

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122618\
 Data File : BF111712.D
 Acq On : 26 Dec 2018 13:29
 Operator : JU/SJ
 Sample : J6498-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1218-S-DH-9-T

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-BF121918.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	2.210	15	21	26	rVB	69434	95602	2.11%	0.235%
2	3.434	226	229	242	rBV	35594	75457	1.67%	0.185%
3	5.122	510	516	522	rBV	184801	245976	5.43%	0.604%
4	5.534	581	586	589	rBV	3913416	3792984	83.81%	9.321%
5	6.540	752	757	762	rBV2	3990161	4285011	94.68%	10.530%
6	6.675	775	780	783	rBV	4452878	4073406	90.00%	10.010%
7	6.898	815	818	822	rVB	1217414	1078638	23.83%	2.651%
8	7.057	841	845	849	rBV	3516573	3140938	69.40%	7.718%
9	7.457	908	913	916	rBV	2759005	2568662	56.75%	6.312%
10	8.181	1032	1036	1040	rBV	1581096	1360071	30.05%	3.342%
11	9.257	1214	1219	1222	rBV	5464743	4525963	100.00%	11.122%
12	9.645	1281	1285	1288	rBV	631696	488730	10.80%	1.201%
13	9.939	1331	1335	1338	rBV	1731587	1528908	33.78%	3.757%
14	10.228	1381	1384	1387	rBV	57712	70893	1.57%	0.174%
15	10.728	1464	1469	1472	rBV	3383873	2947826	65.13%	7.244%
