

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112018\
 Data File : BF110918.D
 Acq On : 21 Nov 2018 3:30
 Operator : JU/SJ
 Sample : J5996-18
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NON-UST-06-A

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-BF110818.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	2.240	21	26	42	rVB	91554	144270	7.75%	0.957%
2	5.187	523	527	541	rBV	48460	81667	4.39%	0.542%
3	5.563	587	591	615	rBV	1538140	1729184	92.88%	11.471%
4	6.575	758	763	782	rBV	1517702	1861660	100.00%	12.350%
5	6.710	782	786	790	rBV	1894751	1788277	96.06%	11.863%
6	6.939	822	825	832	rBV	381852	341091	18.32%	2.263%
7	7.098	848	852	874	rBV	1504398	1392174	74.78%	9.235%
8	7.510	918	922	945	rBV	1041717	1108514	59.54%	7.354%
9	8.222	1040	1043	1058	rBV	326873	417108	22.41%	2.767%
10	9.298	1222	1226	1241	rBV	1898383	1844001	99.05%	12.233%
11	9.692	1287	1293	1303	rVB	115205	132285	7.11%	0.878%
12	9.980	1339	1342	1354	rBV	380818	388640	20.88%	2.578%
13	10.775	1474	1477	1489	rBV	743428	863945	46.41%	5.731%
14	10.874	1491	1494	1502	rVB	31204	35204	1.89%	0.234%
15	11.480	1593	1597	1608	rBV	312150	330846	17.77%	2.195%
16	11.980	1679	1682	1687	rBV	73226	75228	4.04%	0.499%
17	13.063	1861	1866	1869	rBV	1504366	1422034	76.39%	9.433%
18	13.933	2010	2014	2027	rBV	136291	176736	9.49%	1.172%
19	14.133	2044	2048	2058	rBV	313090	322984	17.35%	2.143%
20	14.251	2064	2068	2073	rBV	20961	23776	1.28%	0.158%
21	14.557	2116	2120	2124	rBV	31292	40821	2.19%	0.271%
22	14.868	2169	2173	2177	rBV	51880	50763	2.73%	0.337%
