

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121718\
 Data File : BF111532.D
 Acq On : 17 Dec 2018 11:52
 Operator : JU/SJ
 Sample : J6386-06
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-SS005-0612-01

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-BF121418.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	3.281	201	203	214	rBV	27909	61609	1.33%	0.170%
2	5.016	492	498	506	rBV	164954	246599	5.33%	0.679%
3	5.428	563	568	571	rBV	4341601	4128585	89.25%	11.361%
4	6.445	735	741	755	rBV	3874374	4625610	100.00%	12.728%
5	6.569	757	762	765	rBV	4839278	4340970	93.85%	11.945%
6	6.786	796	799	803	rBV	923499	849079	18.36%	2.336%
7	6.951	822	827	830	rBV	3660608	3397433	73.45%	9.349%
8	7.351	889	895	898	rBV	2751845	2790830	60.33%	7.679%
9	7.392	900	902	906	rVB	128004	101207	2.19%	0.278%
10	8.069	1013	1017	1021	rBV	1177019	1032543	22.32%	2.841%
11	9.151	1195	1201	1204	rBV	4741136	4449166	96.19%	12.243%
12	9.539	1263	1267	1271	rBV	378536	306112	6.62%	0.842%
13	9.745	1297	1302	1308	rVB2	39417	46971	1.02%	0.129%
14	9.821	1311	1315	1323	rBV	1063755	1039918	22.48%	2.862%
15	10.616	1445	1450	1453	rBV	1958531	1867417	40.37%	5.139%
16	11.310	1564	1568	1573	rBV	919062	811987	17.55%	2.234%
17	11.839	1655	1658	1670	rBV	257517	282628	6.11%	0.778%
18	12.551	1770	1779	1783	rBV8	27169	70641	1.53%	0.194%
19	12.627	1788	1792	1798	rBV2	86172	121445	2.63%	0.334%
20	12.892	1833	1837	1841	rBV	2810294	2801713	60.57%	7.709%
21	13.015	1850	1858	1859	rBV8	72477	133338	2.88%	0.367%
