

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032619\
 Data File : BF113302.D
 Acq On : 26 Mar 2019 20:25
 Operator : JU/SJ
 Sample : K2081-16
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4C(6-18)COMP

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-BF032519.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	23	26	40	rVB2	43795	103278	1.92%	0.229%
2	5.328	546	551	554	rBV	4249197	4561634	84.69%	10.099%
3	6.357	720	726	742	rBV	3987860	4893289	90.84%	10.834%
4	6.481	742	747	750	rBV	4346947	4682571	86.93%	10.367%
5	6.698	781	784	794	rVB	1042510	950614	17.65%	2.105%
6	6.857	807	811	815	rBV	3775384	3788474	70.33%	8.388%
7	7.263	875	880	894	rBV	2875085	3386067	62.86%	7.497%
8	7.392	898	902	915	rVV3	39435	111364	2.07%	0.247%
9	7.981	998	1002	1019	rBV	1303442	1261174	23.41%	2.792%
10	9.063	1180	1186	1189	rBV	5045312	5386432	100.00%	11.926%
11	9.451	1248	1252	1257	rBV	292613	262945	4.88%	0.582%
12	9.733	1295	1300	1308	rBV	1416719	1385444	25.72%	3.067%
13	10.516	1429	1433	1447	rBV	2477536	2633385	48.89%	5.830%
14	11.210	1547	1551	1562	rVB	1425473	1399135	25.98%	3.098%
15	11.751	1633	1643	1654	rBV	663196	1049749	19.49%	2.324%
16	12.010	1684	1687	1691	rVB2	54376	59194	1.10%	0.131%
17	12.527	1770	1775	1787	rBV	479275	764490	14.19%	1.693%
18	12.792	1815	1820	1823	rBV	4610131	4563158	84.72%	10.103%