16	11.422	1583	1587	1590	rBV	1815127	1513050	33.43%	3.718%
17	11.945	1673	1676	1679	rBV2	225468	181892	4.02%	0.447%
18	12.633	1790	1793	1796	rBV	234098	188069	4.16%	0.462%
19	12.727	1806	1809	1812	rBV3	63215	60156	1.33%	0.148%
20	12.863	1827	1832	1834	rBV	199082	193397	4.27%	0.475%
21	13.004	1852	1856	1860	rBV	4200715	4083623	90.23%	10.035%
22	13.480	1934	1937	1941	rBV	210995	254703	5.63%	0.626%
23	13.898	2004	2008	2014	rBV3	314036	368697	8.15%	0.906%
24	14.057	2030	2035	2038	rBV	1342884	1372327	30.32%	3.372%
25	14.086	2038	2040	2042	rVB	80805	63313	1.40%	0.156%
26	14.169	2051	2054	2057	rBV2	66577	68129	1.51%	0.167%
27	14.221	2061	2063	2068	rVB	111848	104511	2.31%	0.257%
28	14.533	2113	2116	2120	rVB	182135	191882	4.24%	0.472%
29	14.839	2166	2168	2172	rBV2	113560	100398	2.22%	0.247%
30	15.104	2210	2213	2223	rBV	102059	210781	4.66%	0.518%
31	15.186	2224	2227	2230	rBV	165848	201072	4.44%	0.494%
32	15.545	2283	2288	2291	rBV	940708	1114977	24.64%	2.740%
33	16.021	2366	2369	2373	rBV	119427	144182	3.19%	0.354%

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ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId :
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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

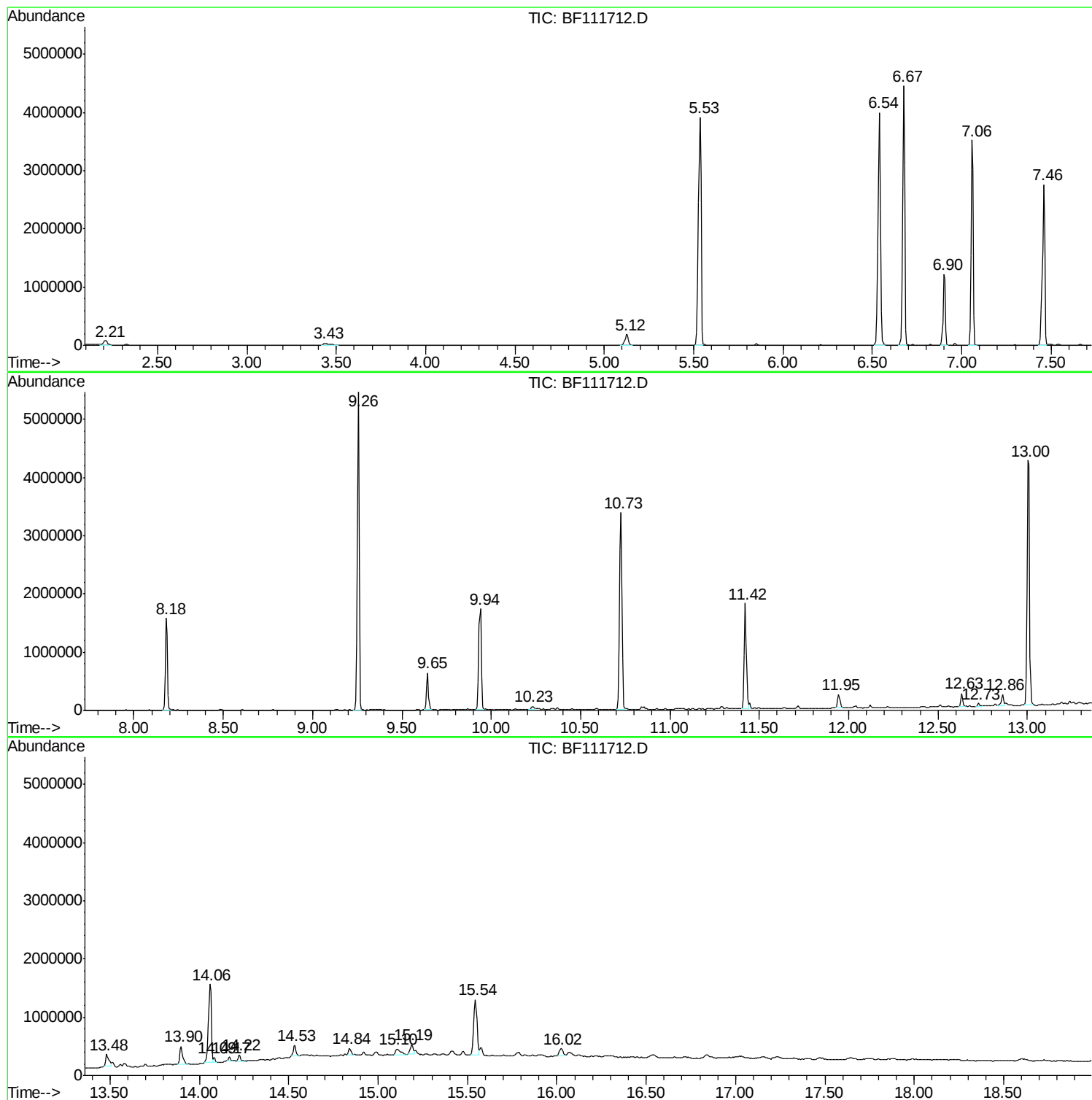
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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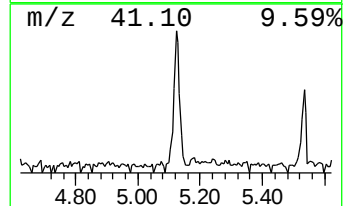
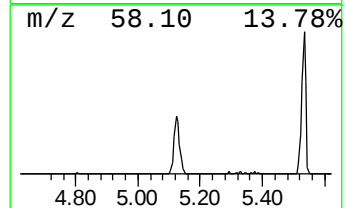
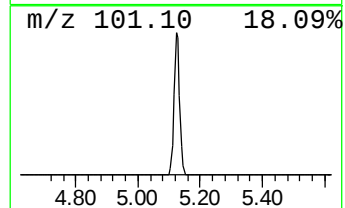
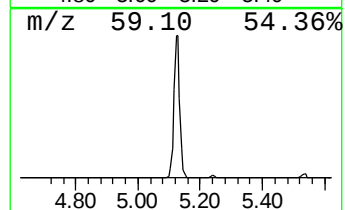
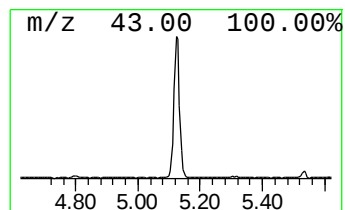
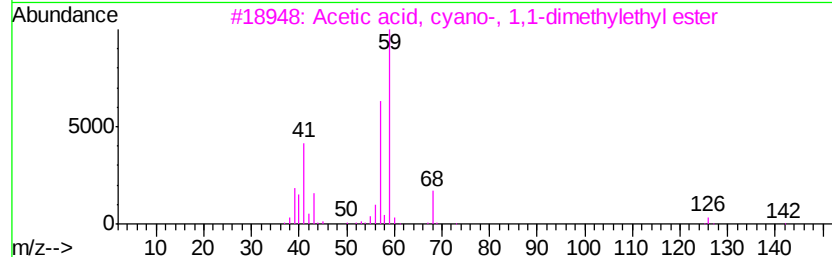
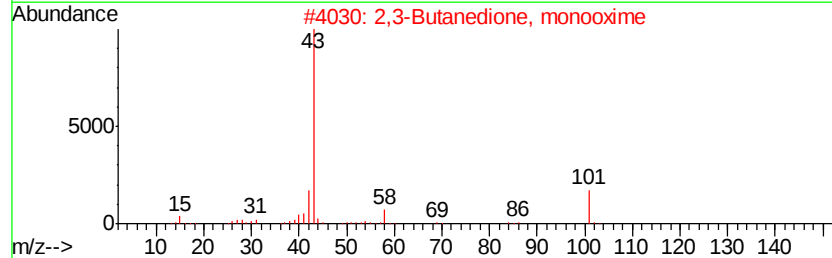
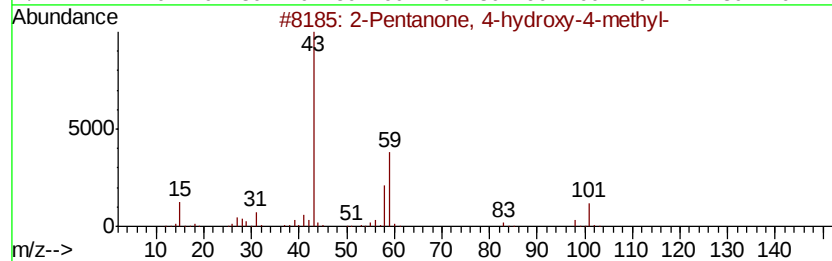
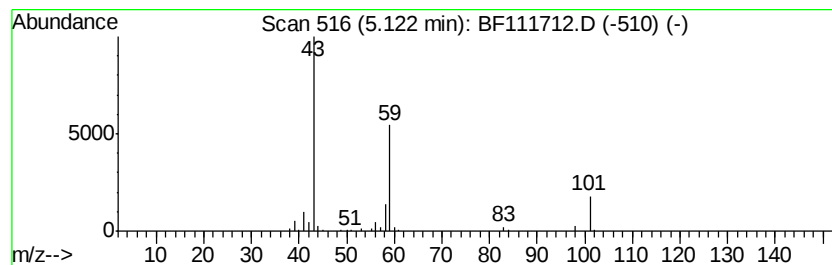
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	4.56 ng	245976	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
5			1,2-Butanediol	90	C4H10O2	000584-03-2	9



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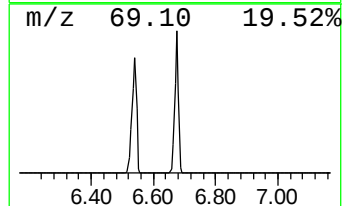
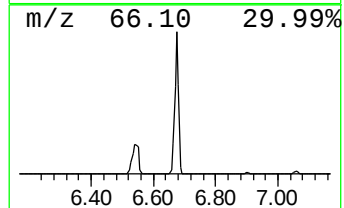
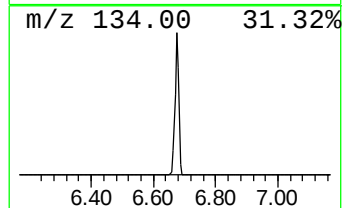
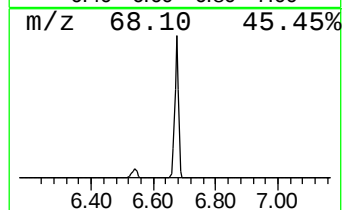
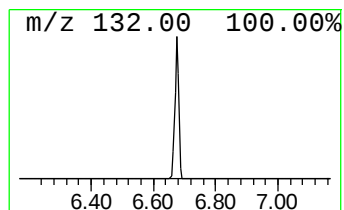
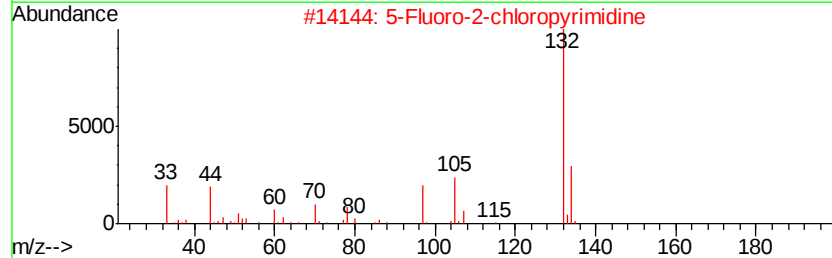
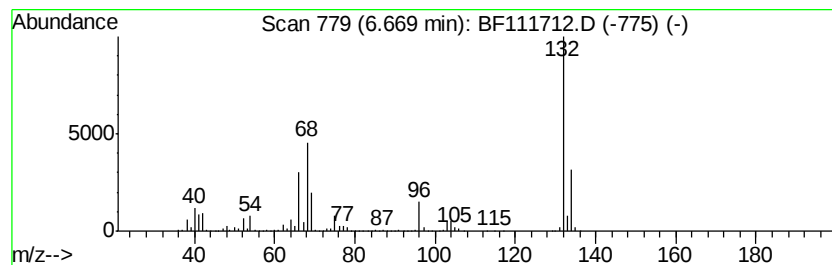