22	13.474	1933	1936	1941	rVB2	35617	48172	1.04%	0.133%
23	13.792	1987	1990	1999	rVB	356854	433708	9.38%	1.193%
24	13.945	2012	2016	2026	rBV	889074	810805	17.53%	2.231%
25	14.115	2042	2045	2051	rBV	71452	82905	1.79%	0.228%
26	14.427	2094	2098	2102	rBV2	104047	135126	2.92%	0.372%
27	14.656	2135	2137	2141	rBV	57451	65576	1.42%	0.180%
28	14.698	2141	2144	2146	rVV	82644	104061	2.25%	0.286%
29	14.721	2146	2148	2154	rVV	119540	149016	3.22%	0.410%
30	14.798	2158	2161	2166	rVB	41220	49087	1.06%	0.135%
31	15.051	2201	2204	2207	rBV	81856	83468	1.80%	0.230%
32	15.386	2256	2261	2265	rBV	642528	785378	16.98%	2.161%
33	15.845	2335	2339	2343	rVB	64021	88254	1.91%	0.243%

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Sample : J6386-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P001-SS005-0612-01

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-BF121418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

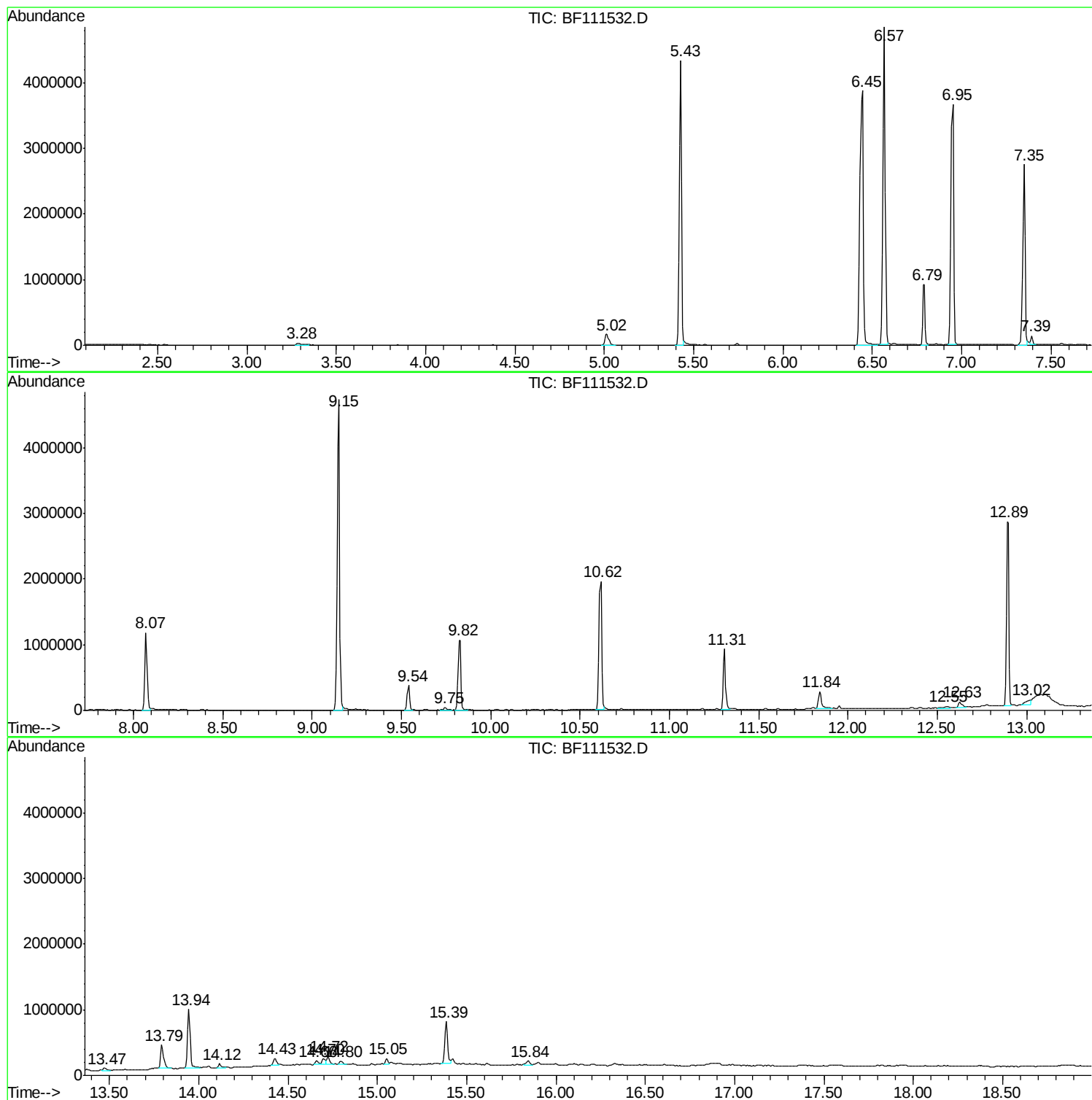
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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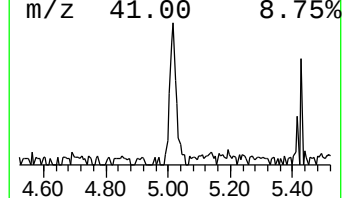
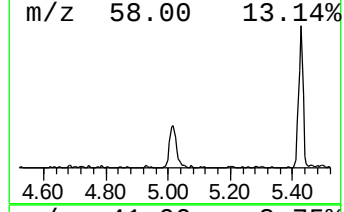
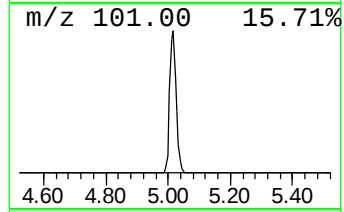
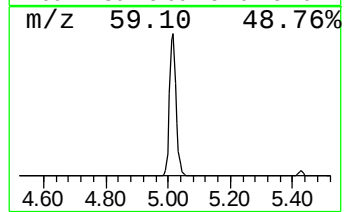
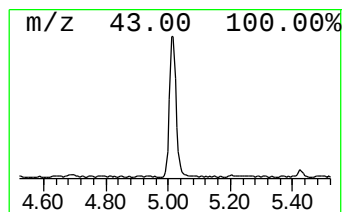
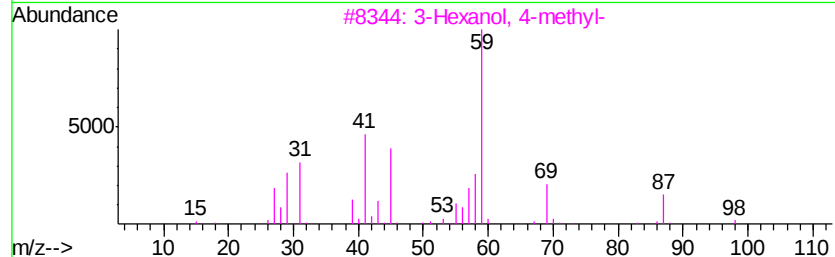
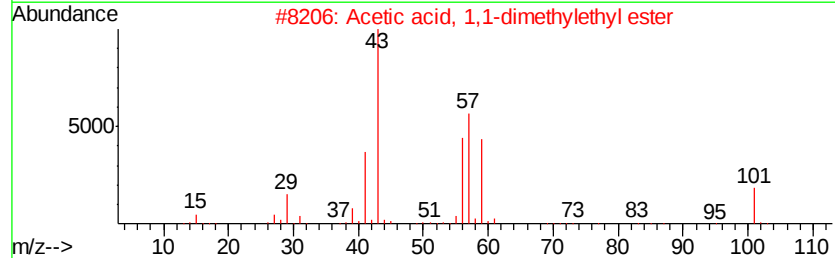
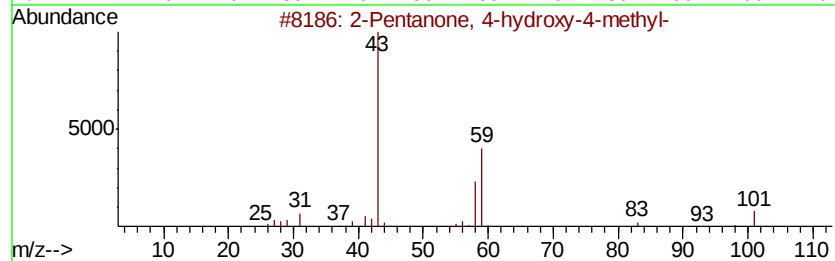
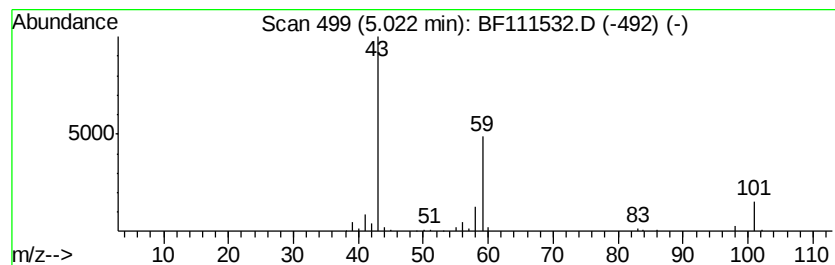