19	13.022	1856	1859	1863	rBV	65948	58997	1.10%	0.131%
20	13.633	1958	1963	1967	rBV3	46079	60501	1.12%	0.134%
21	13.757	1978	1984	1993	rBV4	86717	277343	5.15%	0.614%
22	13.833	1993	1997	2005	rVB	1093106	1108496	20.58%	2.454%
23	14.010	2024	2027	2034	rVB	69426	67830	1.26%	0.150%
24	14.286	2067	2074	2076	rBV5	49015	130074	2.41%	0.288%
25	14.310	2076	2078	2084	rVB	164225	166324	3.09%	0.368%
26	14.604	2125	2128	2136	rVB	203521	198505	3.69%	0.439%
27	14.674	2136	2140	2143	rBV	108850	101706	1.89%	0.225%
28	14.916	2177	2181	2187	rBV	205469	223802	4.15%	0.495%
29	15.233	2230	2235	2239	rBV	838154	1118386	20.76%	2.476%
30	15.663	2303	2308	2313	rBV	120729	173852	3.23%	0.385%
31	16.121	2381	2386	2391	rBV	59866	100741	1.87%	0.223%
32	17.956	2693	2698	2708	rVB5	53149	138125	2.56%	0.306%

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ALS Vial : 6 Sample Multiplier: 1

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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-BF032519.M
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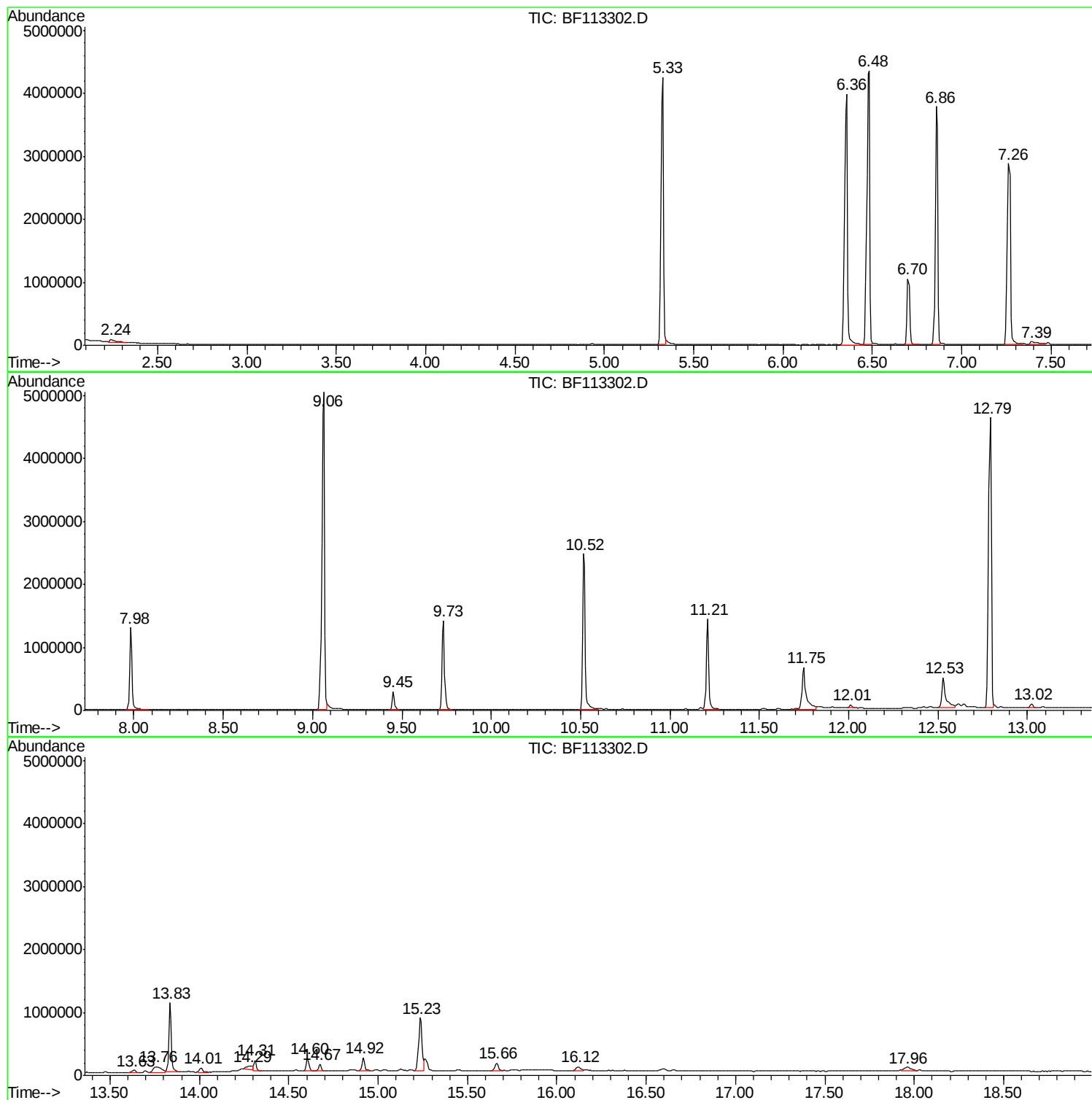
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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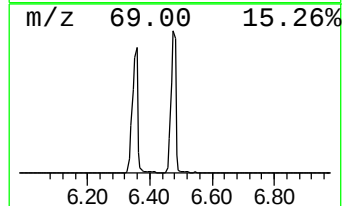
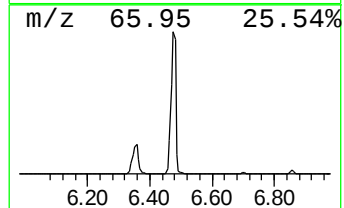
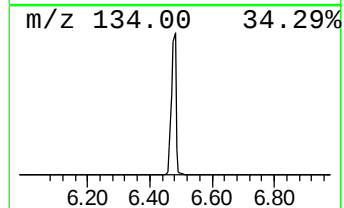