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	75.53 ng	4073410	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	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	10	
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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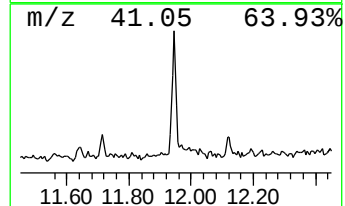
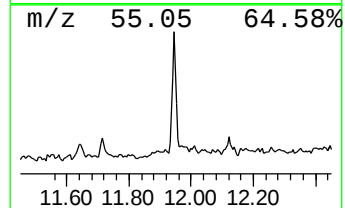
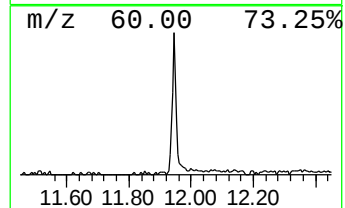
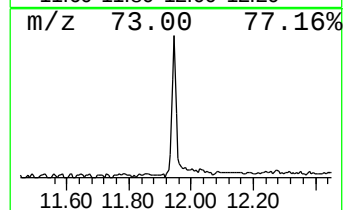
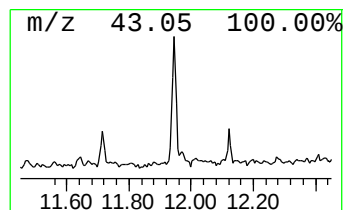
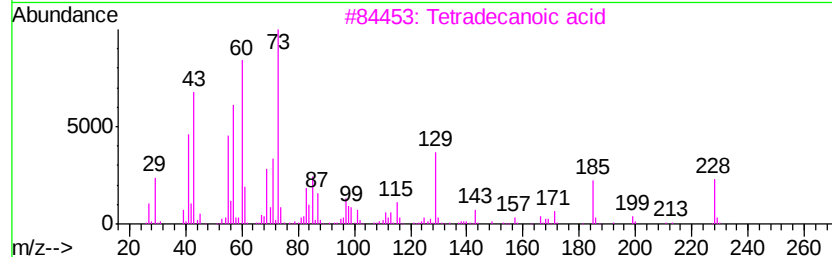
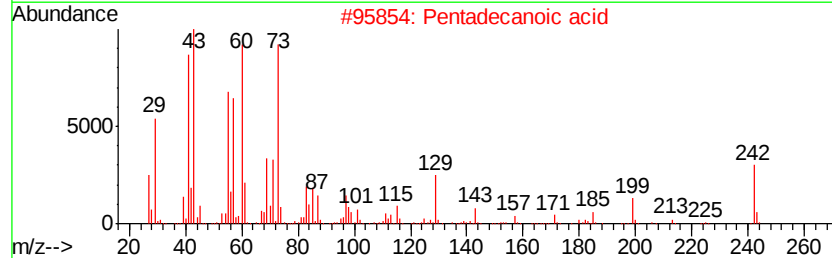
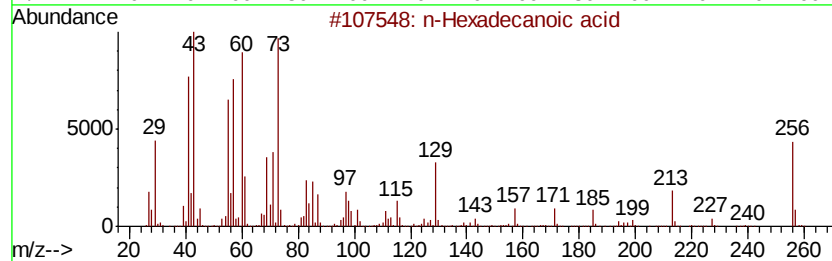
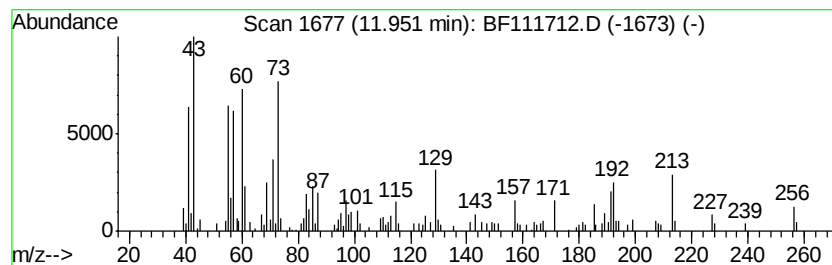
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.40 ng	181892	Phenanthrene-d10	11.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Undecanoic acid	186	C11H22O2	000112-37-8	64



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ALS Vial : 7 Sample Multiplier: 1

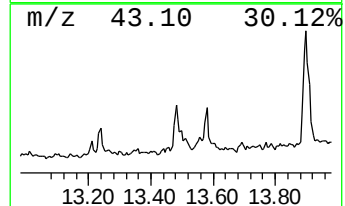
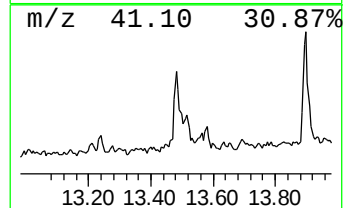
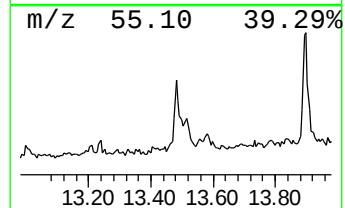
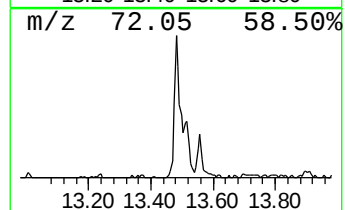
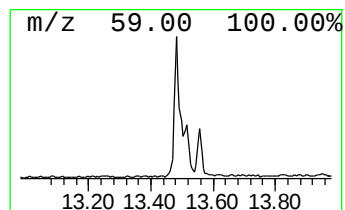
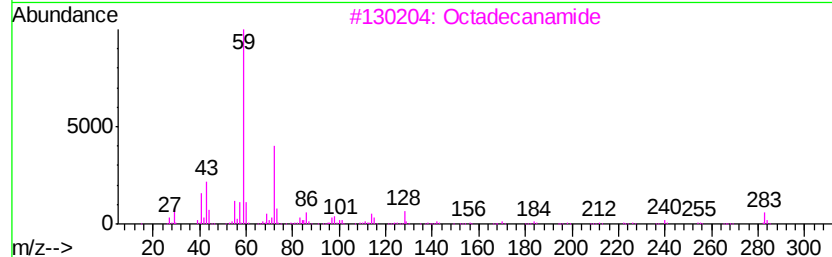
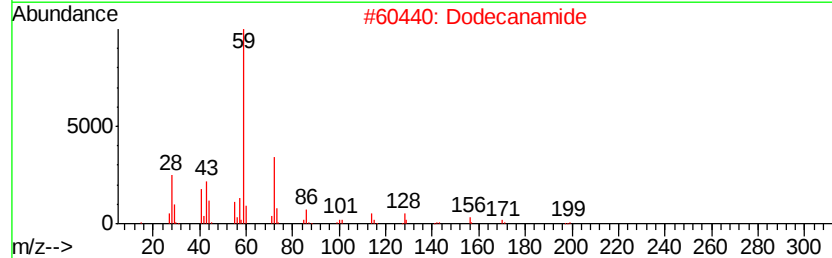