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	5.81 ng	246599	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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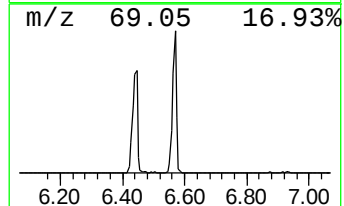
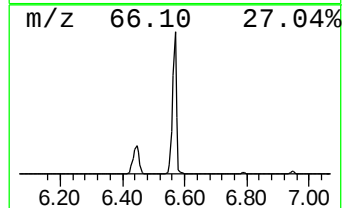
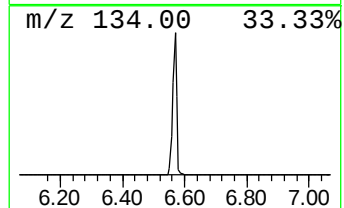
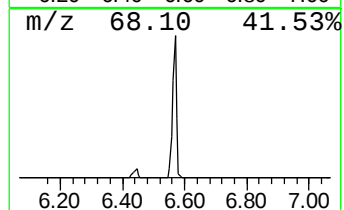
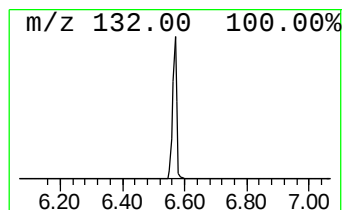
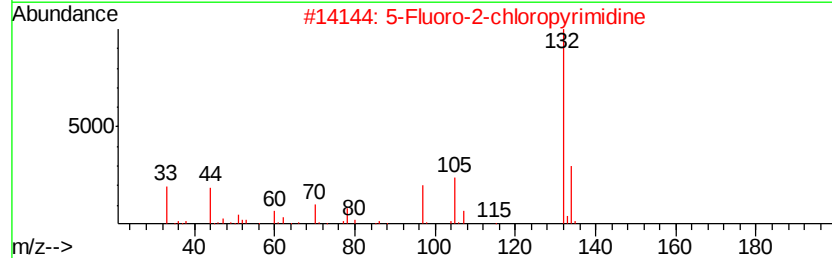
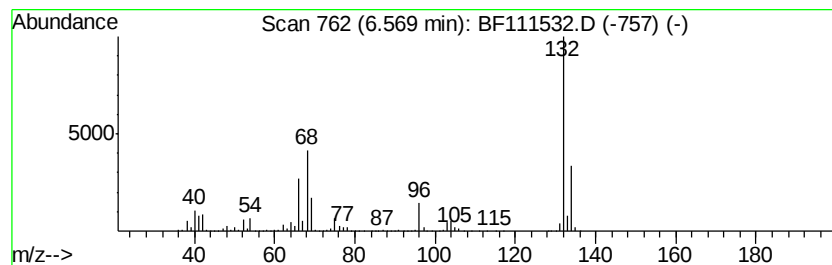
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	102.25 ng	4340970	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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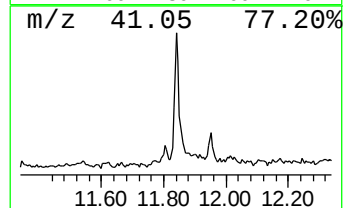
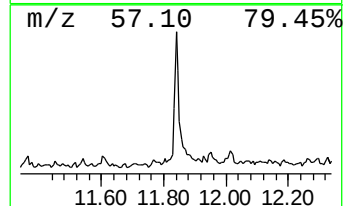
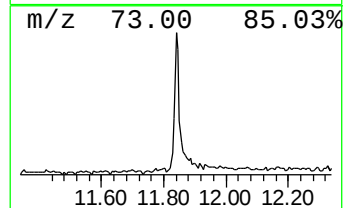
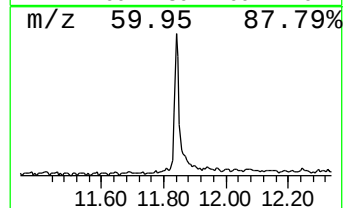
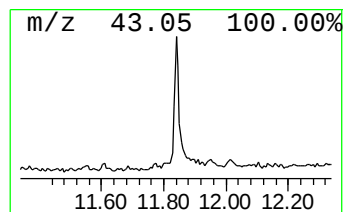
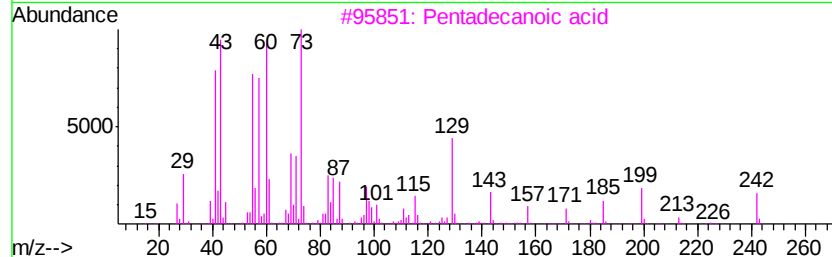
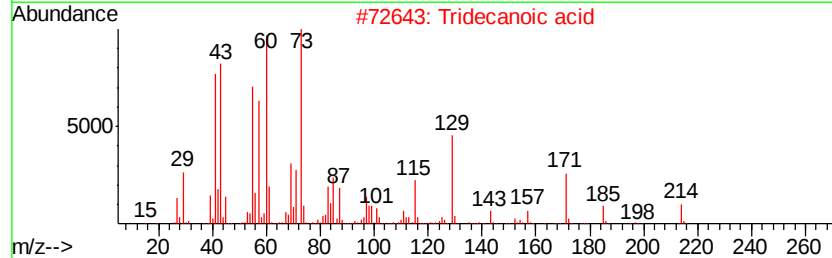
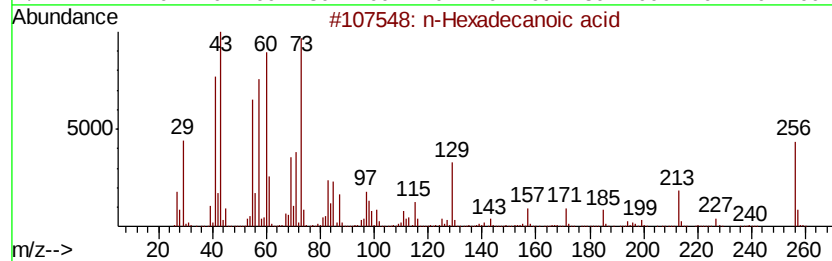
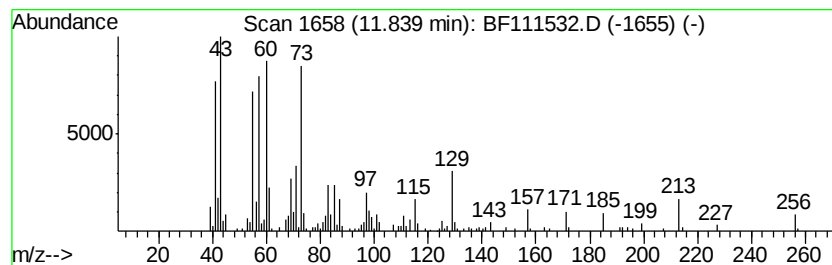
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.84	6.96 ng	282628	Phenanthrene-d10		11.31
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



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Misc :
ALS Vial : 6 Sample Multiplier: 1

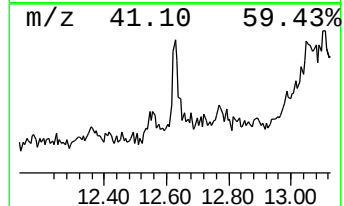
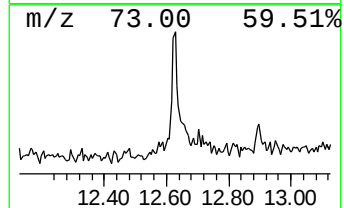
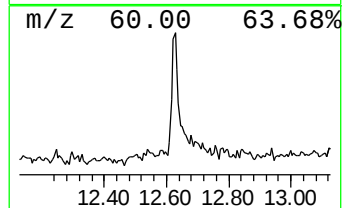
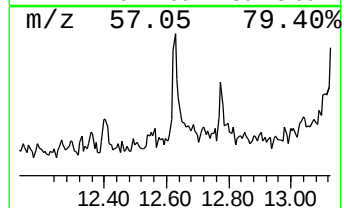
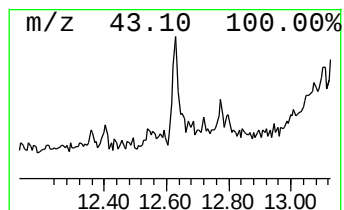
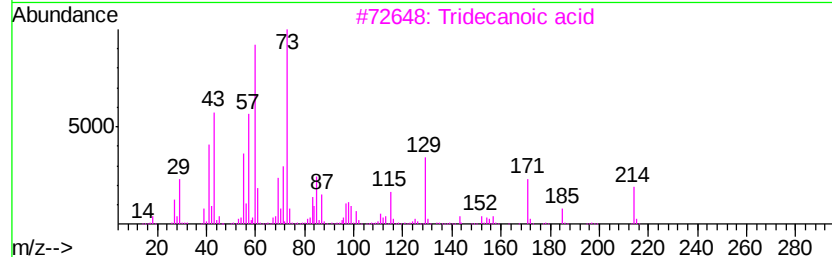