23	15.221	2229	2233	2239	rBV	50495	60087	3.23%	0.399%
24	15.462	2268	2274	2283	rBV8	9164	25585	1.37%	0.170%
25	15.615	2296	2300	2304	rBV	45715	62678	3.37%	0.416%
26	15.668	2304	2309	2321	rVB2	136958	232858	12.51%	1.545%
27	16.062	2372	2376	2382	rBV2	34633	57390	3.08%	0.381%
28	16.133	2382	2388	2395	rVV8	12773	29623	1.59%	0.197%
29	16.592	2461	2466	2470	rBV3	21716	35151	1.89%	0.233%

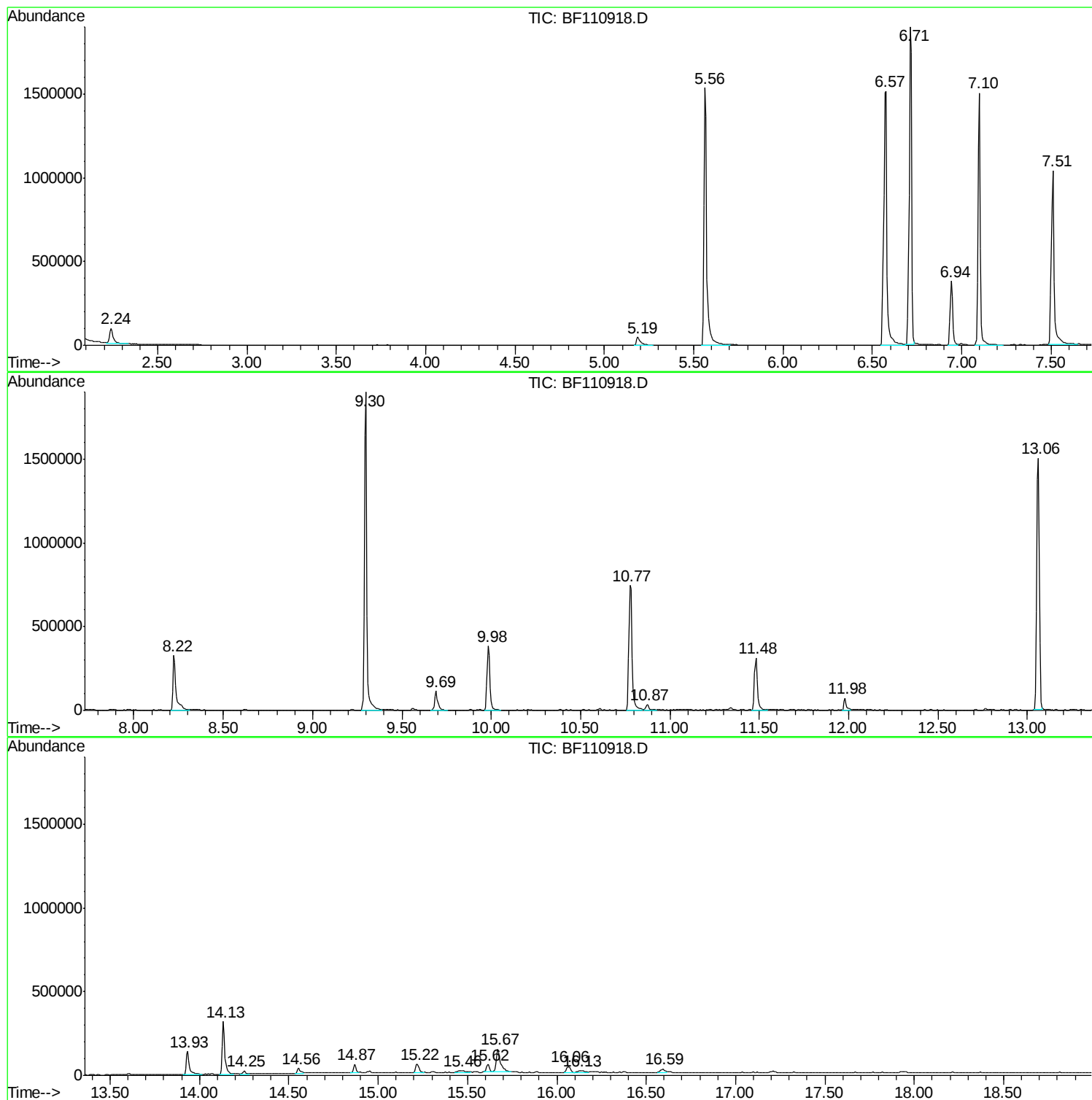
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ALS Vial : 32 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110818.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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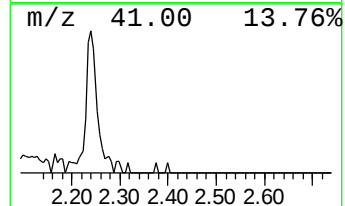
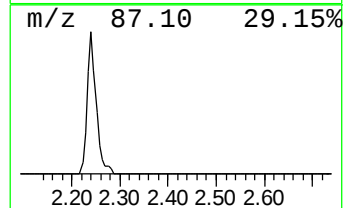
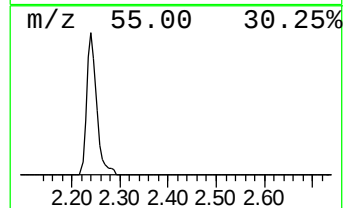
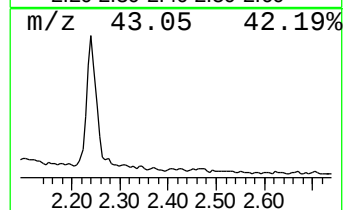
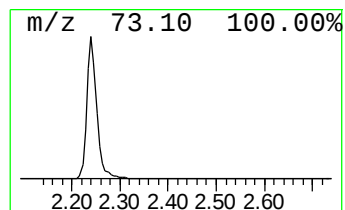
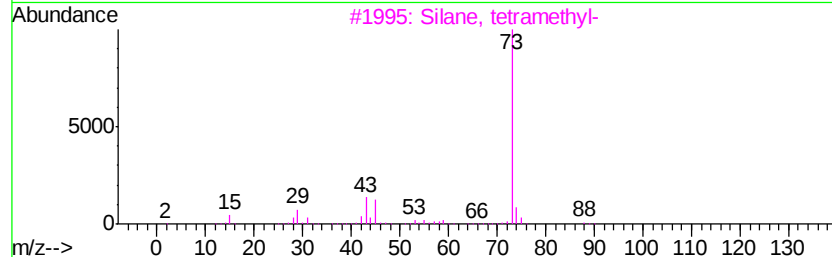
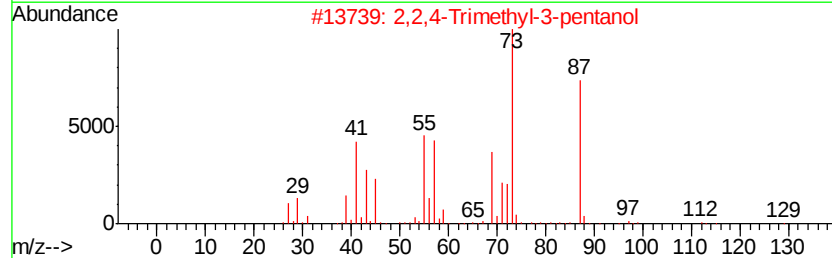
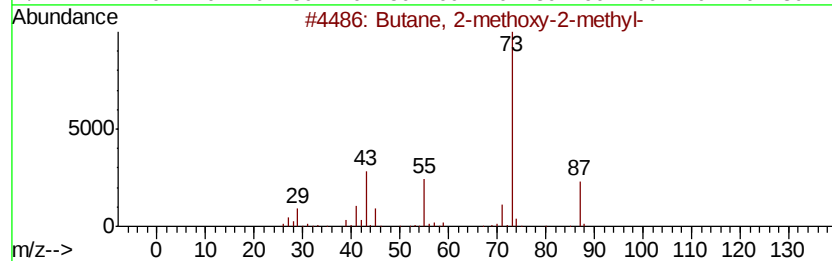
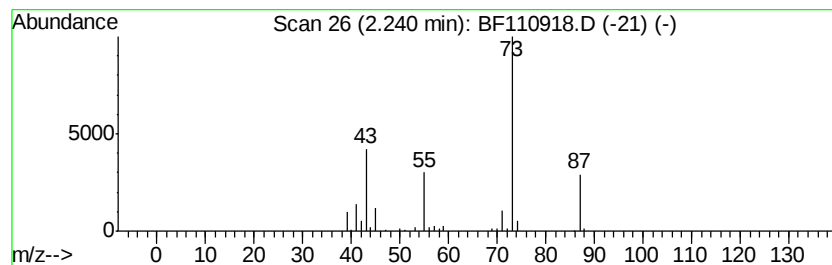
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	8.46 ng	144270	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23



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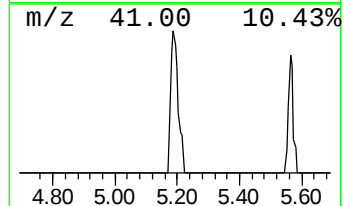
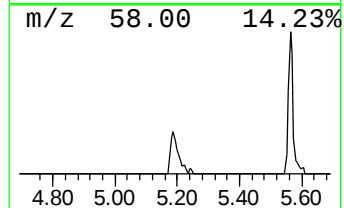
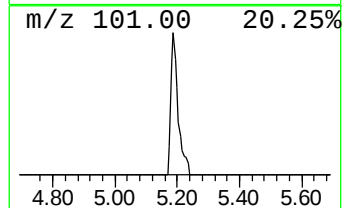
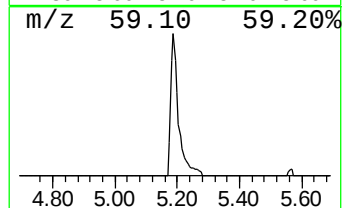
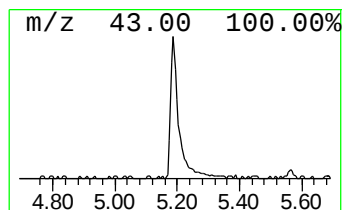
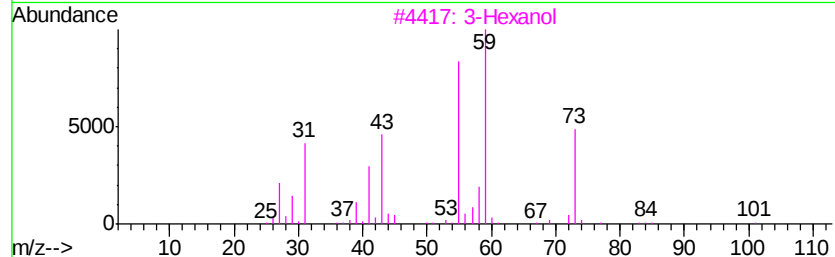
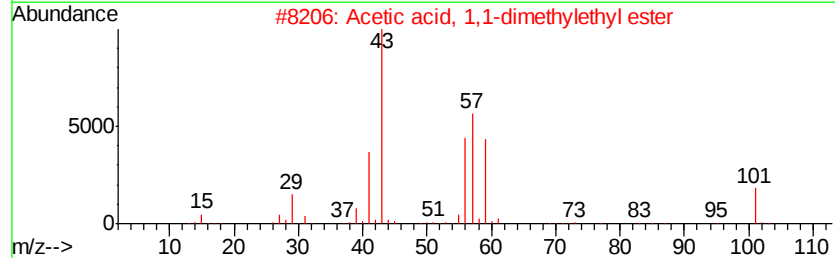
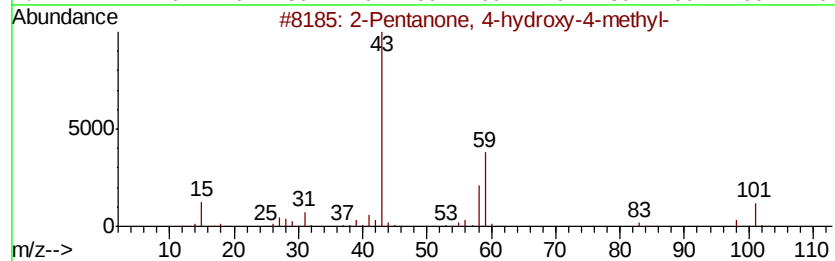