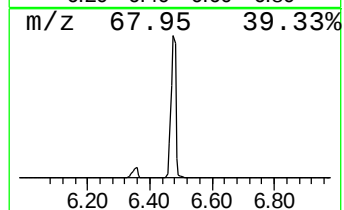
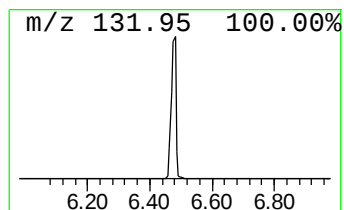
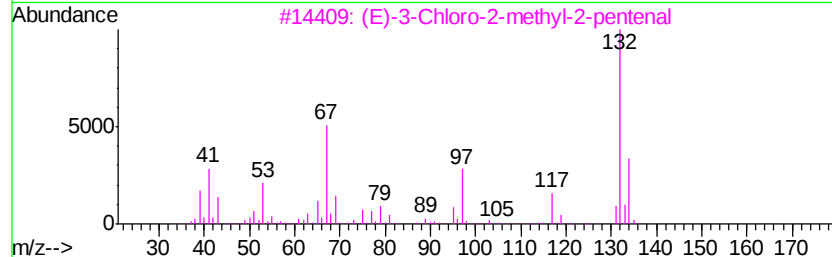
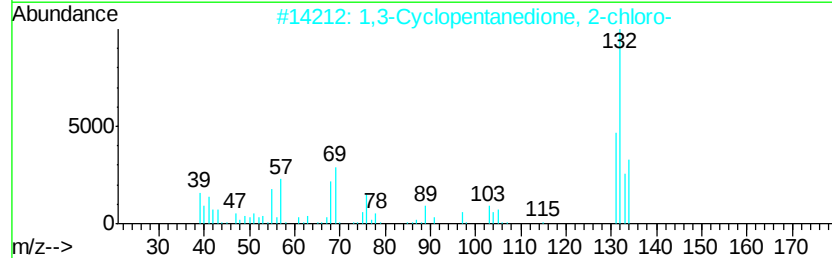
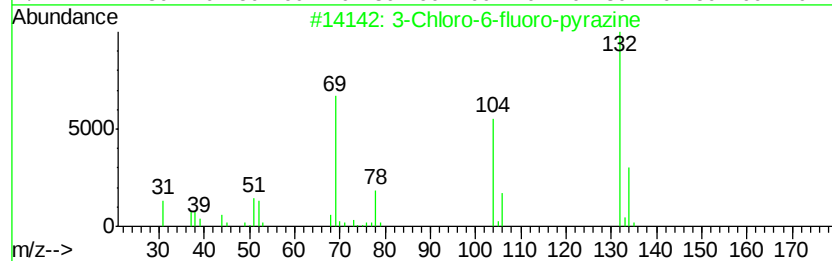
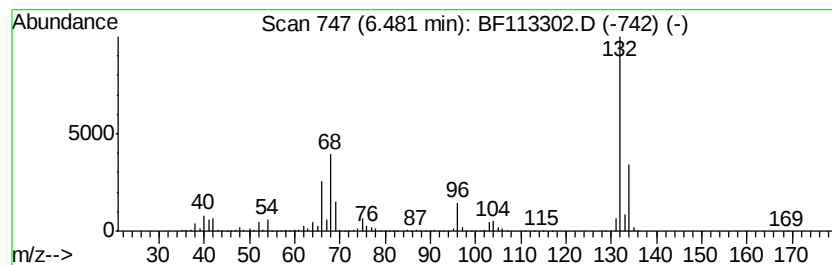
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	98.52 ng	4682570	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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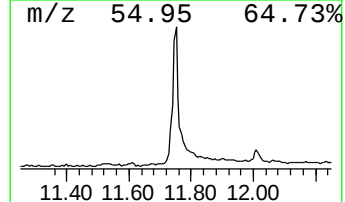
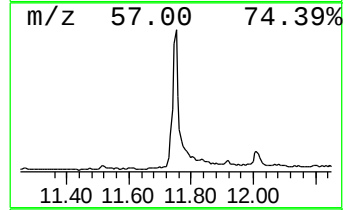
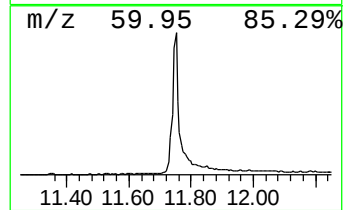
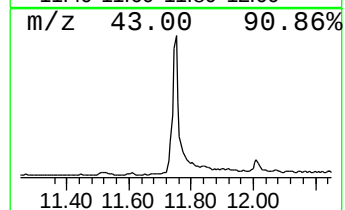
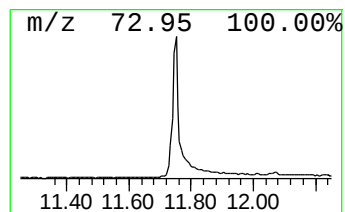
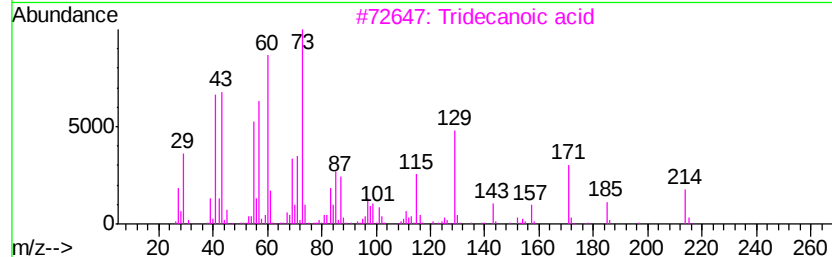
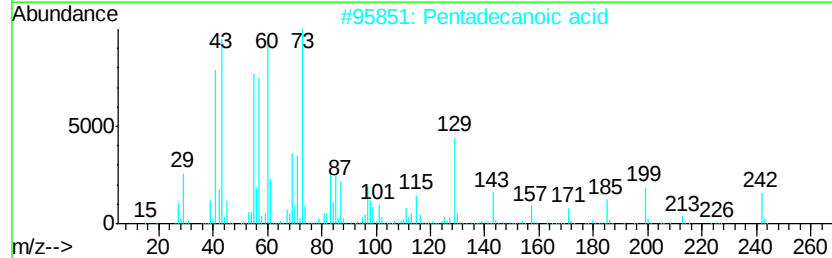
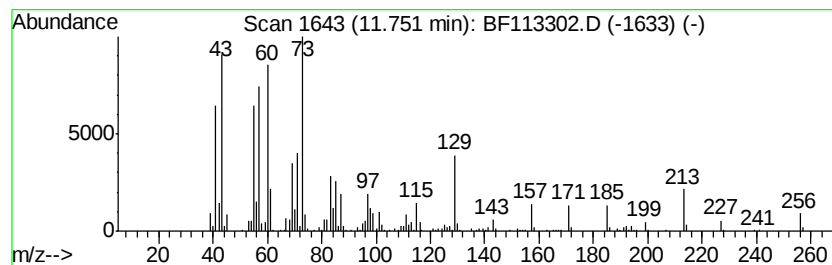
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	15.01 ng	1049750	Phenanthrene-d10	11.21

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	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	92
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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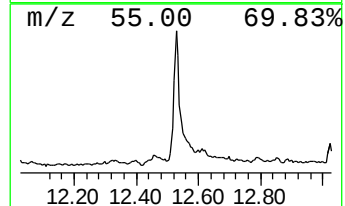
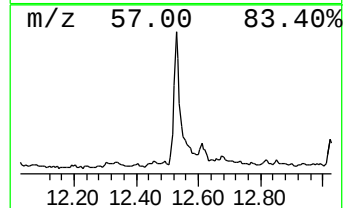
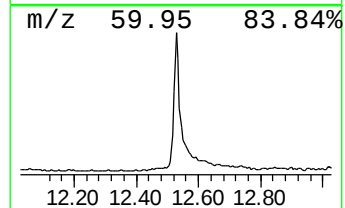
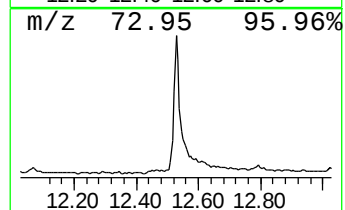
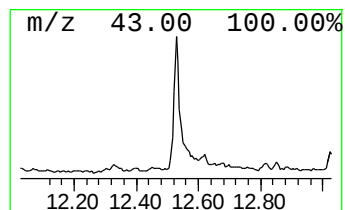
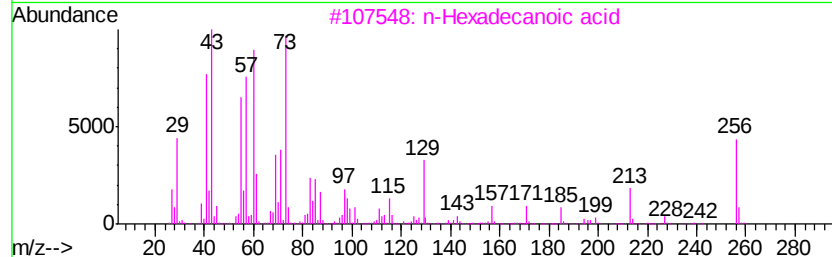