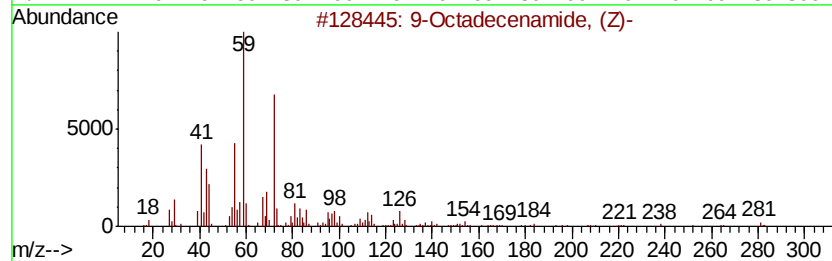
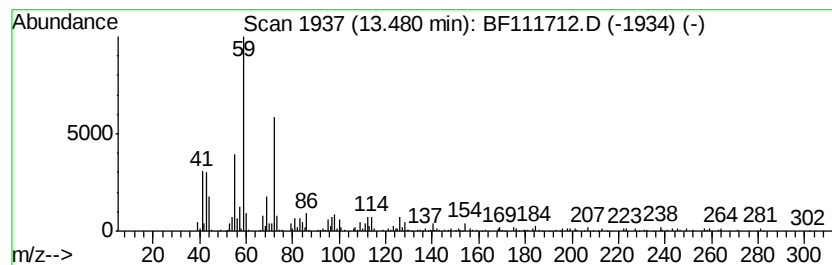
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.48	3.71 ng	254703	Chrysene-d12		14.06
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Dodecanamide	199	C12H25NO	001120-16-7	68
3	Octadecanamide	283	C18H37NO	000124-26-5	59
4	Octanamide	143	C8H17NO	000629-01-6	59
5	Tetradecanamide	227	C14H29NO	000638-58-4	59



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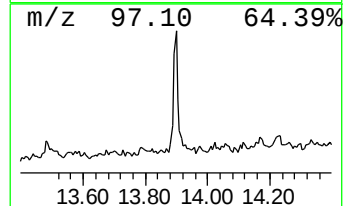
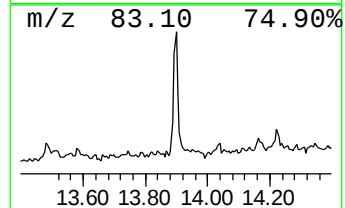
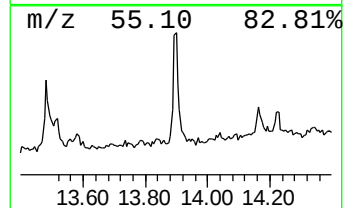
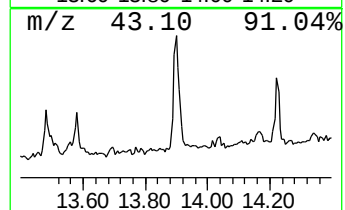
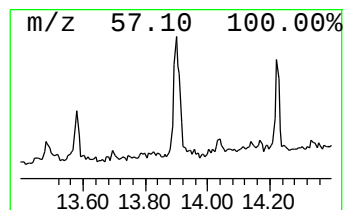
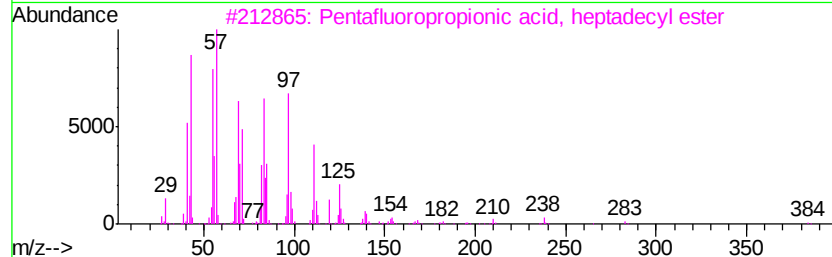
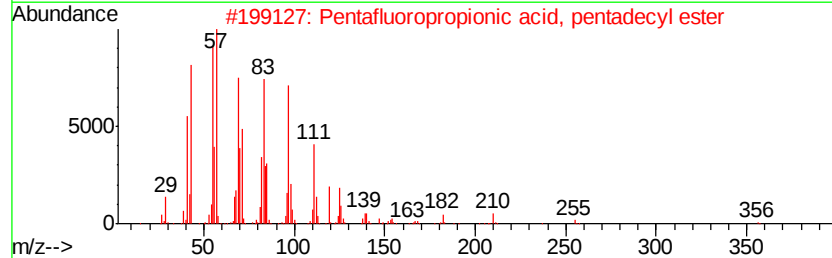
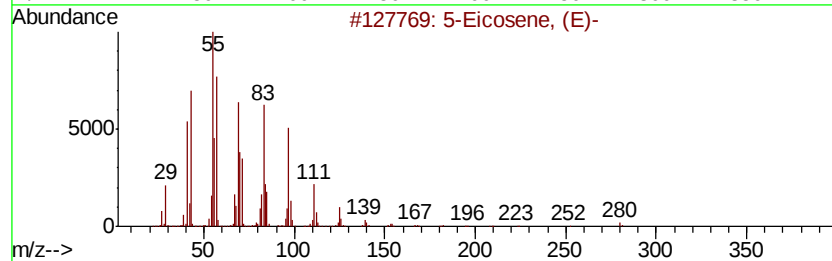
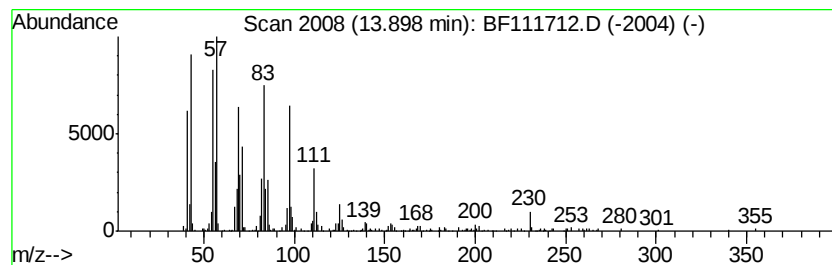
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	5.37 ng	368697	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	95
2	Pentafluoropropionic acid, penta...		374	C18H31F5O2	959092-08-1	93
3	Pentafluoropropionic acid, hepta...		402	C20H35F5O2	959218-78-1	91
4	Cyclotetracosane		336	C24H48	000297-03-0	91