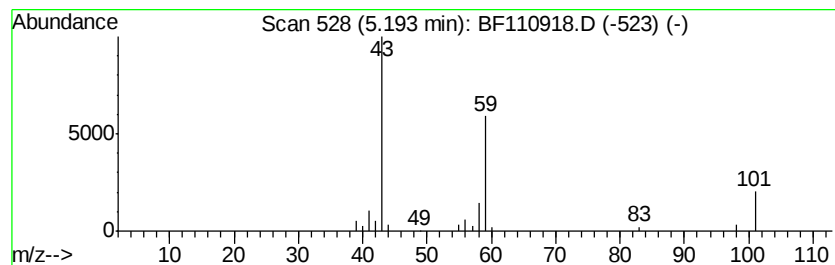
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	4.79 ng	81667	1,4-Dichlorobenzene-d4	6.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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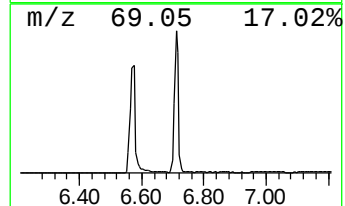
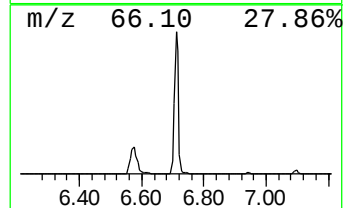
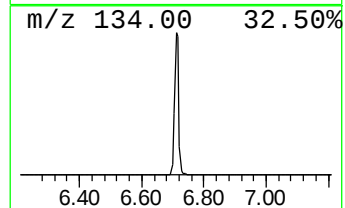
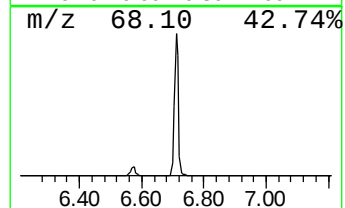
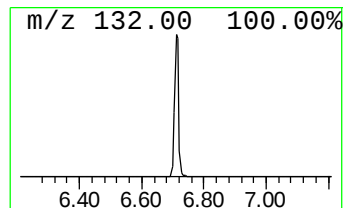
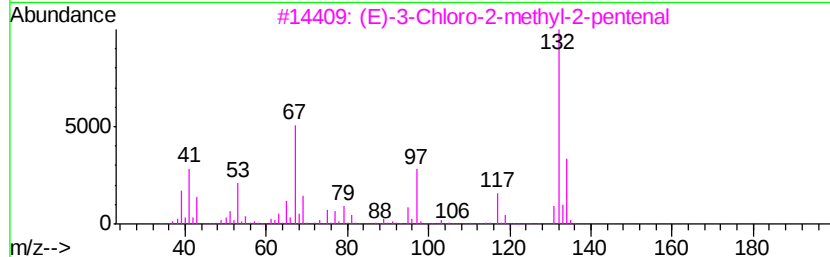
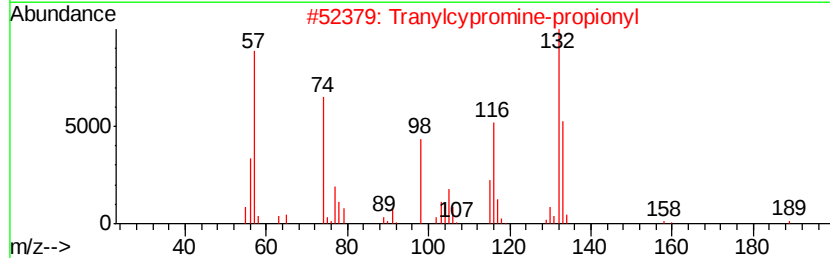
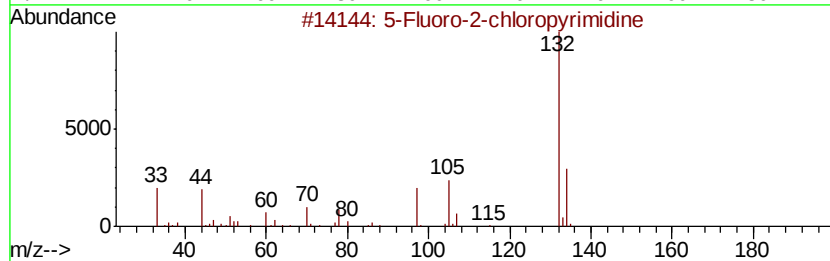
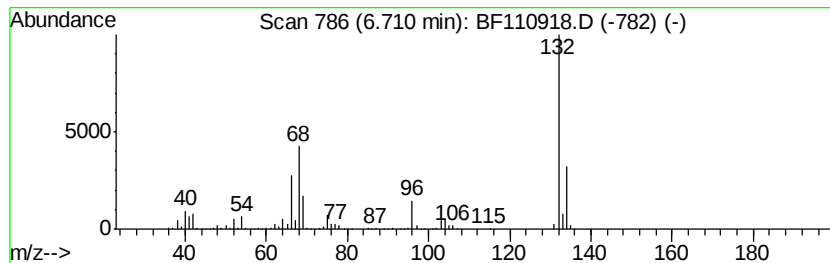
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Peak Number 3 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	104.86 ng	1788280	1,4-Dichlorobenzene-d4	6.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	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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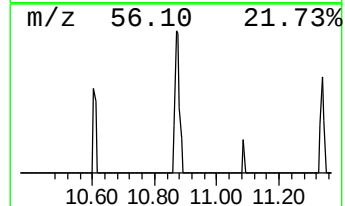
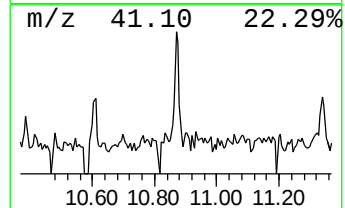
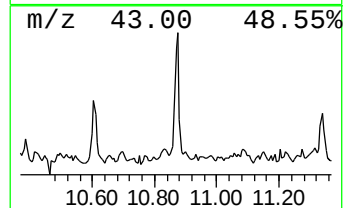
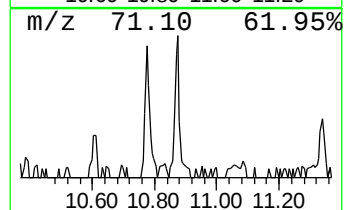
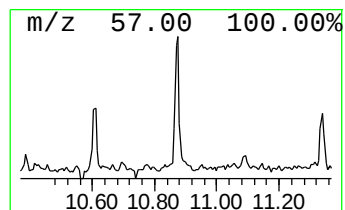
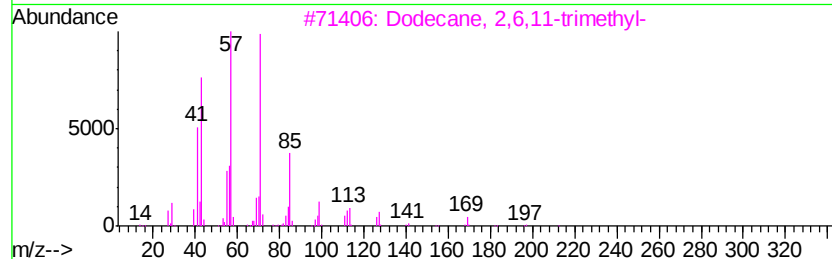
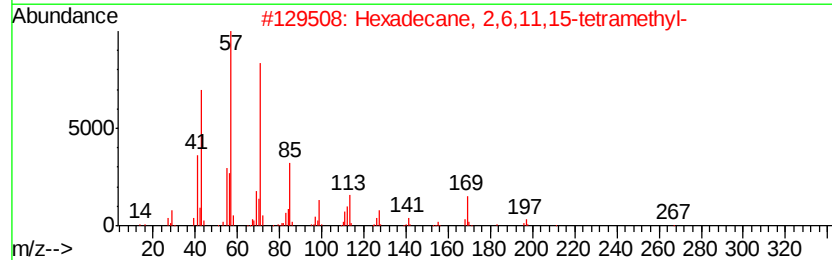
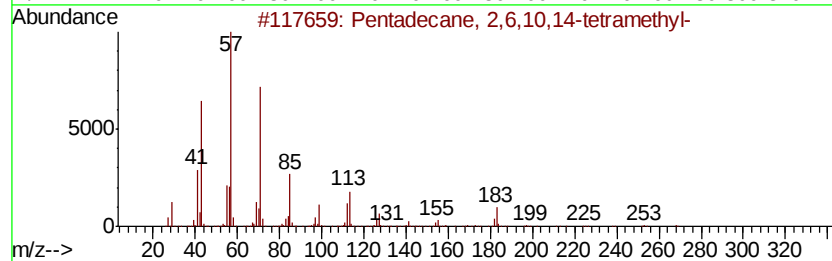
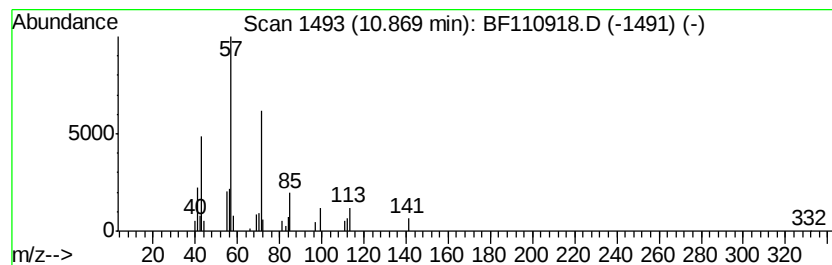
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Peak Number 5 Pentadecane, 2,6,10,14-tetr... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	2.13 ng	35204	Phenanthrene-d10	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	90