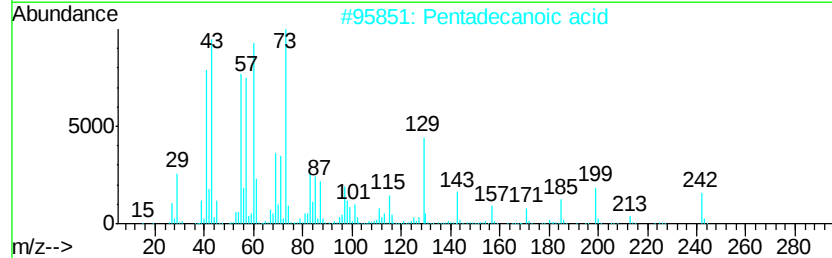
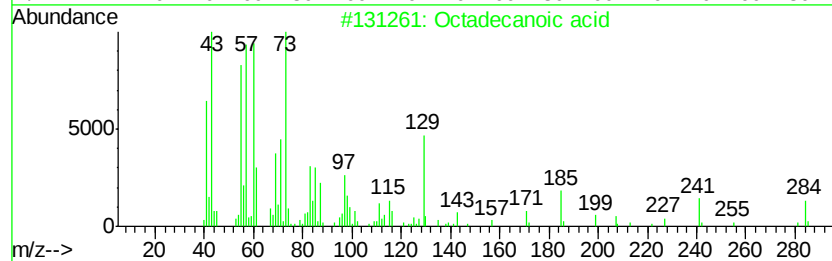
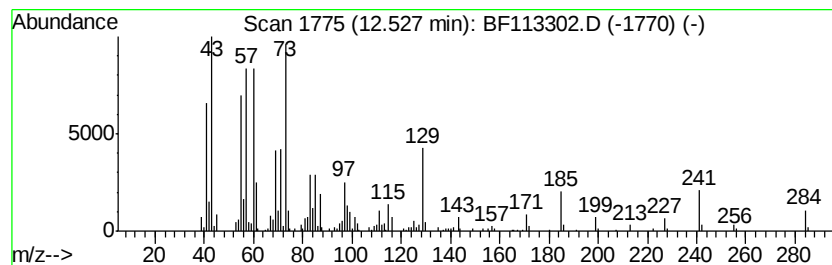
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.53	13.79 ng	764490	Chrysene-d12		13.83	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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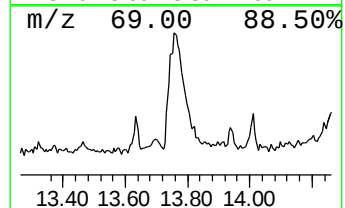
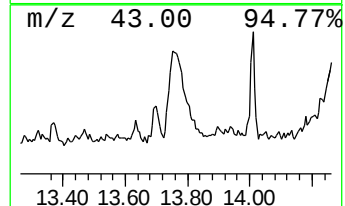
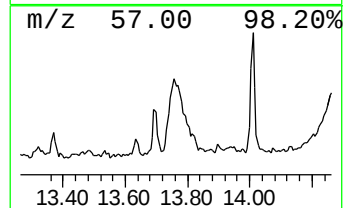
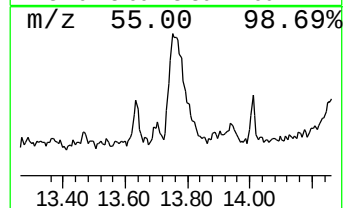
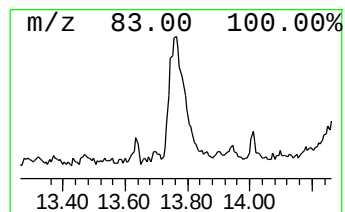
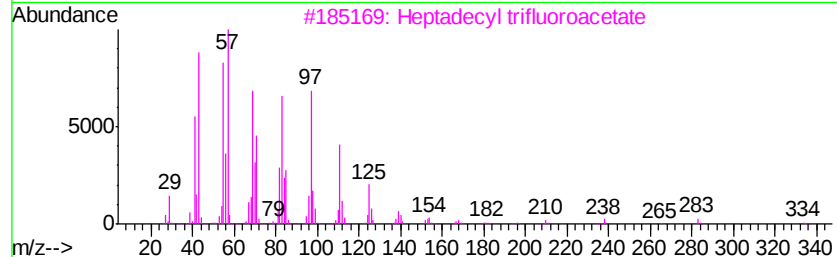
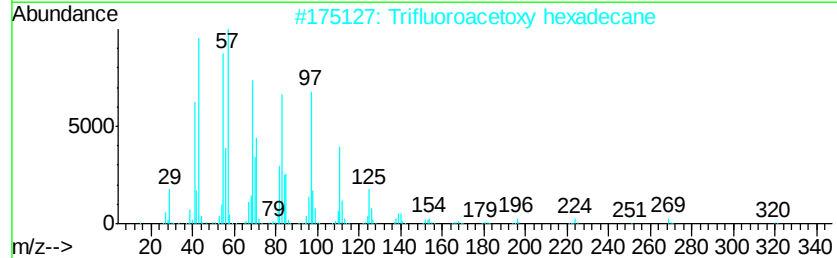
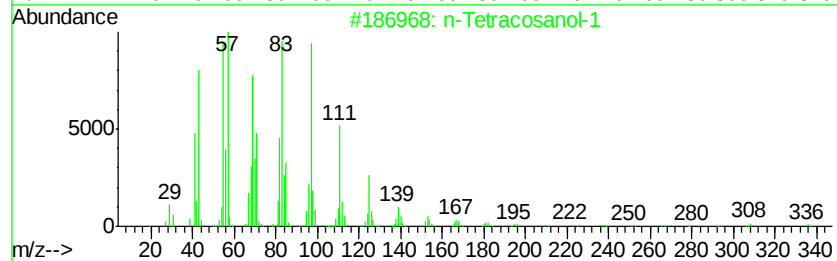
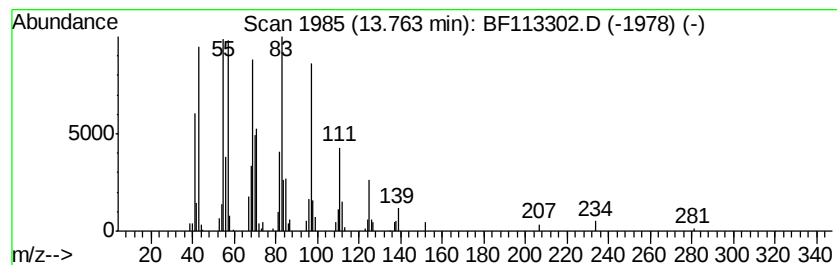
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.76	5.00 ng	277343	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93



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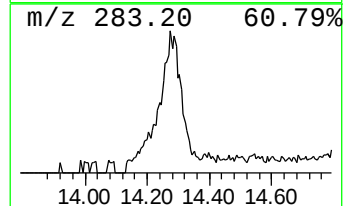
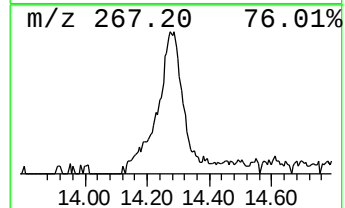
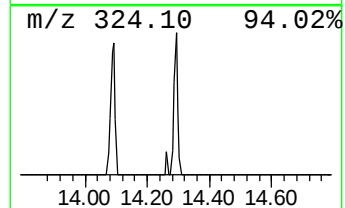
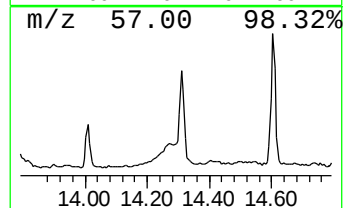
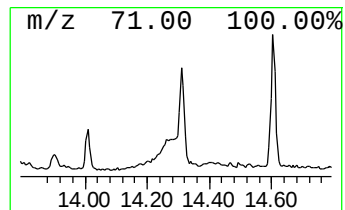
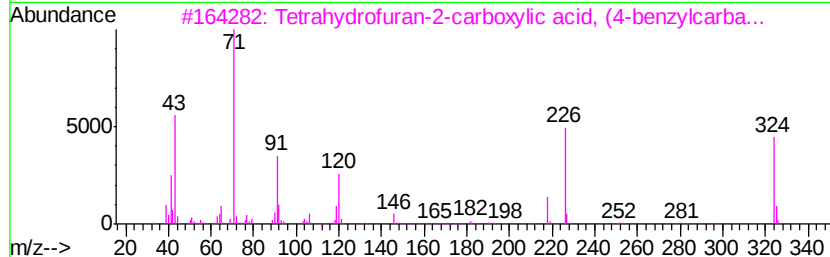
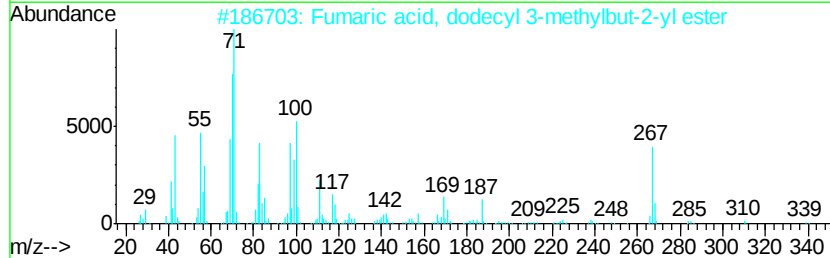
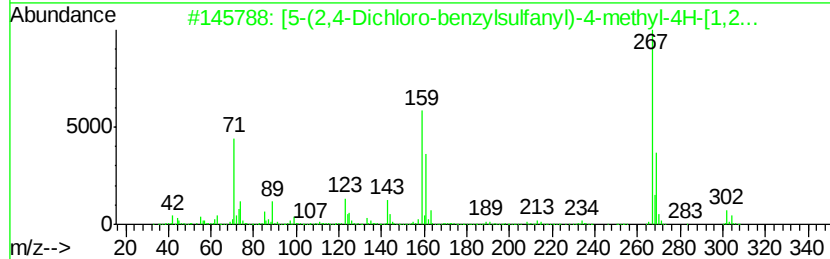
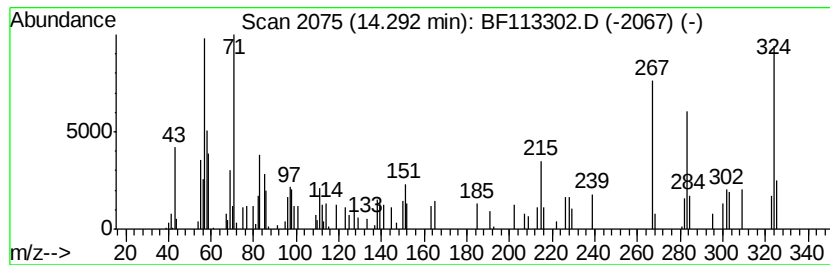