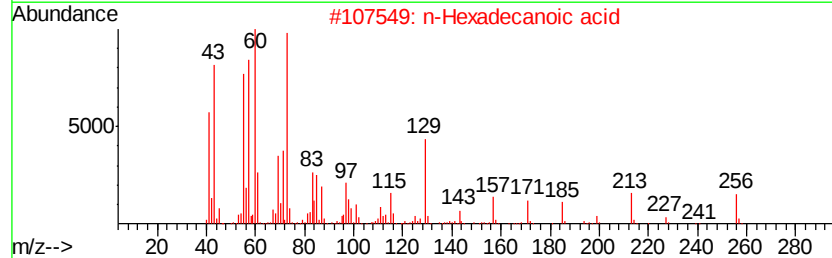
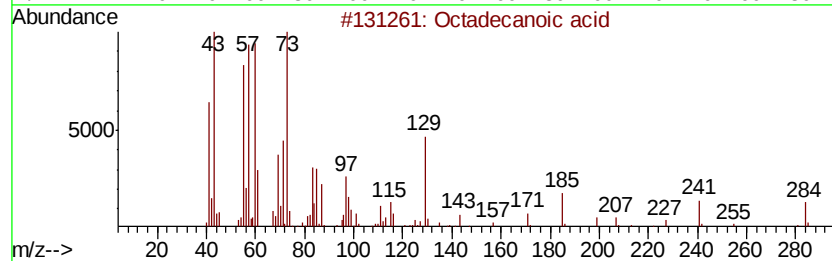
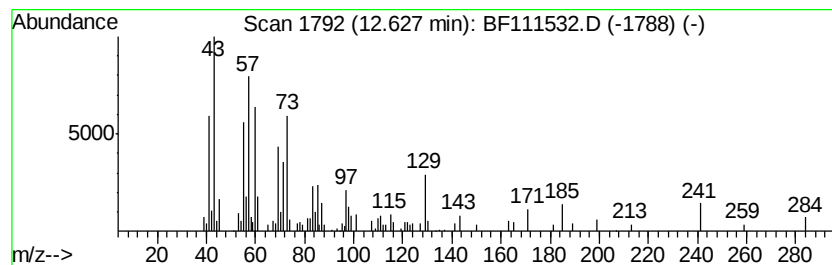
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.63	3.00 ng	121445	Chrysene-d12		13.94	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3		Tridecanoic acid	214	C13H26O2	000638-53-9	53
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5		Dodecanoic acid	200	C12H24O2	000143-07-7	47



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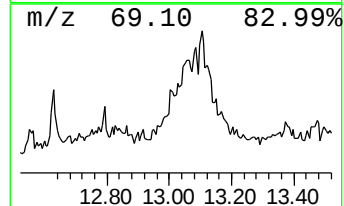
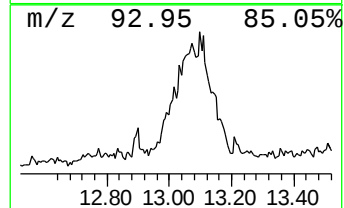
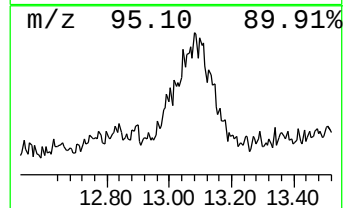
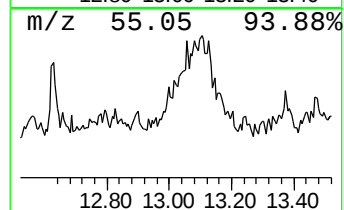
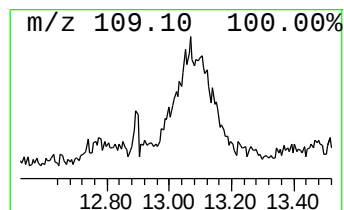
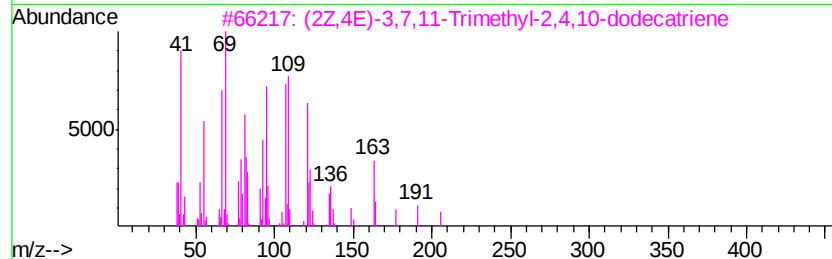
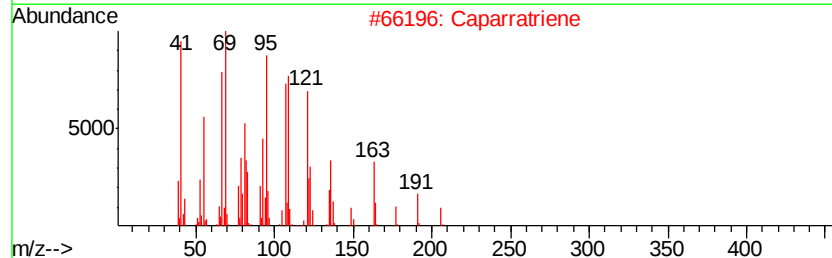
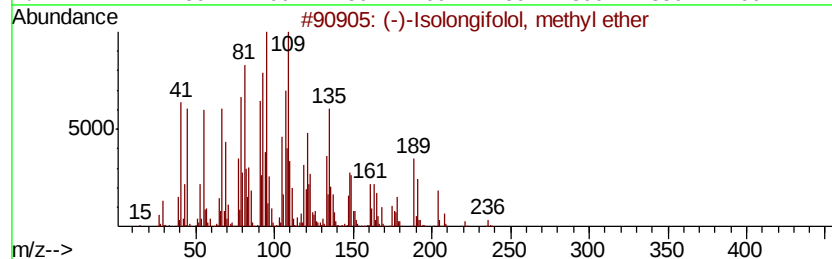
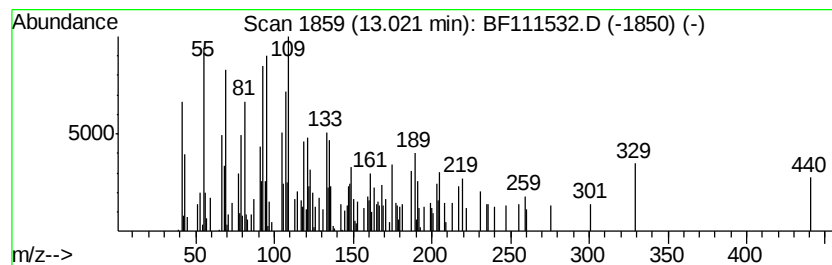
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (-)-Isolongifolol, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.02	3.29 ng	133338	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1 (-)-Isolongifolol, methyl ether		236	C16H28O	1000333-80-8	64
2 Caparratriene		206	C15H26	1000374-08-7	45
3 (2Z,4E)-3,7,11-Trimethyl-2,4,10-...		206	C15H26	172549-29-0	45
4 6.beta.Bicyclo[4.3.0]nonane, 5.b...		332	C15H25I	1000195-85-9	38
5 Dimethyl[bis[(4,8,8-trimethyldec...		500	C32H56O2Si	1000364-69-0	35



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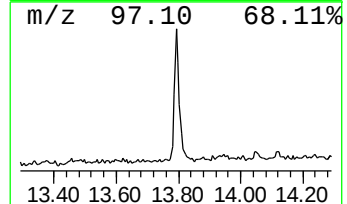
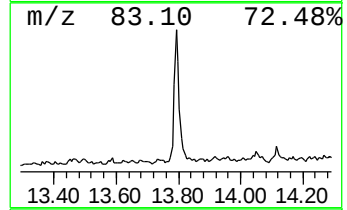