2		Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	87
3		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
4		Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	83
5		Tridecane, 5-propyl-	226	C16H34	055045-11-9	78



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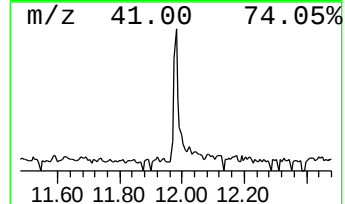
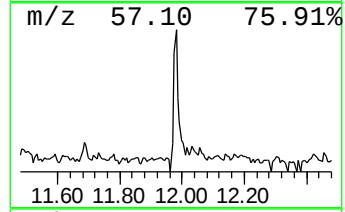
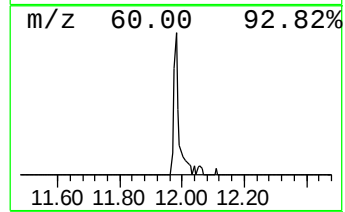
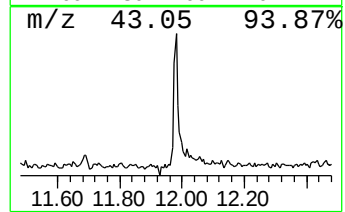
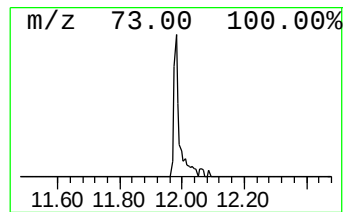
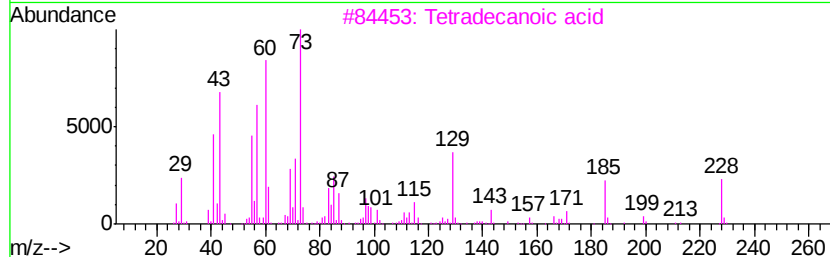
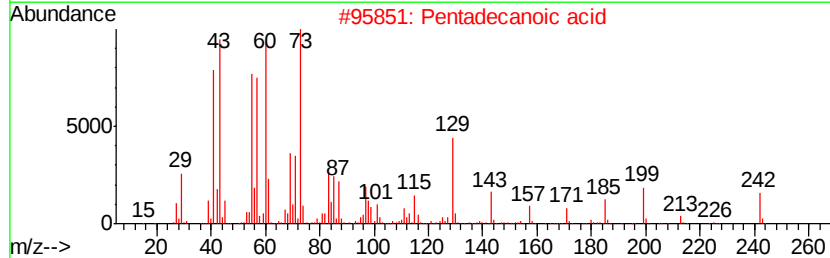
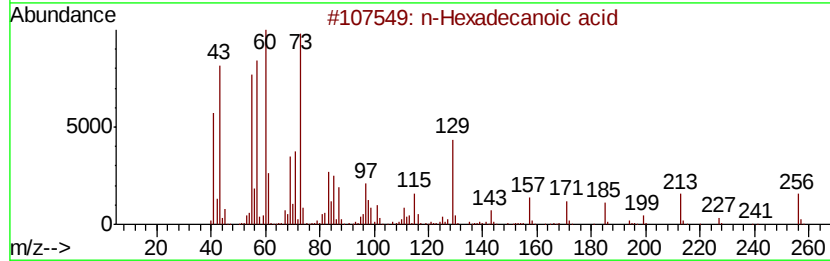
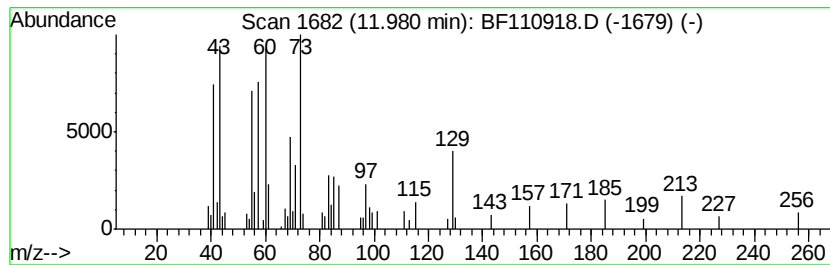
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.98	4.55 ng	75228	Phenanthrene-d10	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



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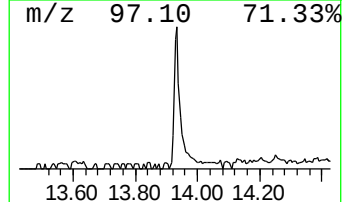
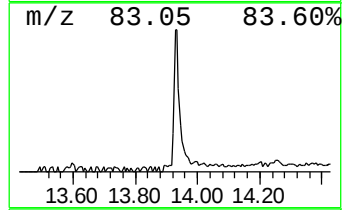
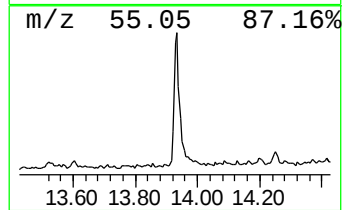
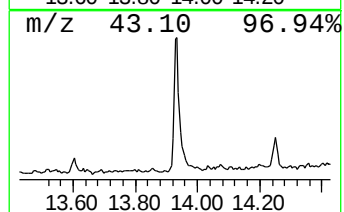
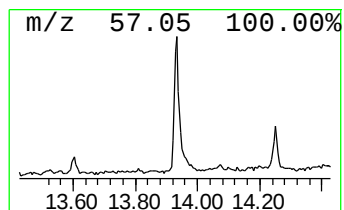
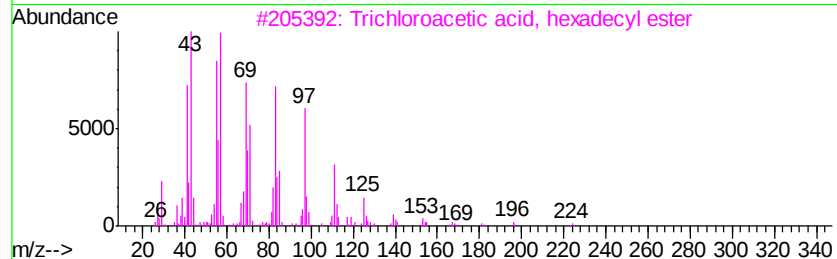
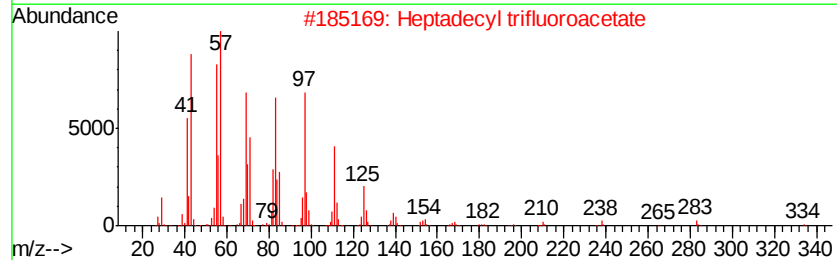
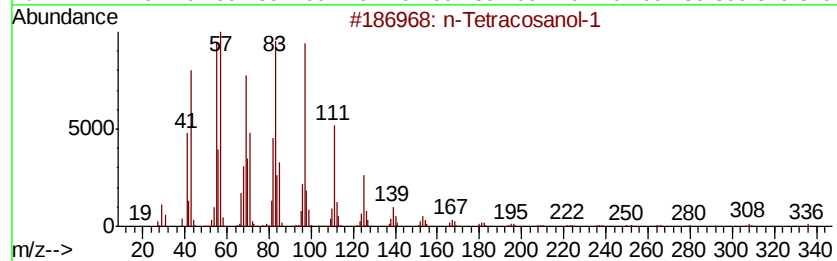
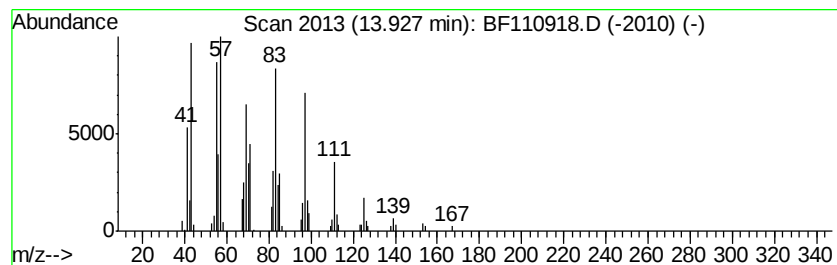
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	10.94 ng	176736	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5		1-Docosene	308	C22H44	001599-67-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112018\
Data File : BF110918.D
Acq On : 21 Nov 2018 3:30
Operator : JU/SJ