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown14.29 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.35 ng	130074	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	[5-(2,4-Dichloro-benzylsulfanyl)...	302	C11H12Cl2N4S	1000276-01-0	38
2		Fumaric acid, dodecyl 3-methylbu...	354	C21H38O4	1000348-08-4	22
3		Tetrahydrofuran-2-carboxylic aci...	324	C19H20N2O3	1000316-12-3	16
4		Phenylpropylamine, N-acetyl-3,4,...	267	C14H21N04	112369-97-8	11
5		2-Benzylidenehydrazono-3-methyl-...	267	C15H13N3S	1000146-59-1	11



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ClientSampleId :
S4C(6-18)COMP

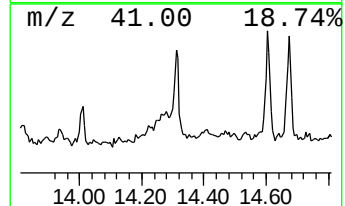
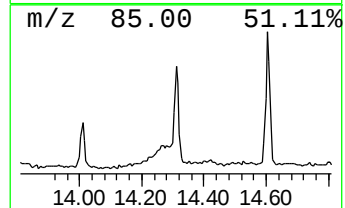
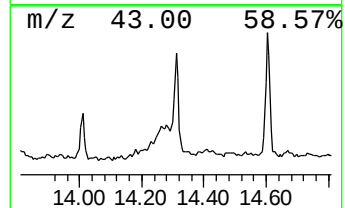
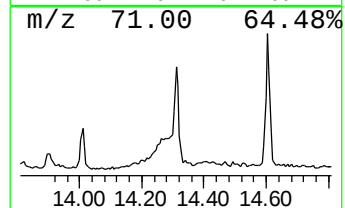
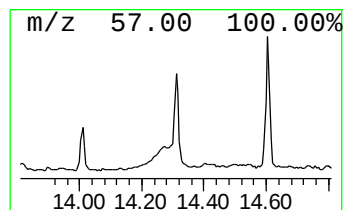
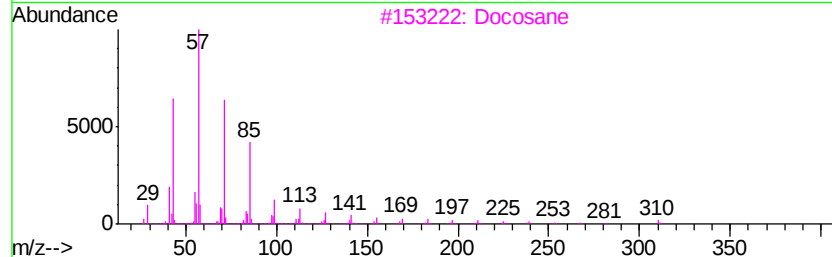
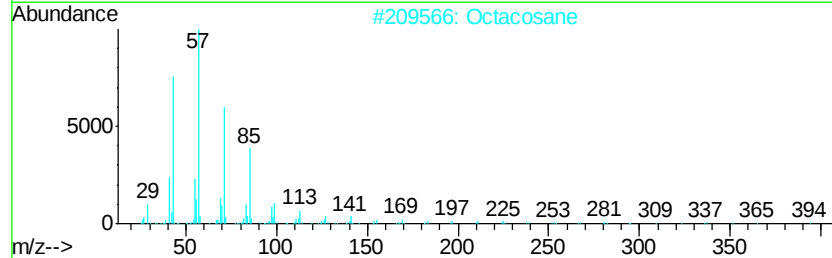
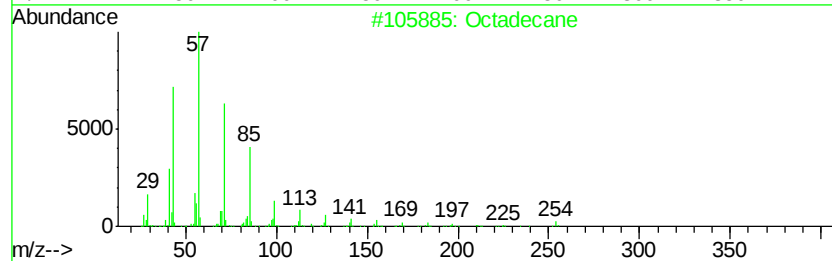
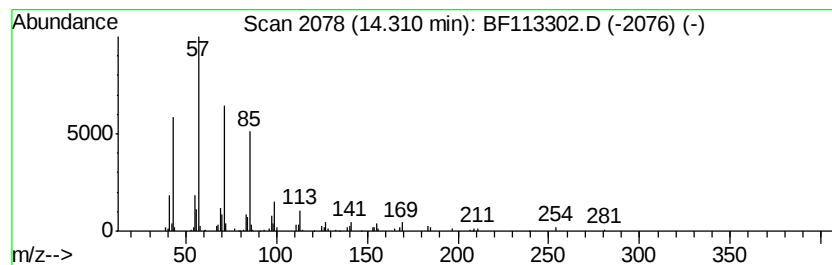
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.31	3.00 ng	166324	Chrysene-d12	13.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	96
2	Octacosane		394	C28H58	000630-02-4	91
3	Docosane		310	C22H46	000629-97-0	91
4	Heneicosane		296	C21H44	000629-94-7	87
5	Nonadecane		268	C19H40	000629-92-5	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032619\
Data File : BF113302.D