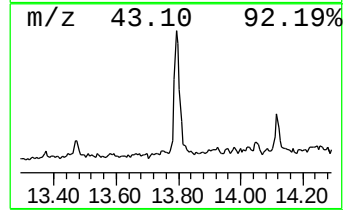
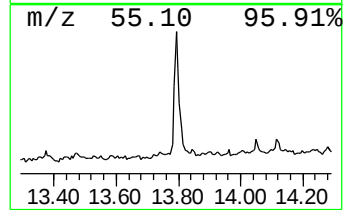
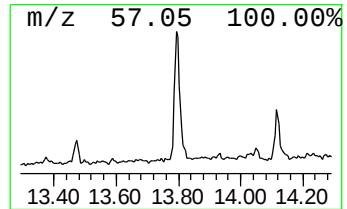
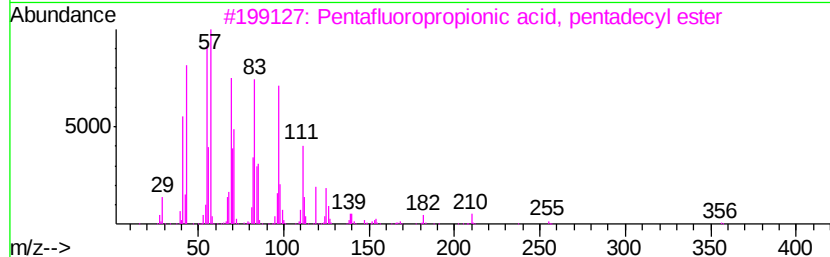
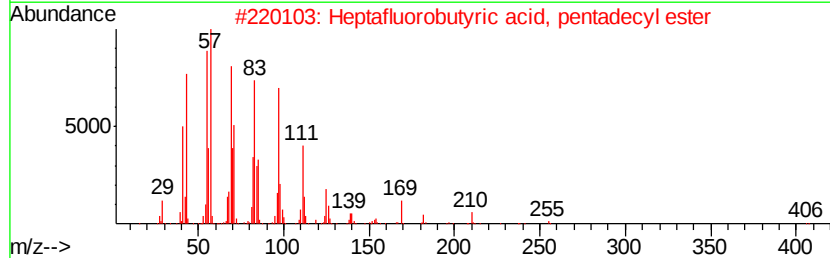
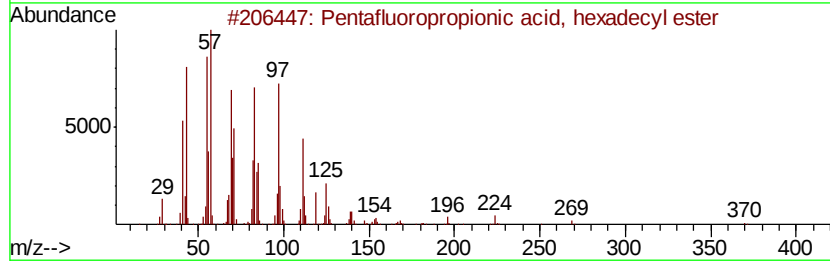
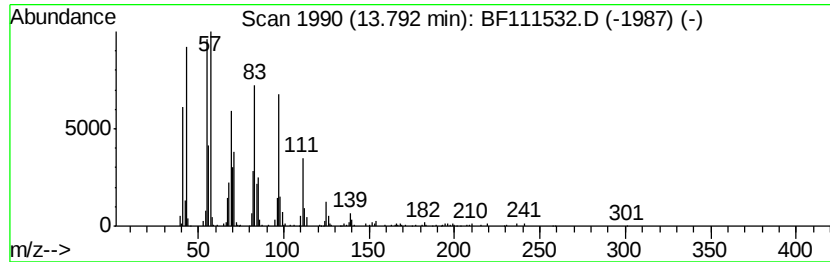
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	10.70 ng	433708	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4		Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111532.D
Acq On : 17 Dec 2018 11:52
Operator : JU/SJ
Sample : J6386-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

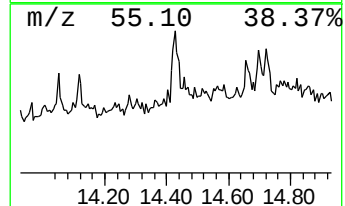
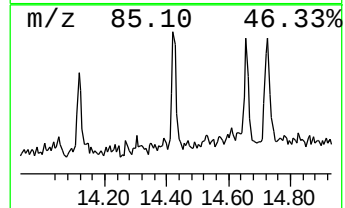
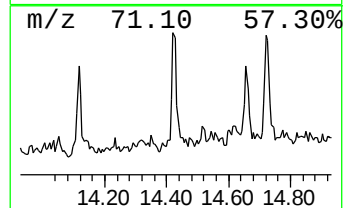
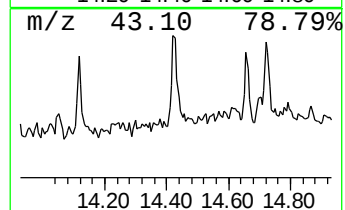
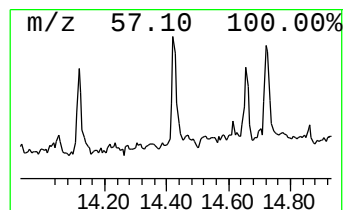
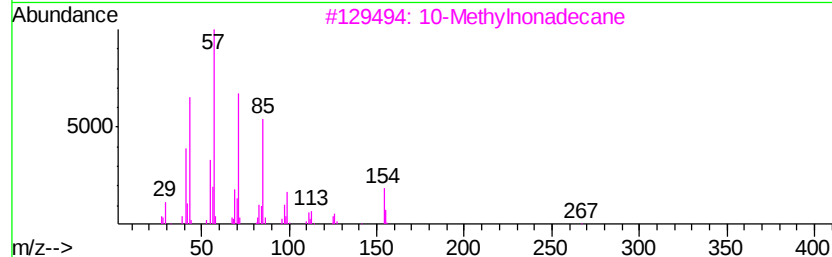
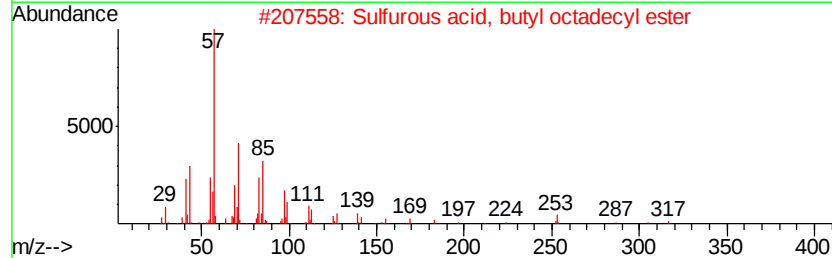
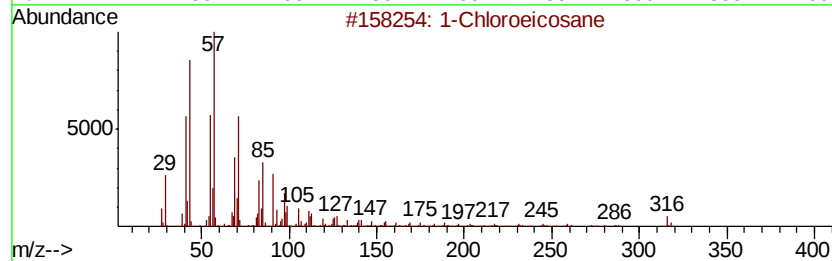
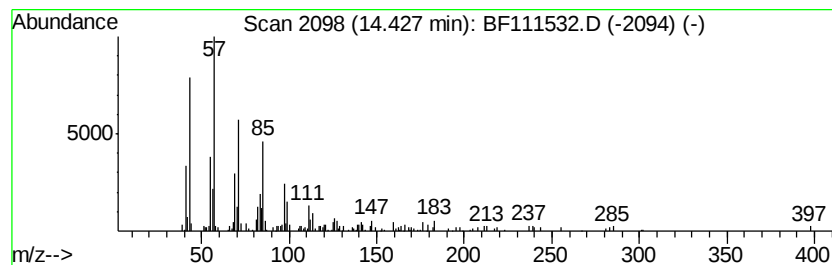
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Chloroeicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.43	3.33 ng	135126	Chrysene-d12	13.94		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Chloroeicosane	316	C20H41Cl	042217-02-7	91
2		Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	90
3		10-Methylnonadecane	282	C20H42	056862-62-5	87
4		Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	86
5		Tetratetracontane	619	C44H90	007098-22-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111532.D