Sample : J5996-18
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NON-UST-06-A

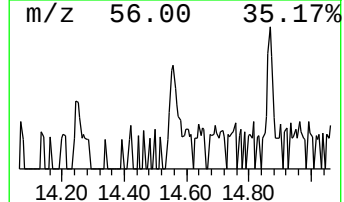
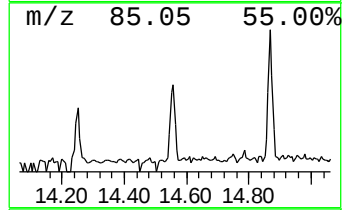
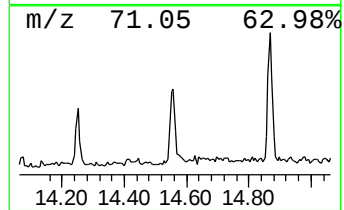
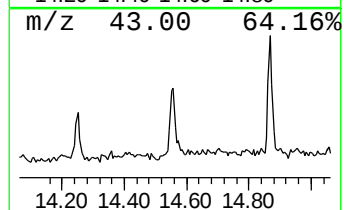
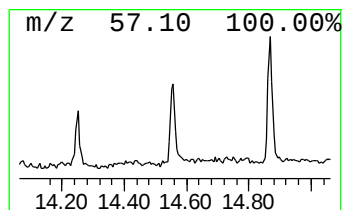
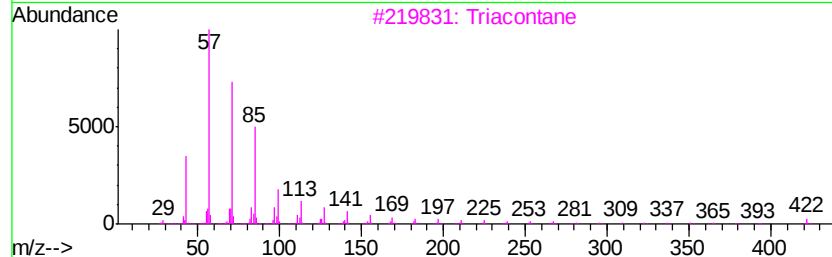
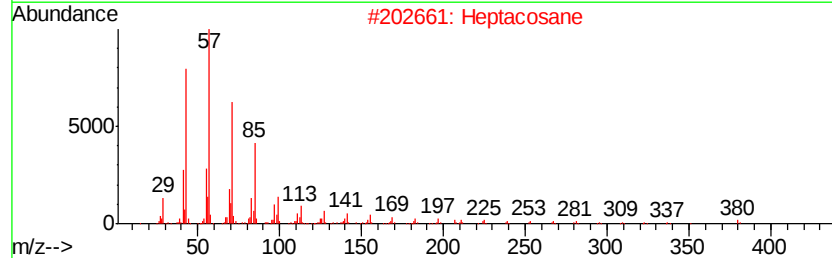
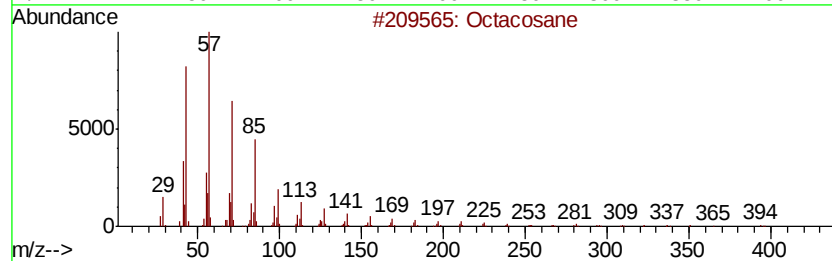
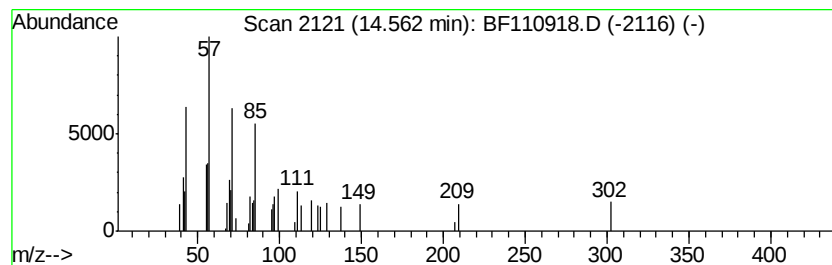
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.53 ng	40821	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Heptacosane	380	C27H56	000593-49-7	87
3		triacontane	422	C30H62	000638-68-6	86
4		Hentriacontane	437	C31H64	000630-04-6	86
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112018\
Data File : BF110918.D
Acq On : 21 Nov 2018 3:30
Operator : JU/SJ
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ClientSampleId :
NON-UST-06-A

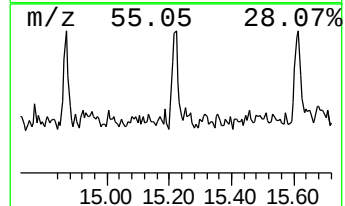
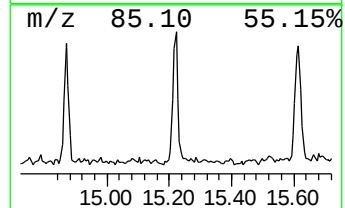
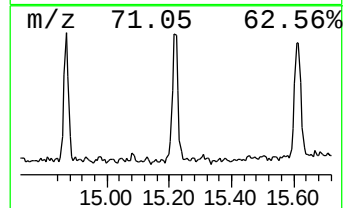
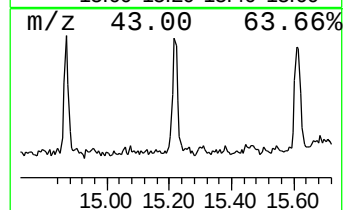
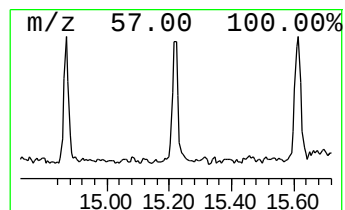
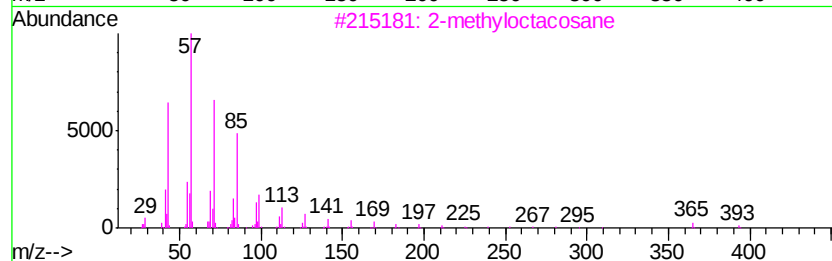
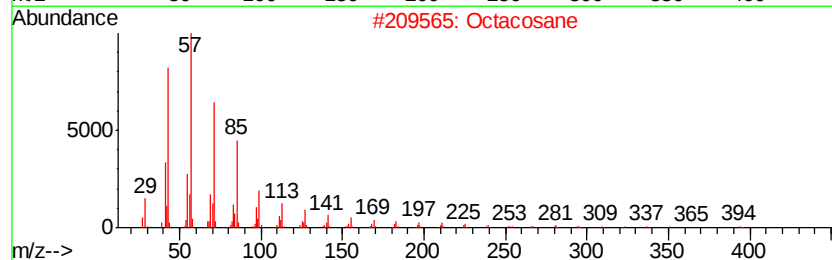
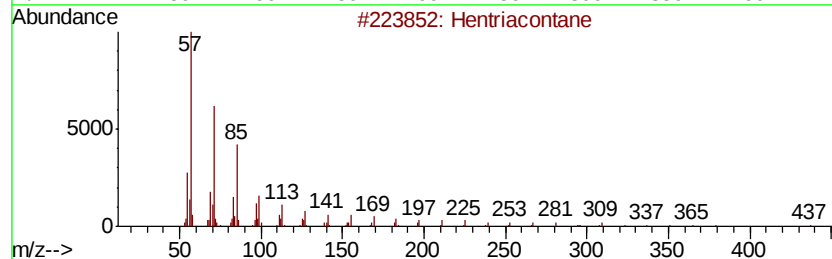
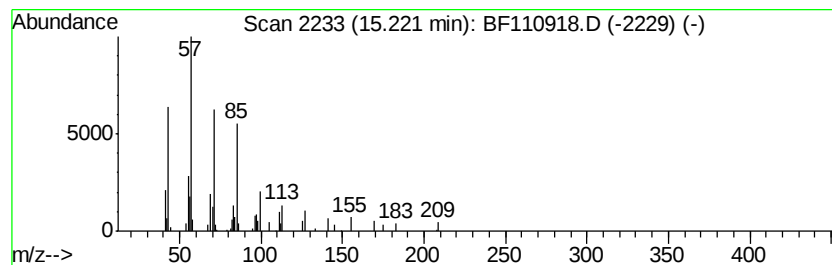
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	5.16 ng	60087	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	90
2		Octacosane	394	C28H58	000630-02-4	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Tetratetracontane	619	C44H90	007098-22-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112018\