5	1-Tricosene		322	C23H46	018835-32-0	91



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ALS Vial : 7 Sample Multiplier: 1

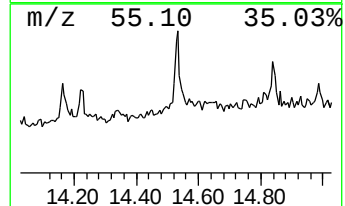
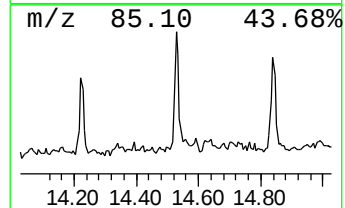
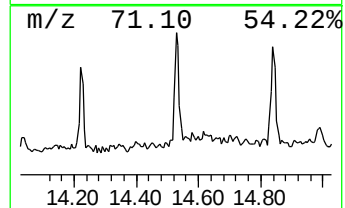
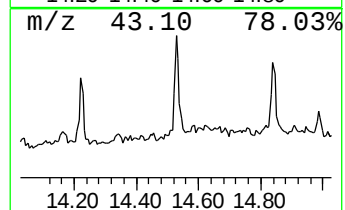
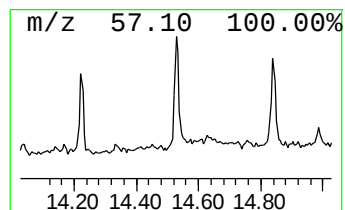
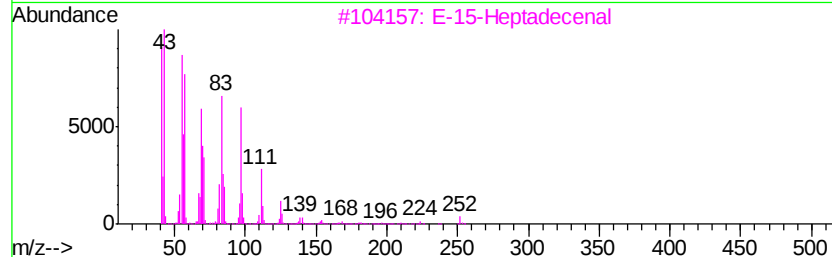
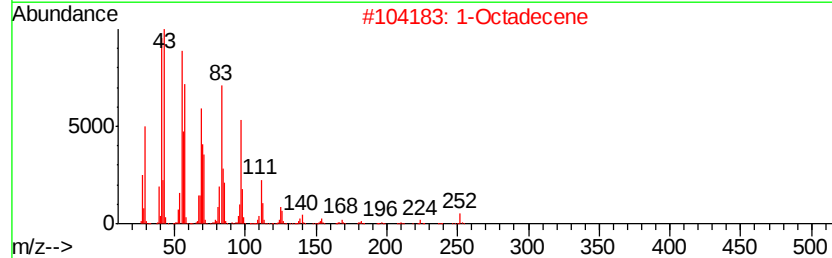
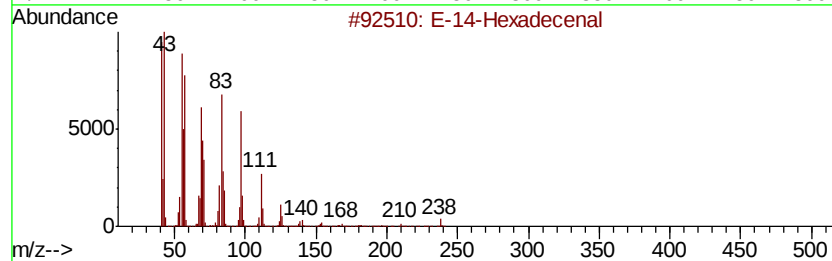
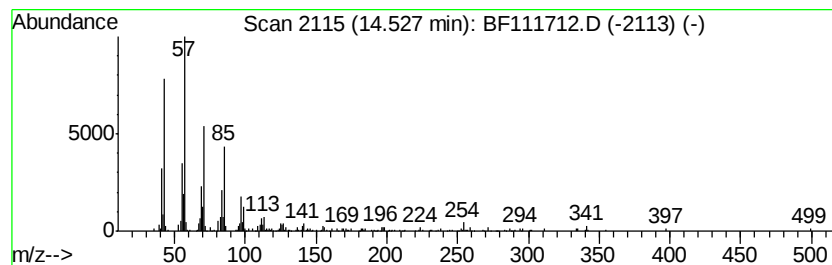
Instrument :
BNA_F
ClientSampleId :
SSSI-1218-S-DH-9-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 E-14-Hexadecenal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.80 ng	191882	Chrysene-d12	14.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	E-14-Hexadecenal	238 C16H30O	330207-53-9	94
2	1-Octadecene	252 C18H36	000112-88-9	94
3	E-15-Heptadecenal	252 C17H32O	1000130-97-9	94
4	Heptadecane	240 C17H36	000629-78-7	93
5	Octadecane	254 C18H38	000593-45-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111712.D
Acq On : 26 Dec 2018 13:29
Operator : JU/SJ
Sample : J6498-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