Acq On : 17 Dec 2018 11:52
Operator : JU/SJ
Sample : J6386-06
Misc :
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Instrument :
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ClientSampleId :
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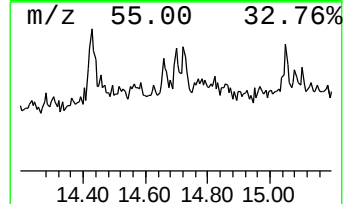
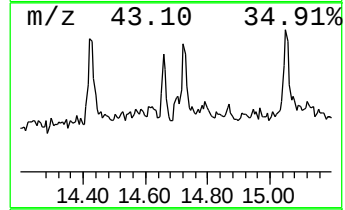
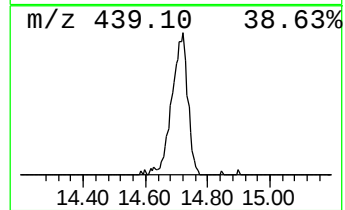
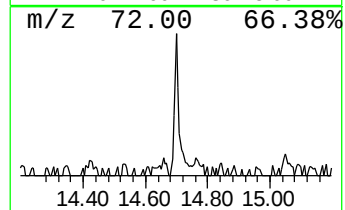
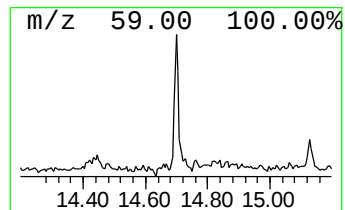
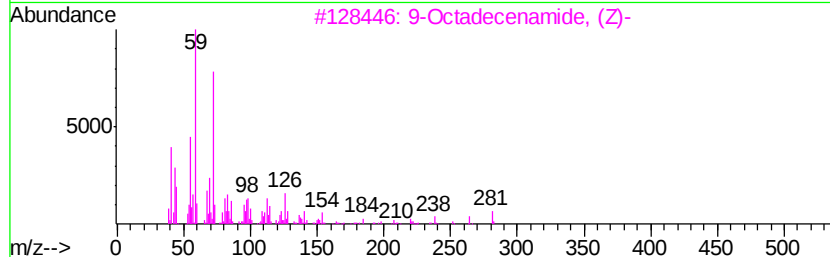
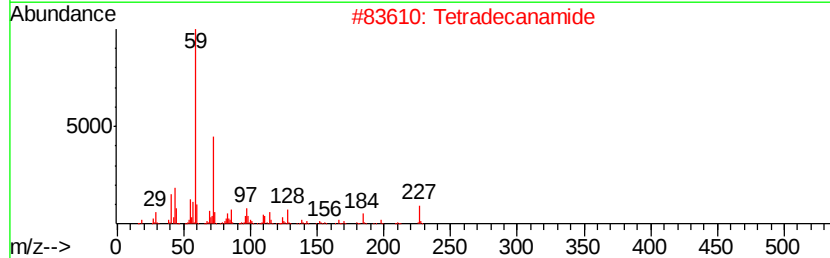
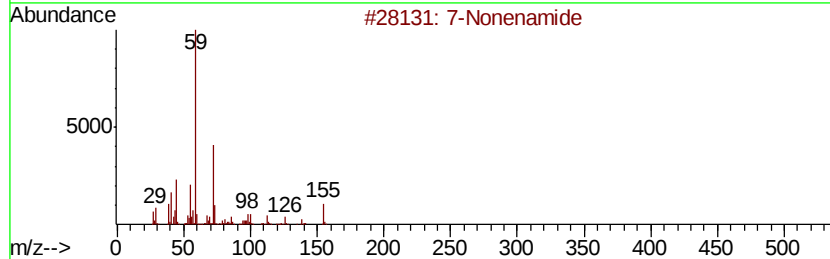
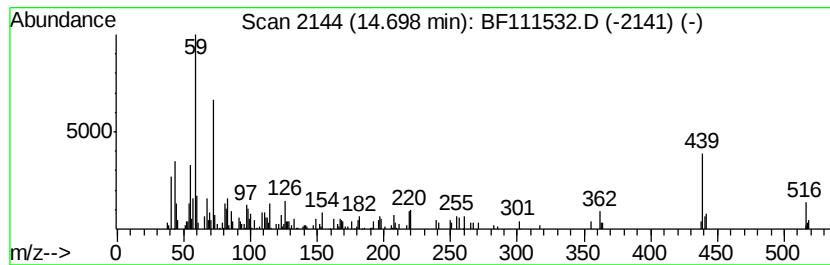
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.70 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	2.65 ng	104061	Perylene-d12	15.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Nonenamide	155	C9H17NO	090949-53-4	43
2			Tetradecanamide	227	C14H29NO	000638-58-4	43
3			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	37
4			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	37
5			Hexadecanamide	255	C16H33NO	000629-54-9	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111532.D
Acq On : 17 Dec 2018 11:52
Operator : JU/SJ
Sample : J6386-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

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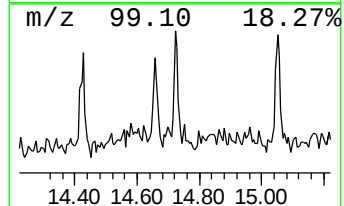
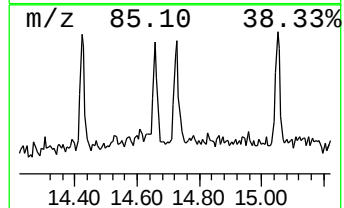
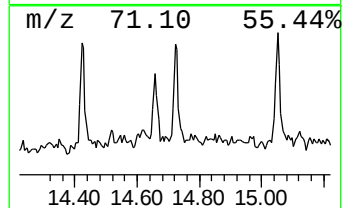
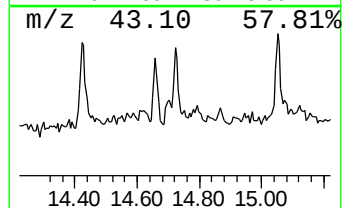