Acq On : 26 Mar 2019 20:25
Operator : JU/SJ
Sample : K2081-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4C(6-18)COMP

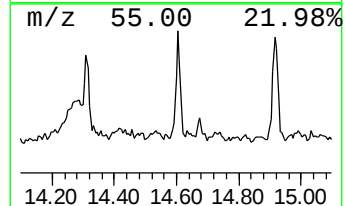
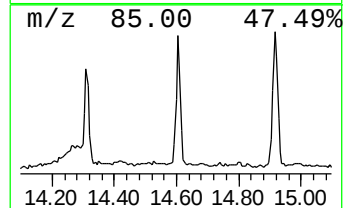
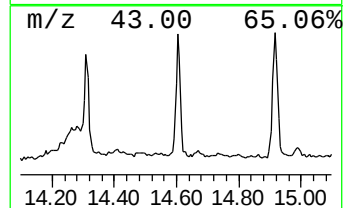
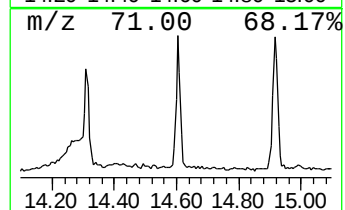
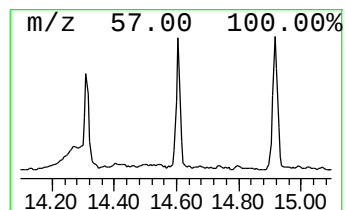
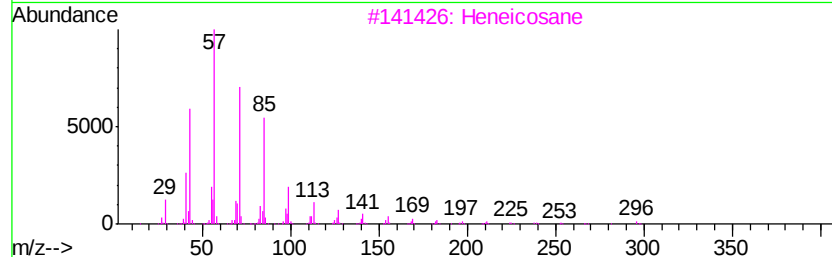
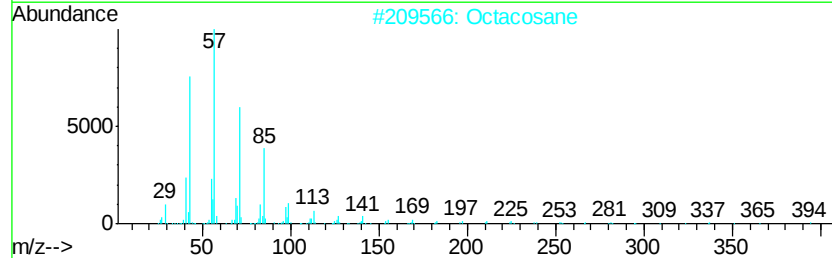
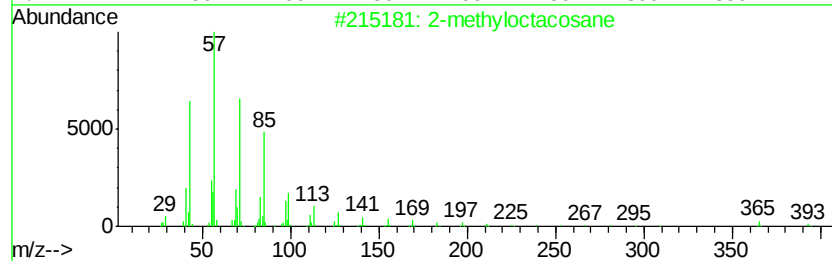
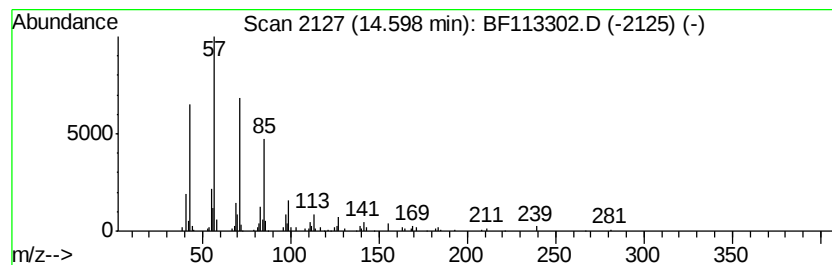
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	3.55 ng	198505	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Triacontane	422	C30H62	000638-68-6	90
5		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032619\
Data File : BF113302.D
Acq On : 26 Mar 2019 20:25
Operator : JU/SJ
Sample : K2081-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4C(6-18)COMP

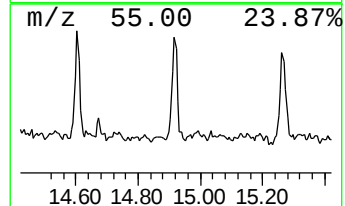
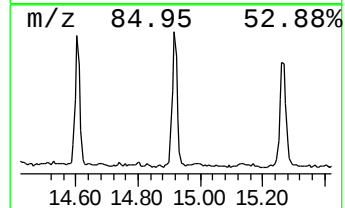
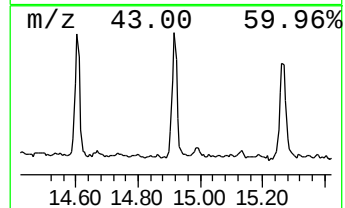
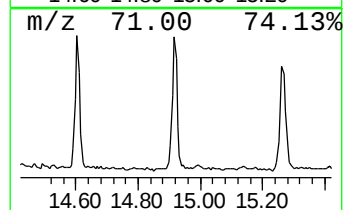
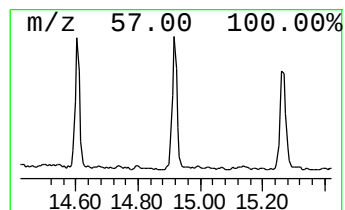
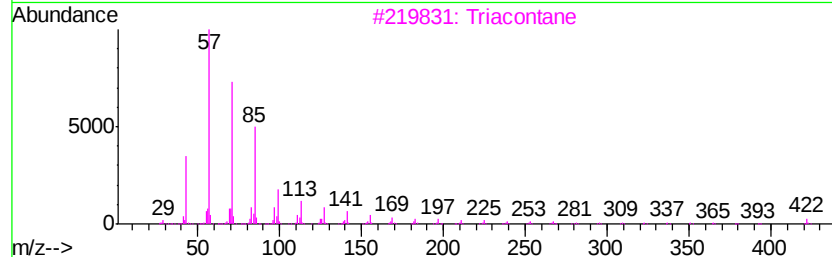
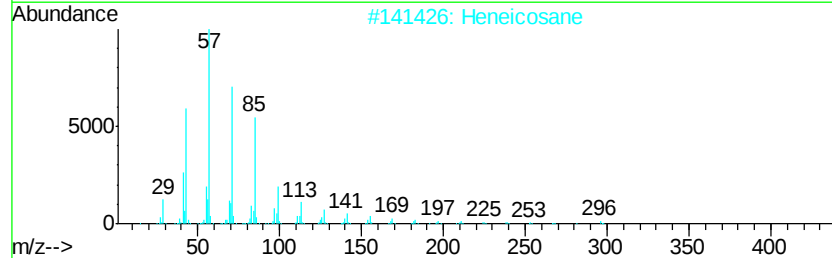
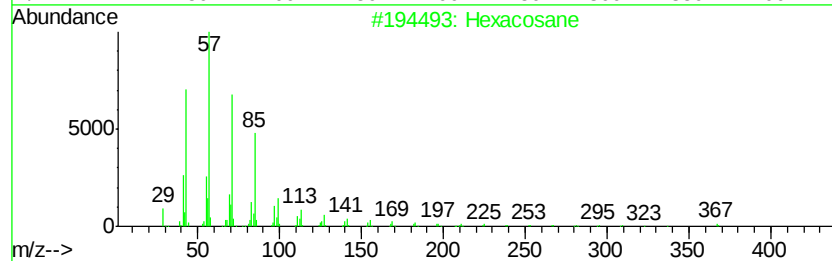
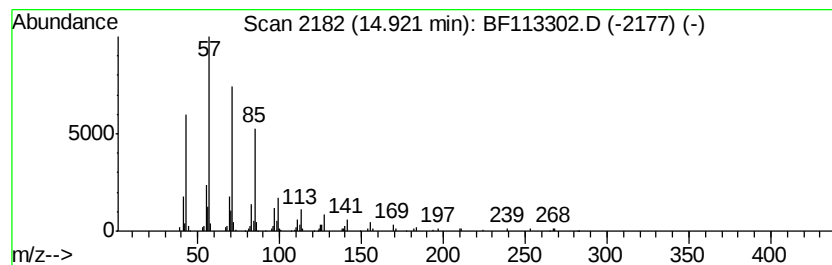