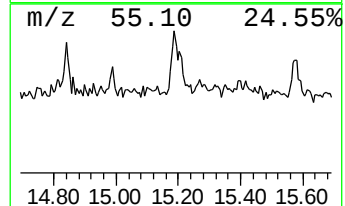
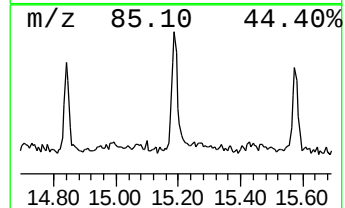
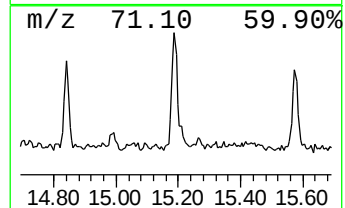
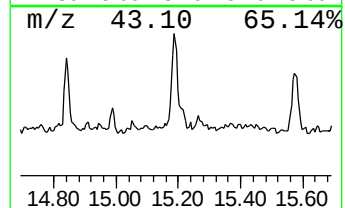
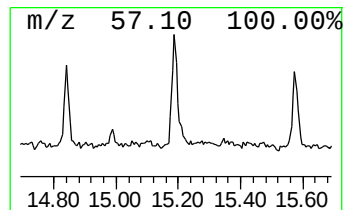
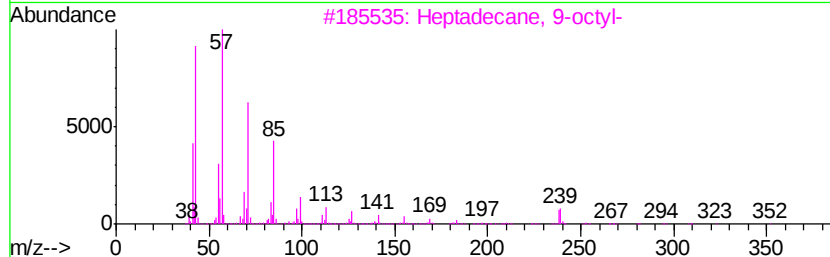
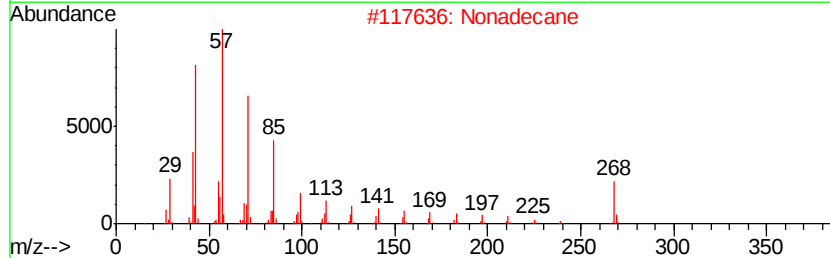
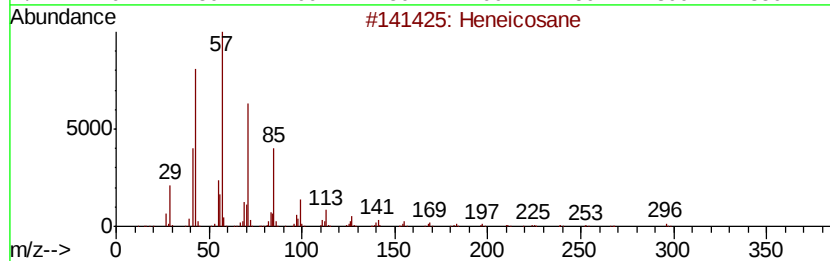
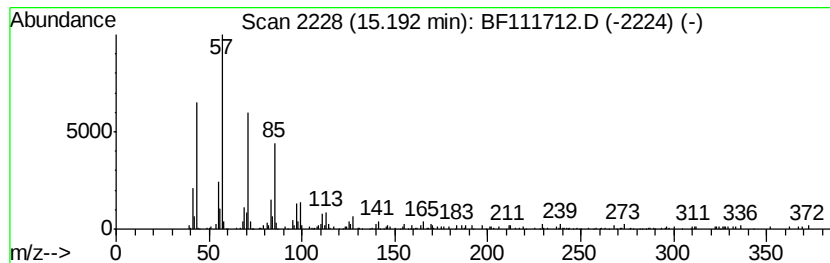
Instrument :
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ClientSampleId :
SSSI-1218-S-DH-9-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.19	3.61 ng	201072	Perylene-d12	15.54	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Nonadecane	268	C19H40	000629-92-5	93
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
 Data File : BF111712.D
 Acq On : 26 Dec 2018 13:29
 Operator : JU/SJ
 Sample : J6498-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1218-S-DH-9-T

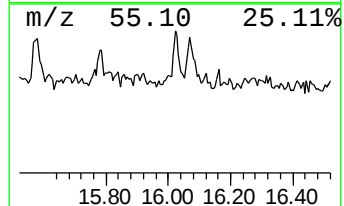
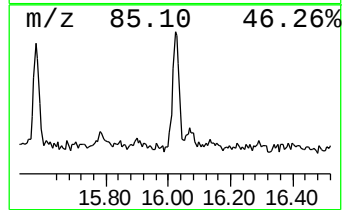
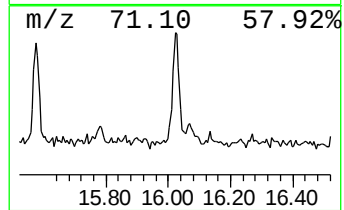
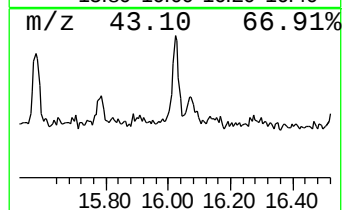
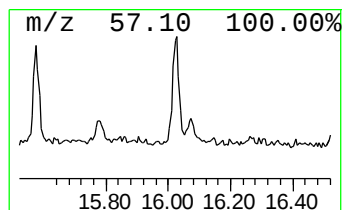
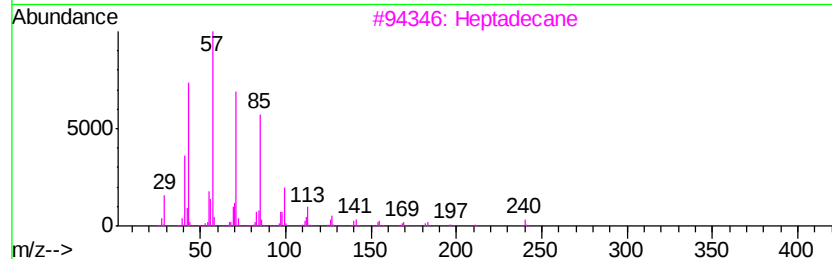
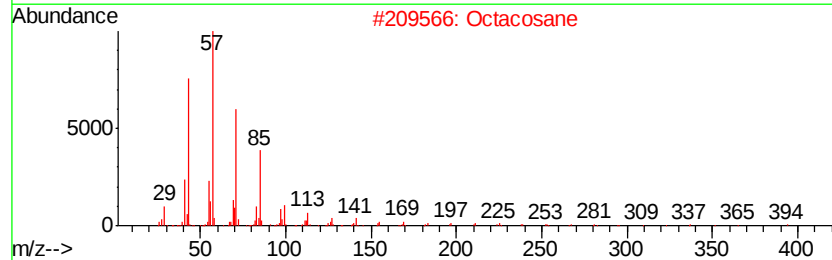
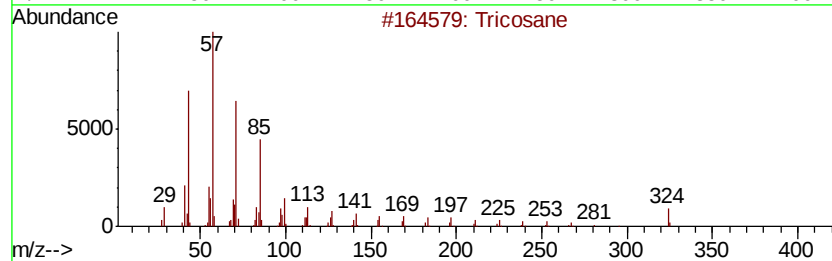