Data File : BF110918.D
Acq On : 21 Nov 2018 3:30
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ClientSampleId :
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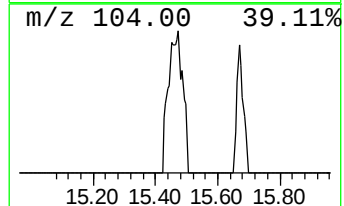
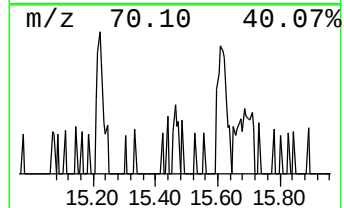
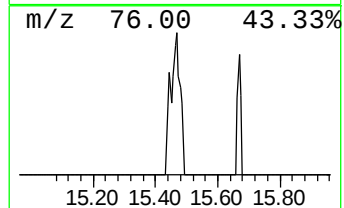
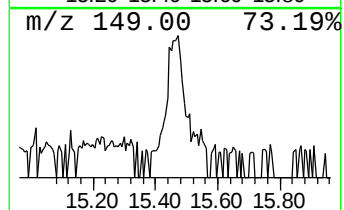
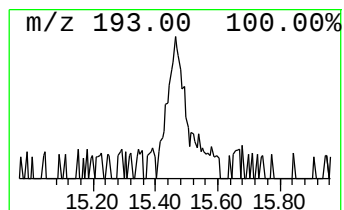
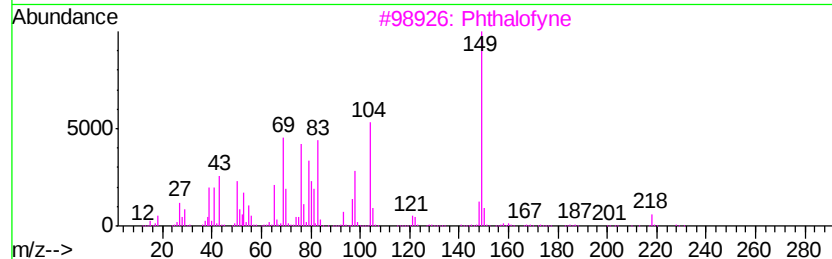
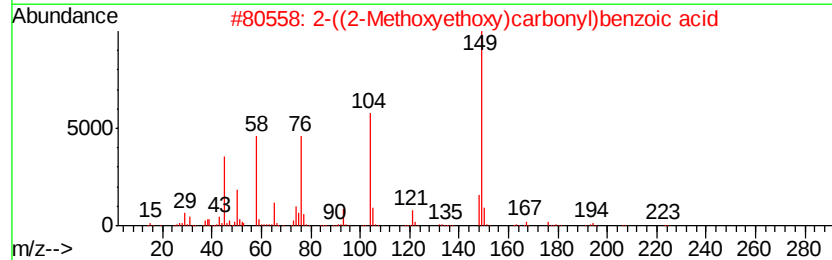
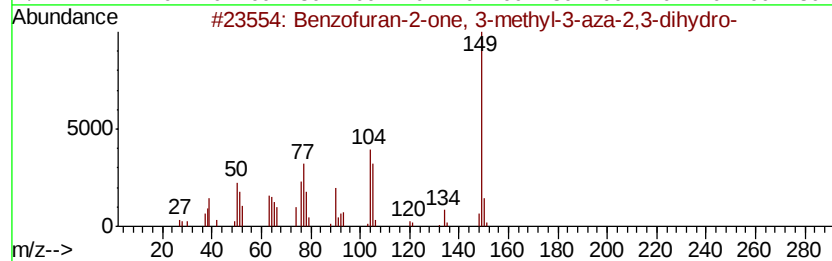
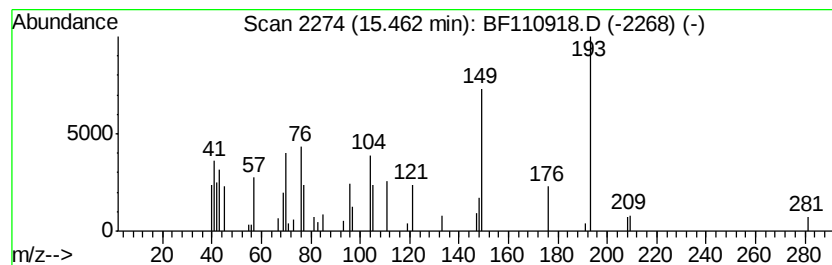
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.46 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	2.20 ng	25585	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzofuran-2-one, 3-methyl-3-aza...	149	C8H7N02	1000289-12-2	25
2		2-((2-Methoxyethoxy)carbonyl)ben...	224	C11H12O5	1000373-52-0	17
3		Phthalofyne	246	C14H14O4	000131-67-9	17
4		2-Hydroxy-1-isoindolinone	149	C8H7N02	1000289-12-0	14
5		3-Amino-2,3-dihydrobenzoic acid,...	250	C14H22N2O2	1000375-81-8	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112018\
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Acq On : 21 Nov 2018 3:30
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Misc :
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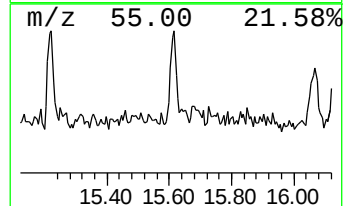
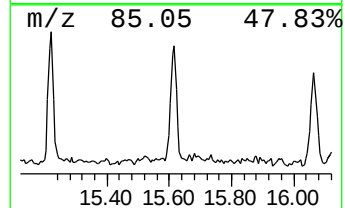
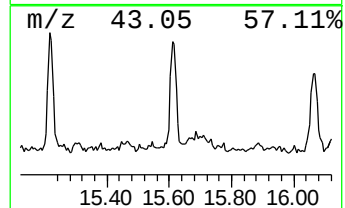
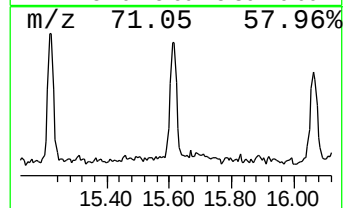
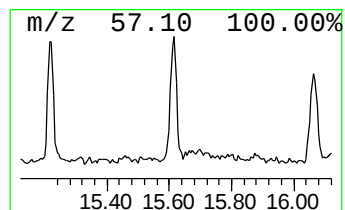
