

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
 Data File : BF122661.D
 Acq On : 11 Dec 2020 14:04
 Operator : JU/CG
 Sample : L5033-06
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CS-48

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-BF120520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122661.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	498	505	513	rBV	36334	47208	1.12%	0.135%
2	5.457	569	573	591	rBV	2831577	2727577	64.52%	7.805%
3	6.469	740	745	760	rBV2	2685891	3132461	74.10%	8.963%
4	6.840	804	808	811	rBV	1062537	897419	21.23%	2.568%
5	7.398	898	903	906	rBV	1881303	1853578	43.84%	5.304%
6	8.122	1022	1026	1041	rBV	1342458	1191777	28.19%	3.410%
7	9.198	1204	1209	1212	rBV	3937039	3600055	85.16%	10.301%
8	9.592	1272	1276	1283	rBV	137451	135558	3.21%	0.388%
9	9.875	1320	1324	1336	rBV	1463386	1407482	33.29%	4.027%
10	10.663	1454	1458	1473	rBV	1499345	1543982	36.52%	4.418%
11	11.316	1565	1569	1573	rVB	55776	56788	1.34%	0.162%
12	11.363	1573	1577	1583	rBV	1639746	1453755	34.39%	4.160%
13	11.745	1639	1642	1647	rBV	53054	72274	1.71%	0.207%
14	11.898	1661	1668	1689	rVB	1455958	2340696	55.37%	6.698%
15	12.157	1709	1712	1718	rVB	153590	165242	3.91%	0.473%
16	12.210	1718	1721	1727	rVB	82035	94413	2.23%	0.270%
17	12.475	1763	1766	1772	rBV2	36806	55740	1.32%	0.159%
18	12.545	1774	1778	1781	rBV	126544	148500	3.51%	0.425%
19	12.586	1781	1785	1786	rBV3	56647	64346	1.52%	0.184%
20	12.680	1795	1801	1814	rBV	1685751	2725724	64.47%	7.799%
21	12.951	1842	1847	1850	rBV	4467187	4227581	100.00%	12.097%
22	13.698	1969	1974	1987	rVB4	50381	106884	2.53%	0.306%
23	13.910	2005	2010	2021	rBV2	108186	324966	7.69%	0.930%
24	14.004	2022	2026	2033	rVB	1456022	1441801	34.10%	4.125%
25	14.451	2095	2102	2119	rBV8	226442	876078	20.72%	2.507%
26	14.704	2140	2145	2154	rVB2	65141	147879	3.50%	0.423%
27	15.104	2206	2213	2222	rBV2	131702	278389	6.59%	0.797%
28	15.468	2269	2275	2288	rBV	1126115	2060977	48.75%	5.897%
29	16.939	2519	2525	2531	rVB3	64677	134522	3.18%	0.385%