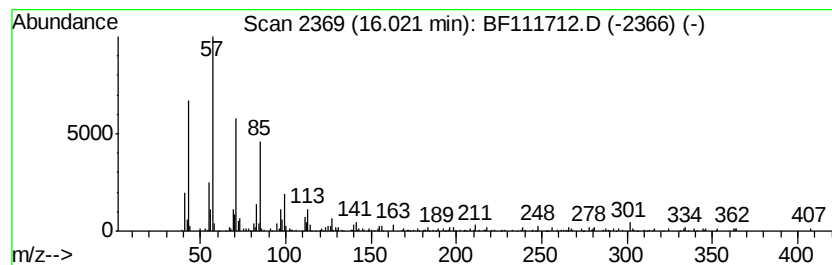
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.59 ng	144182	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane		324	C23H48	000638-67-5	90
2	Octacosane		394	C28H58	000630-02-4	90
3	Heptadecane		240	C17H36	000629-78-7	87
4	Tetradecane, 2,6,10-trimethyl-		240	C17H36	014905-56-7	87
5	Hentriacontane		437	C31H64	000630-04-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122618\
Data File : BF111712.D
Acq On : 26 Dec 2018 13:29
Operator : JU/SJ
Sample : J6498-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SSSI-1218-S-DH-9-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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...	5.12	4.6 ng		245976	1	6.90	1078640	20.0
unknown6.67	6.67	75.5 ng		4073410	1	6.90	1078640	20.0
n-Hexadecanoic acid	11.95	2.4 ng		181892	4	11.42	1513050	20.0
9-Octadecenamide, ...	13.48	3.7 ng		254703	5	14.06	1372330	20.0
5-Eicosene, (E)-	13.90	5.4 ng		368697	5	14.06	1372330	20.0
E-14-Hexadecenal	14.53	2.8 ng		191882	5	14.06	1372330	20.0
Heneicosane	15.19	3.6 ng		201072	6	15.54	1114980	20.0
Tricosane	16.02	2.6 ng		144182	6	15.54	1114980	20.0