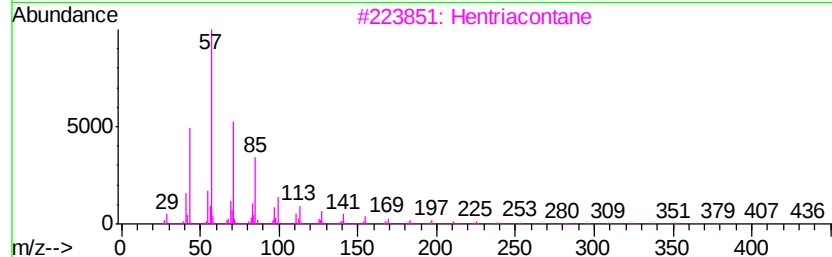
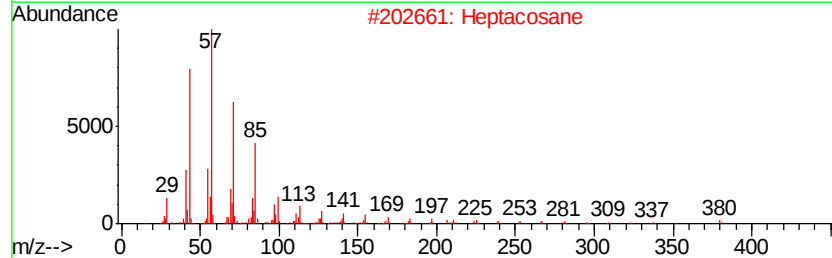
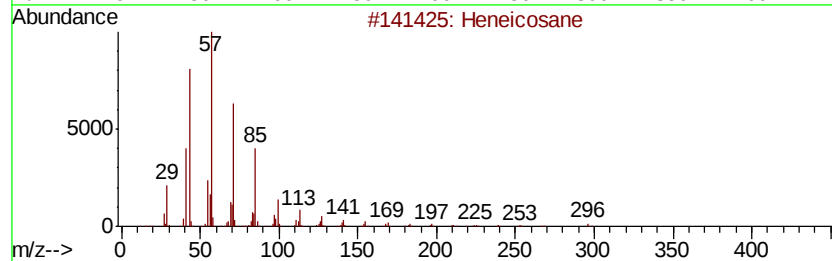
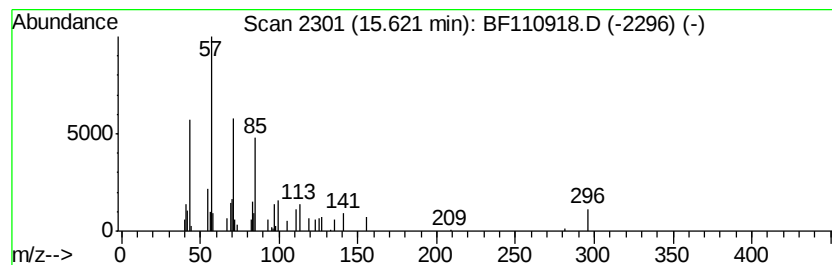
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	5.38 ng	62678	Perylene-d12	15.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	93
2	Heptacosane		380	C27H56	000593-49-7	87
3	Hentriacontane		437	C31H64	000630-04-6	87
4	Eicosane		282	C20H42	000112-95-8	86
5	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112018\
Data File : BF110918.D
Acq On : 21 Nov 2018 3:30
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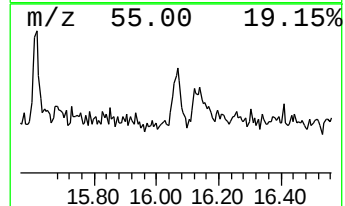
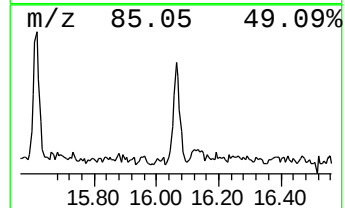
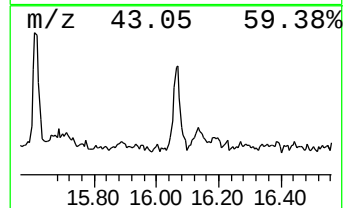
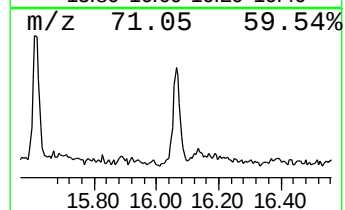
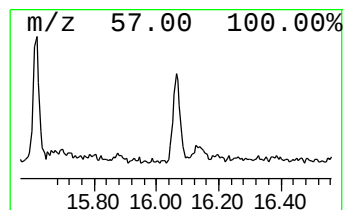
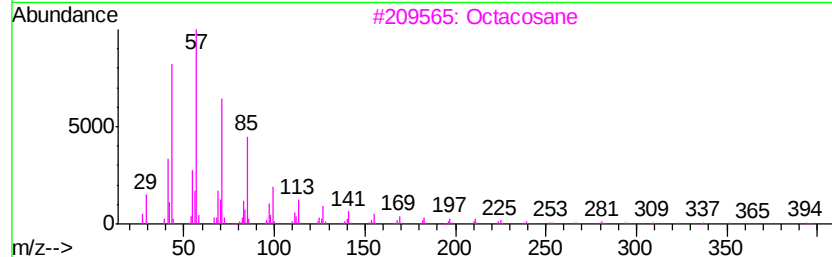
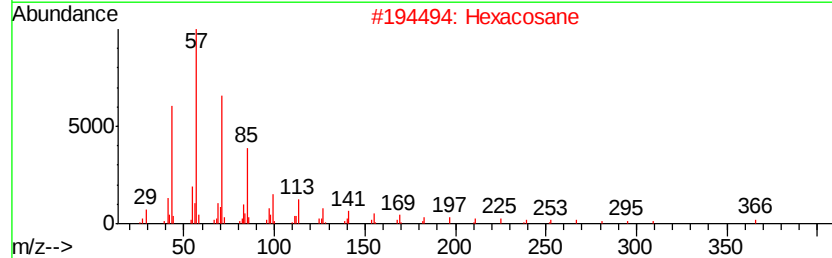
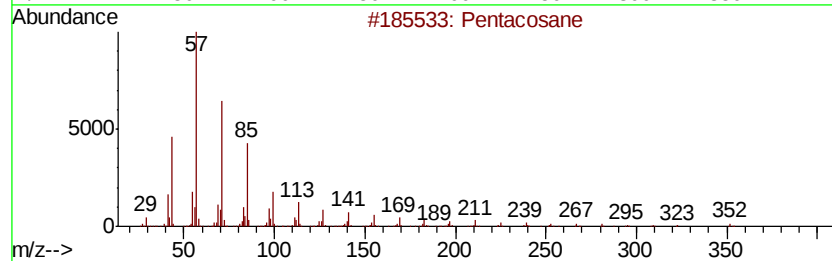
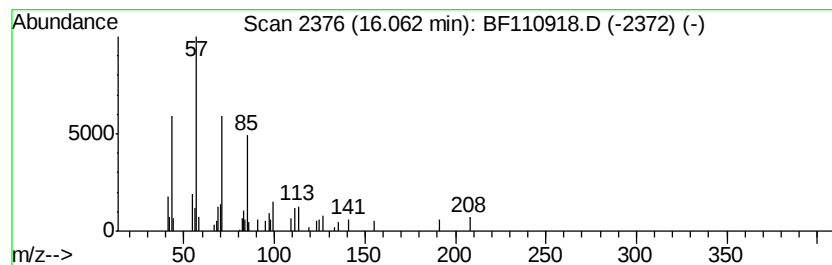
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	4.93 ng	57390	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	87
2		Hexacosane	366	C26H54	000630-01-3	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Hentriacontane	437	C31H64	000630-04-6	86
5		Triacontane	422	C30H62	000638-68-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112018\
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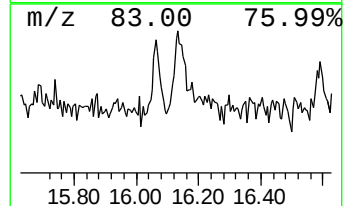
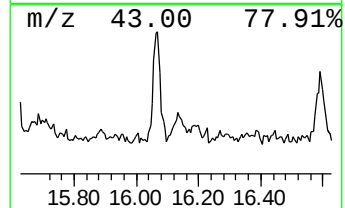
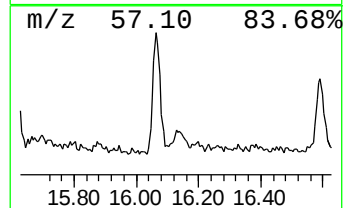
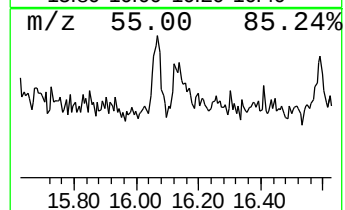
