ng		621166	4	11.32	3839230	20.0
Heptadecyl triflu...	13.82	6.4 ng		1045720	5	13.96	3258830	20.0
Triacontyl triflu...	14.45	3.0 ng		488575	5	13.96	3258830	20.0