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	4.00 ng	223802	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Hexatriacontane	507	C36H74	000630-06-8	91
5		Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032619\
Data File : BF113302.D
Acq On : 26 Mar 2019 20:25
Operator : JU/SJ
Sample : K2081-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4C(6-18)COMP

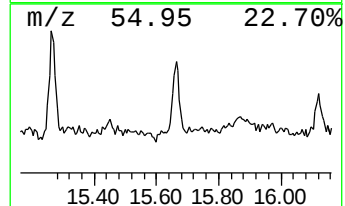
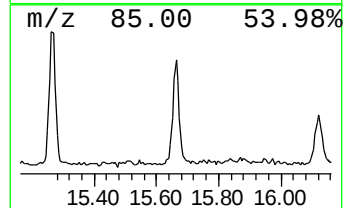
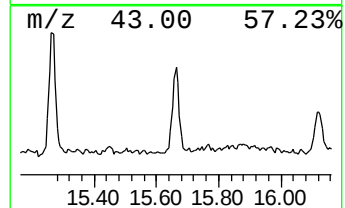
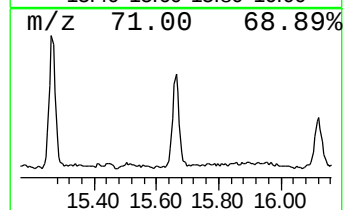
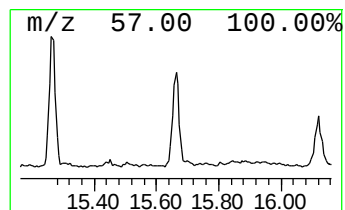
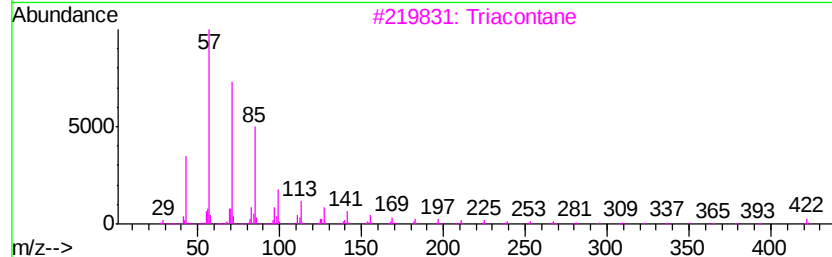
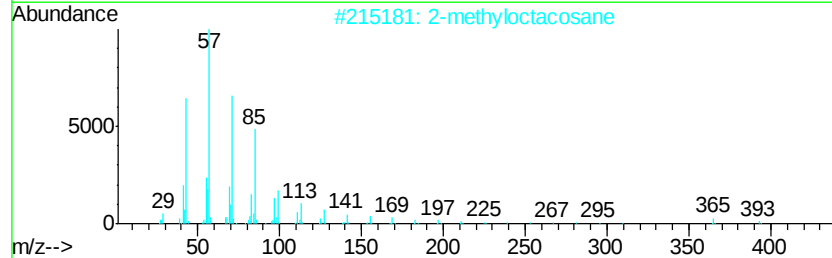
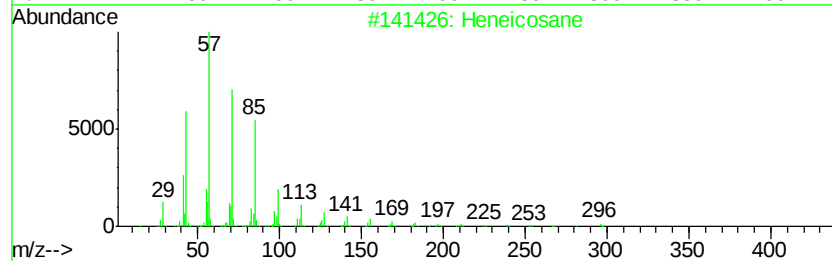
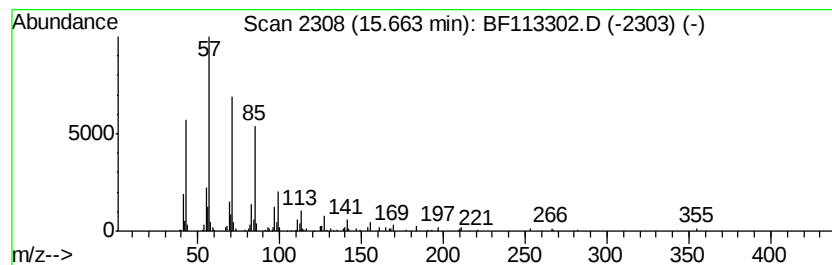
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	3.11 ng	173852	Perylene-d12	15.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032619\
Data File : BF113302.D
Acq On : 26 Mar 2019 20:25
Operator : JU/SJ
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S4C(6-18)COMP

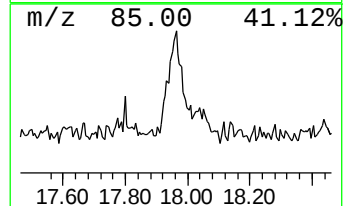
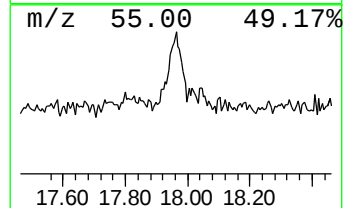
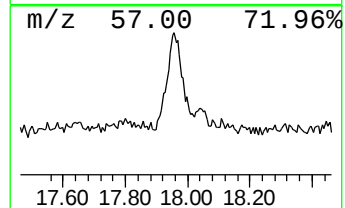
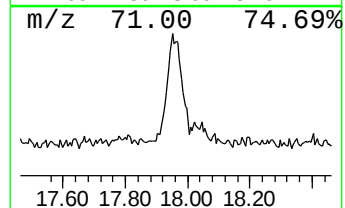
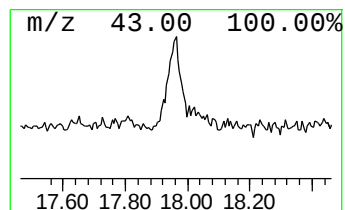
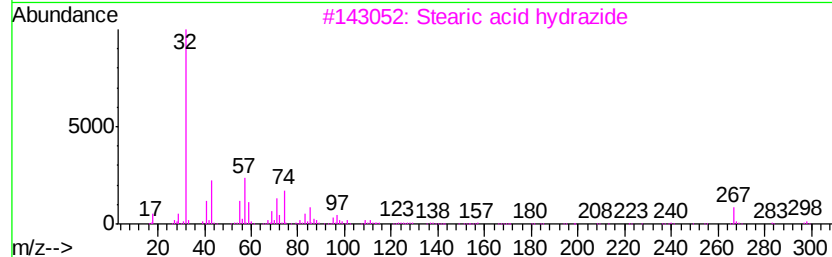
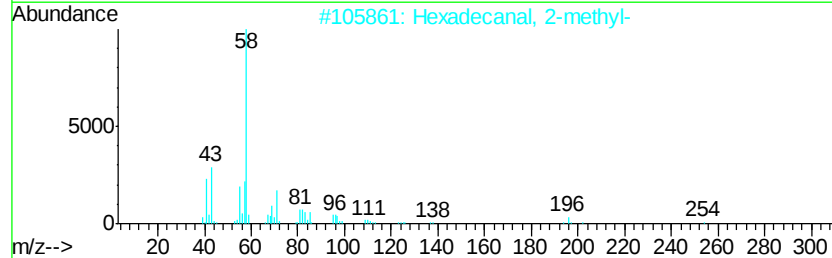
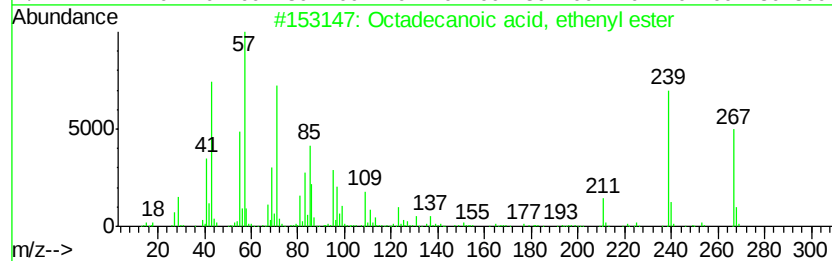
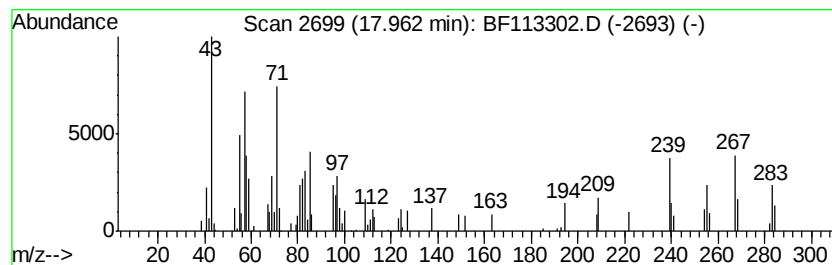