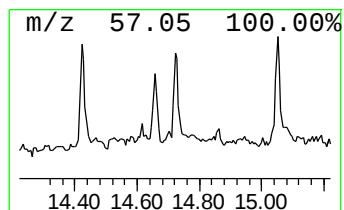
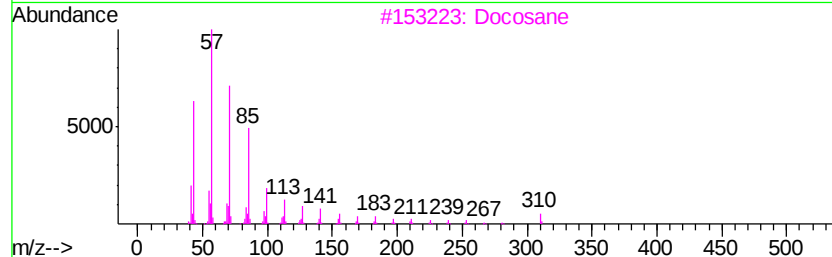
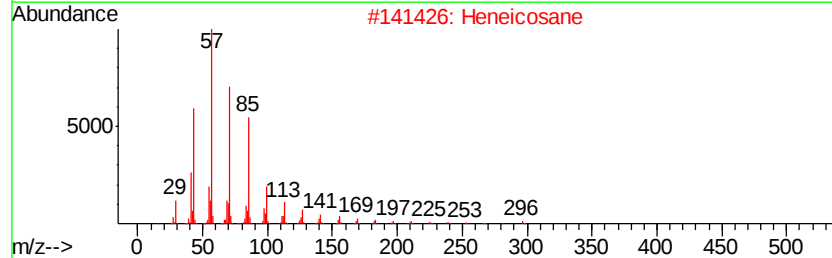
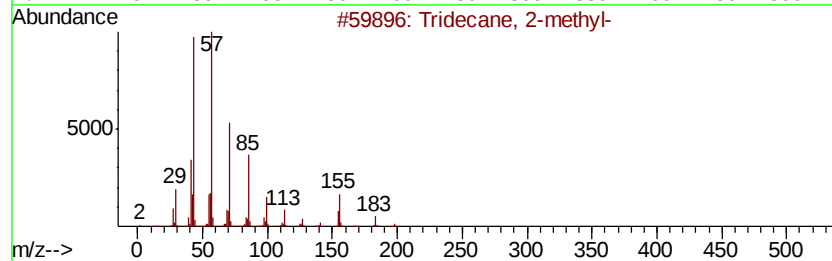
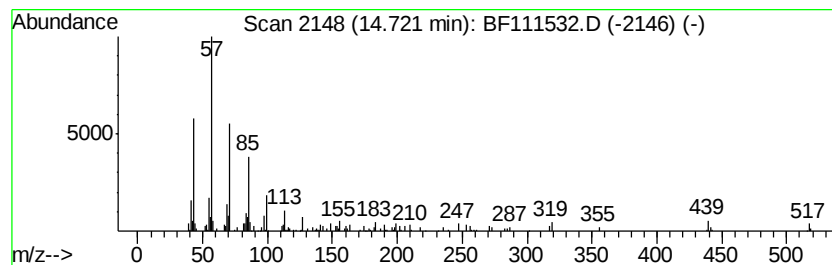
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tridecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.79 ng	149016	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	74
2		Heneicosane	296	C21H44	000629-94-7	72
3		Docosane	310	C22H46	000629-97-0	72
4		Tetracosane	338	C24H50	000646-31-1	72
5		Eicosane, 2-methyl-	296	C21H44	001560-84-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
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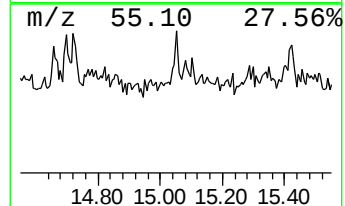
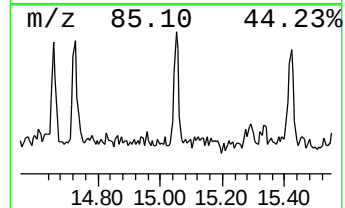
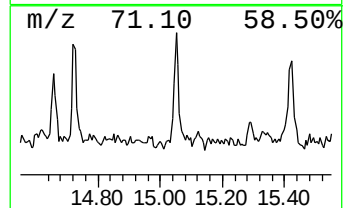
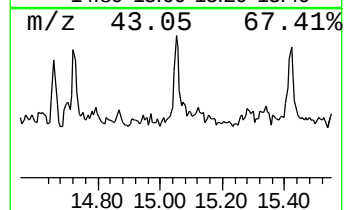
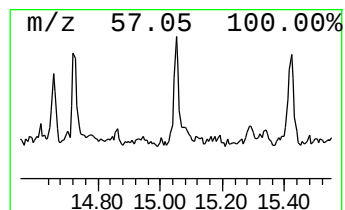
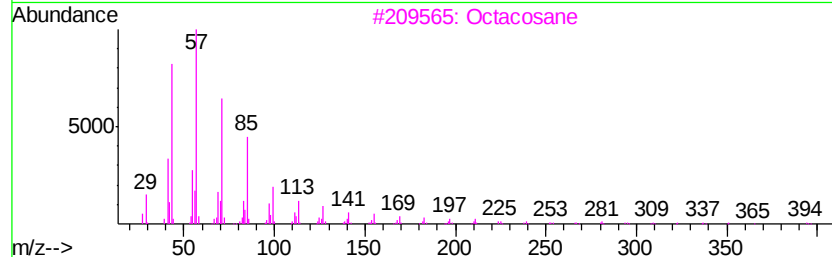
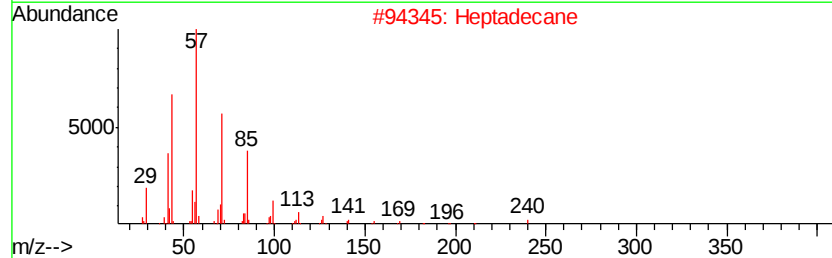
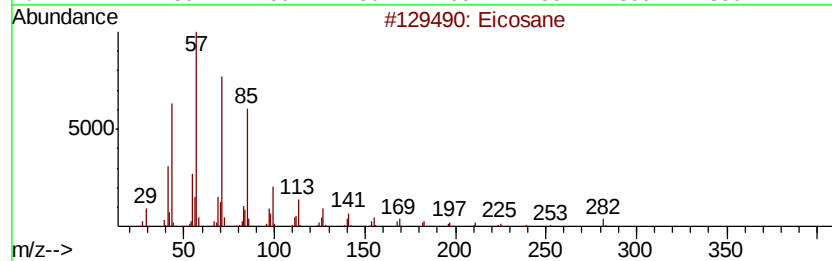
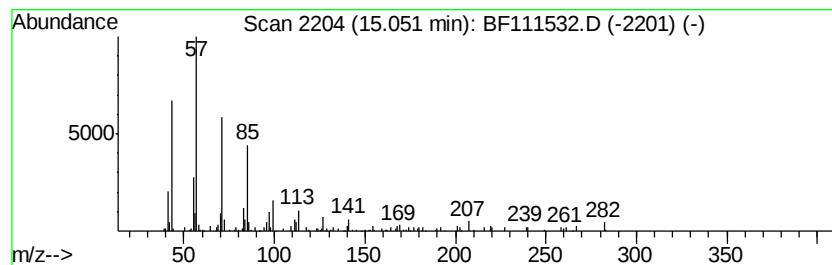
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	2.13 ng	83468	Perylene-d12	15.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Heptadecane	240 C17H36	000629-78-7	91
3	Octacosane	394 C28H58	000630-02-4	87
4	Heneicosane	296 C21H44	000629-94-7	87
5	Pentacosane	352 C25H52	000629-99-2	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
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Misc :