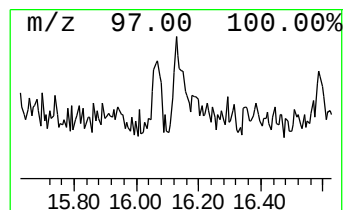
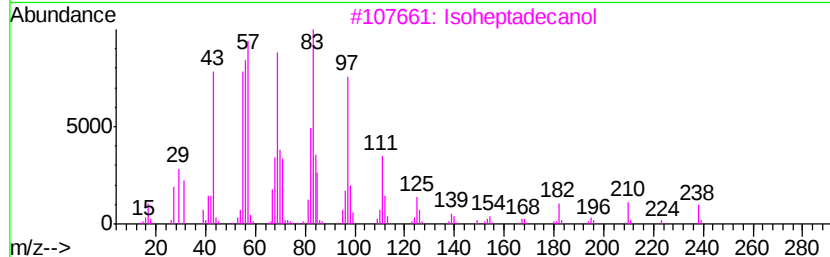
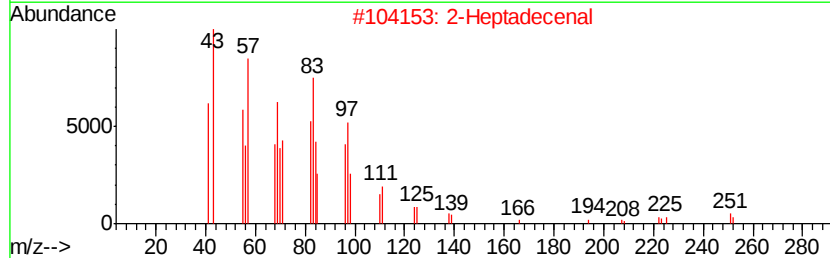
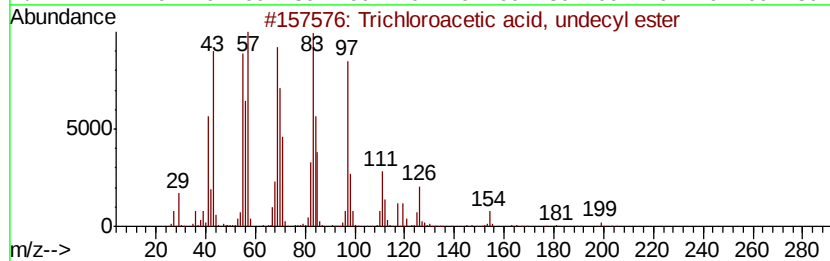
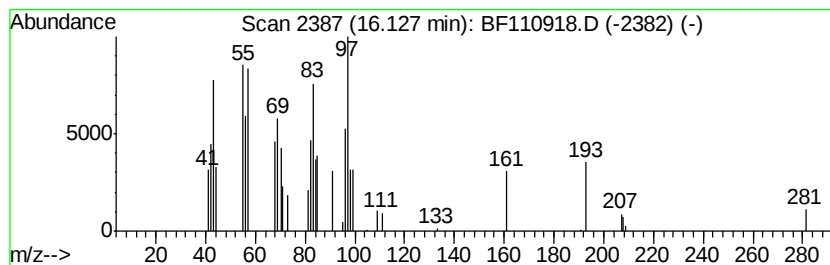
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Trichloroacetic acid, undec... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.54 ng	29623	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	52
2			2-Heptadecenal	252	C17H32O	1000143-48-6	49
3			Isoheptadecanol	256	C17H36O	057289-07-3	47
4			Formic acid, undecyl ester	200	C12H24O2	1000368-25-0	46
5			Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112018\
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ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NON-UST-06-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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
Butane, 2-methoxy...	2.24	8.5	ng	144270	1	6.94	341091	20.0
2-Pentanone, 4-hy...	5.19	4.8	ng	81667	1	6.94	341091	20.0
unknown6.71	6.71	104.9	ng	1788280	1	6.94	341091	20.0
Pentadecane, 2,6,...	10.87	2.1	ng	35204	4	11.48	330846	20.0
n-Hexadecanoic acid	11.98	4.5	ng	75228	4	11.48	330846	20.0
n-Tetracosanol-1	13.93	10.9	ng	176736	5	14.13	322984	20.0
Octacosane	14.56	2.5	ng	40821	5	14.13	322984	20.0
Hentriacontane	15.22	5.2	ng	60087	6	15.67	232858	20.0
unknown15.46	15.46	2.2	ng	25585	6	15.67	232858	20.0
Heneicosane	15.62	5.4	ng	62678	6	15.67	232858	20.0
Pentacosane	16.06	4.9	ng	57390	6	15.67	232858	20.0
Trichloroacetic a...	16.13	2.5	ng	29623	6	15.67	232858	20.0