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.96 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	2.47 ng	138125	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	46
2		Hexadecanal, 2-methyl-	254	C17H34O	055019-46-0	22
3		Stearic acid hydrazide	298	C18H38N2O	004130-54-5	22
4		Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	14
5		S-[2-[N,N-Dimethylamino]ethylpyr...	245	C10H19N3O2S	1000212-14-2	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032619\
 Data File : BF113302.D
 Acq On : 26 Mar 2019 20:25
 Operator : JU/SJ
 Sample : K2081-16
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4C(6-18)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.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
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n-Hexadecanoic acid	11.75	15.0	ng	1049750	4	11.21	1399140	20.0
Octadecanoic acid	12.53	13.8	ng	764490	5	13.83	1108500	20.0
n-Tetracosanol-1	13.76	5.0	ng	277343	5	13.83	1108500	20.0
unknown14.29	14.29	2.4	ng	130074	5	13.83	1108500	20.0
Octadecane	14.31	3.0	ng	166324	5	13.83	1108500	20.0
2-methyloctacosane	14.60	3.5	ng	198505	6	15.23	1118390	20.0
Hexacosane	14.92	4.0	ng	223802	6	15.23	1118390	20.0
Heneicosane	15.66	3.1	ng	173852	6	15.23	1118390	20.0
unknown17.96	17.96	2.5	ng	138125	6	15.23	1118390	20.0