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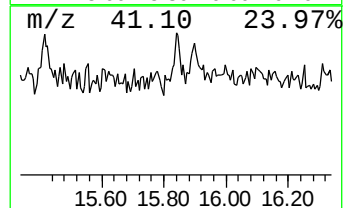
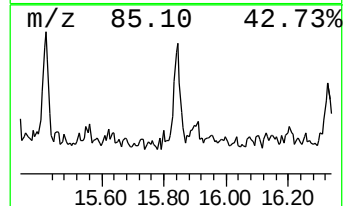
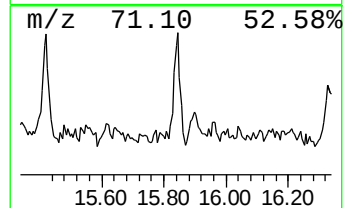
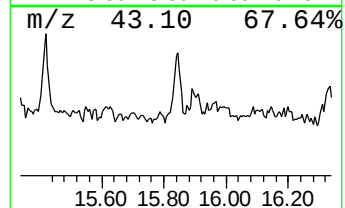
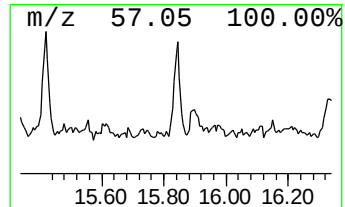
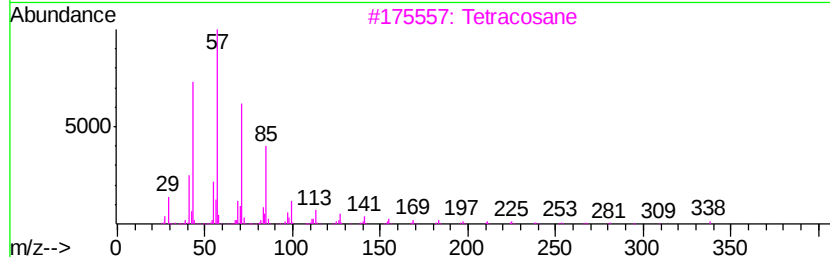
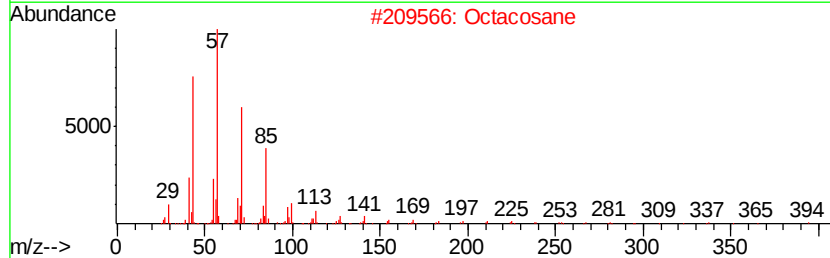
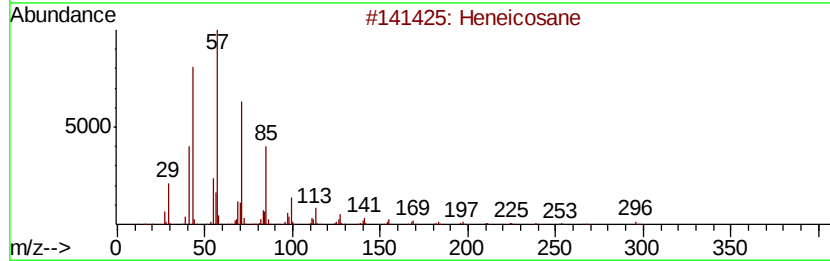
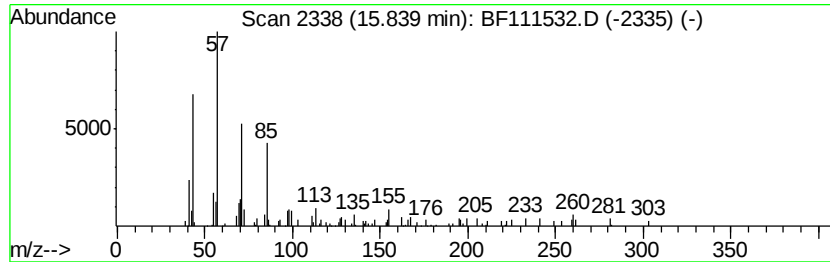
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.84	2.25 ng	88254	Perylene-d12		15.39
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	64
2	Octacosane	394	C28H58	000630-02-4	64
3	Tetracosane	338	C24H50	000646-31-1	64
4	Pentadecane	212	C15H32	000629-62-9	64
5	Heptadecane	240	C17H36	000629-78-7	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121718\
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 Acq On : 17 Dec 2018 11:52
 Operator : JU/SJ
 Sample : J6386-06
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.57	6.57	102.3	ng	4340970	1	6.79	849079	20.0
n-Hexadecanoic acid	11.84	7.0	ng	282628	4	11.31	811987	20.0
Octadecanoic acid	12.63	3.0	ng	121445	5	13.94	810805	20.0
(-)-Isolongifolol...	13.02	3.3	ng	133338	5	13.94	810805	20.0
Pentafluoropropio...	13.79	10.7	ng	433708	5	13.94	810805	20.0
1-Chloroeicosane	14.43	3.3	ng	135126	5	13.94	810805	20.0
unknown14.70	14.70	2.6	ng	104061	6	15.39	785378	20.0
Tridecane, 2-methyl-	14.72	3.8	ng	149016	6	15.39	785378	20.0
Eicosane	15.05	2.1	ng	83468	6	15.39	785378	20.0
Heneicosane	15.84	2.3	ng	88254	6	15.39	785378	20.0