30	17.698	2642	2654	2667	rBV3	206087	891755	21.09%	2.552%
31	18.433	2767	2779	2790	rBV2	225253	743259	17.58%	2.127%

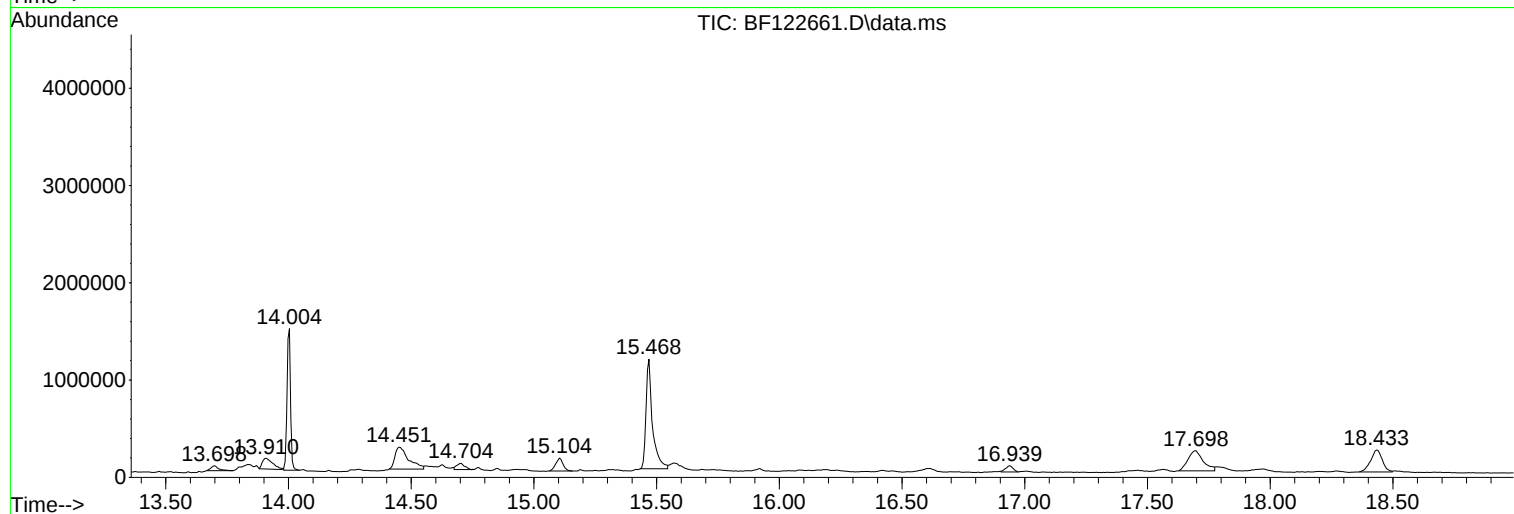
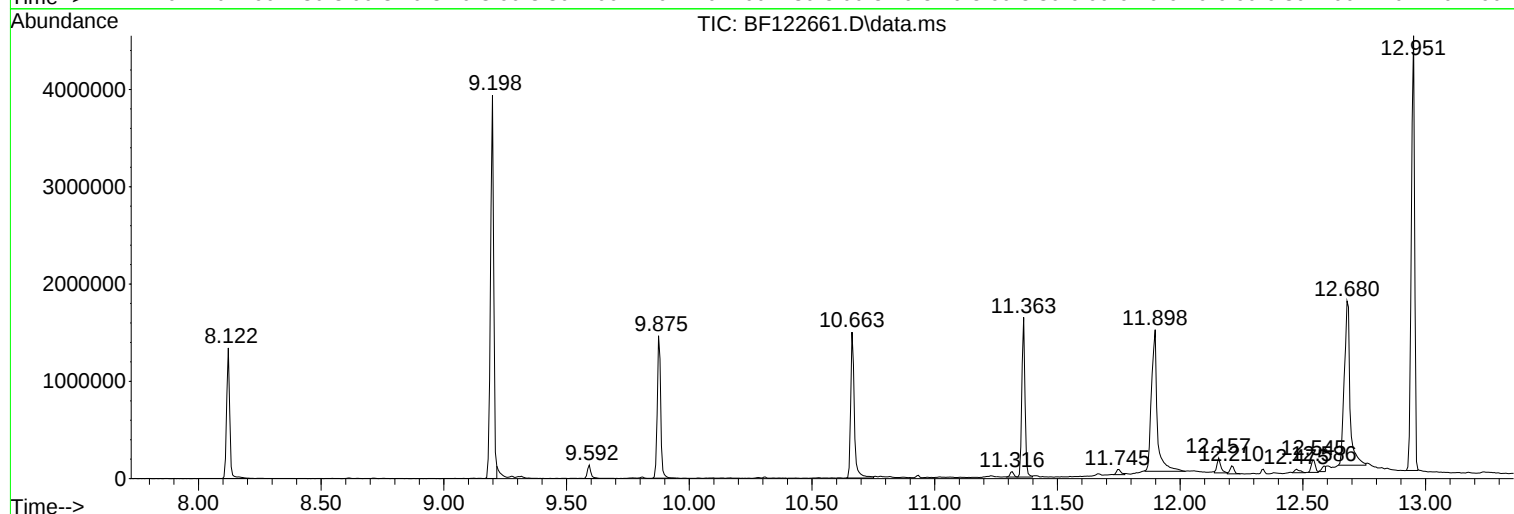
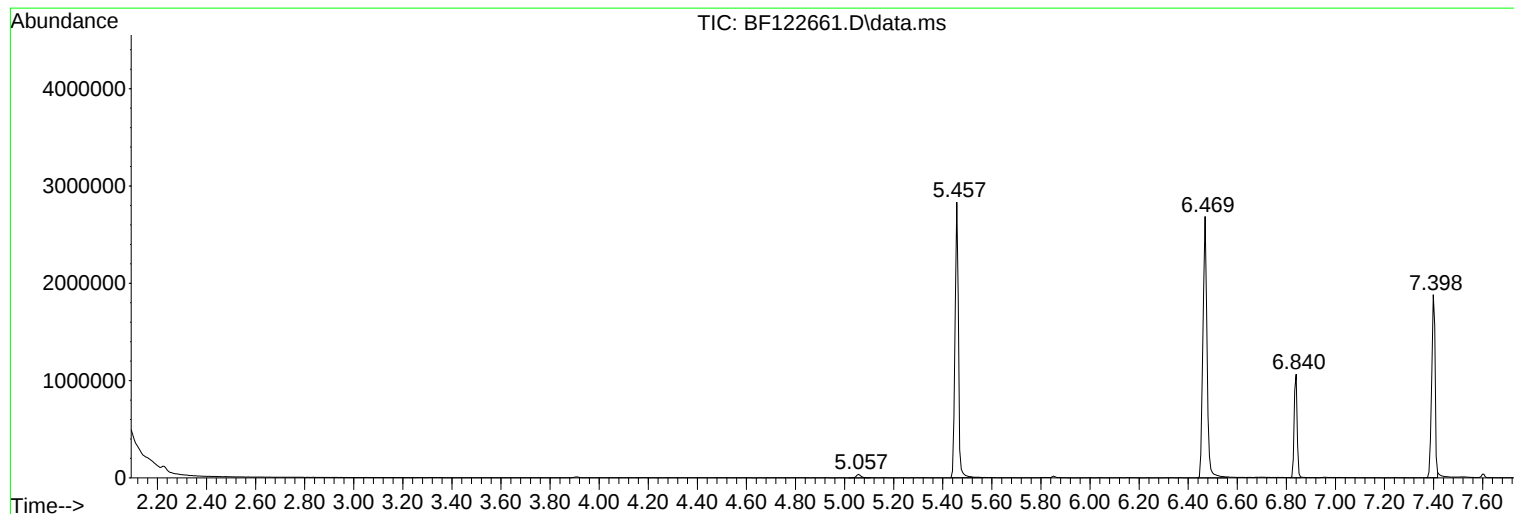
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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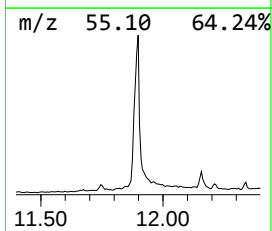
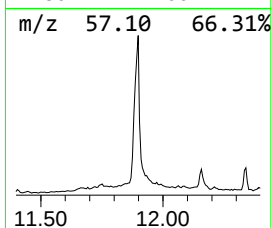
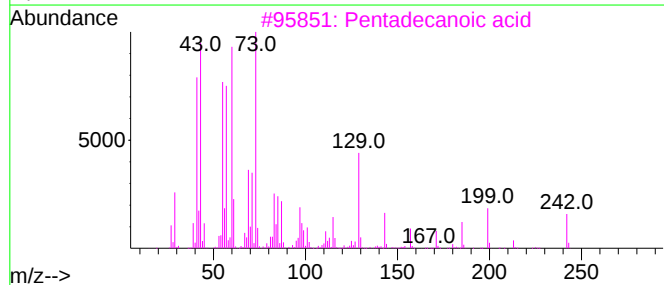
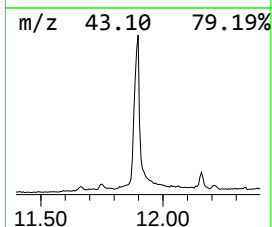
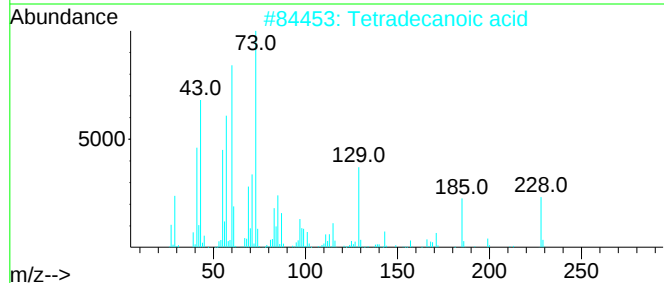
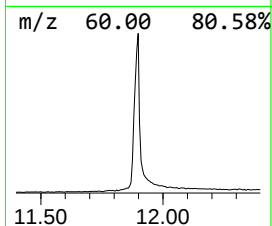
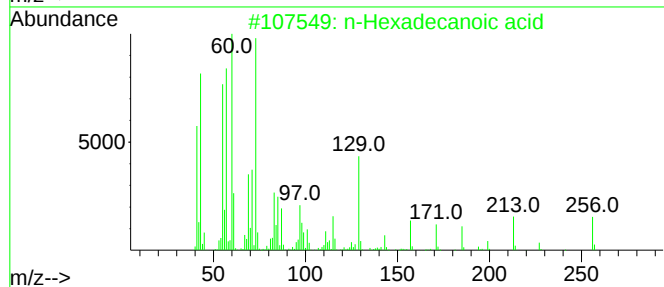
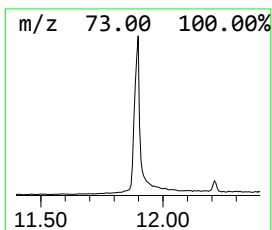
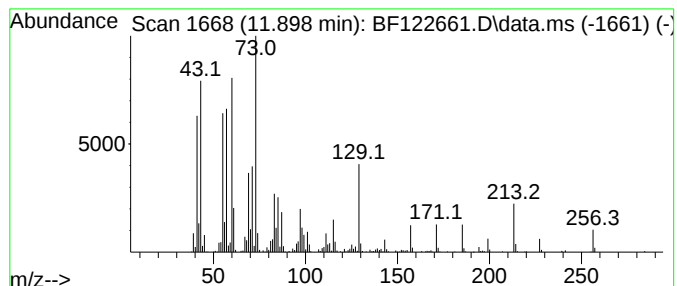
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	32.20 ng	2340700	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	91
5			Octadecanoic acid	284	C18H36O2	000057-11-4	81



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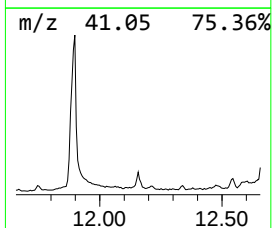
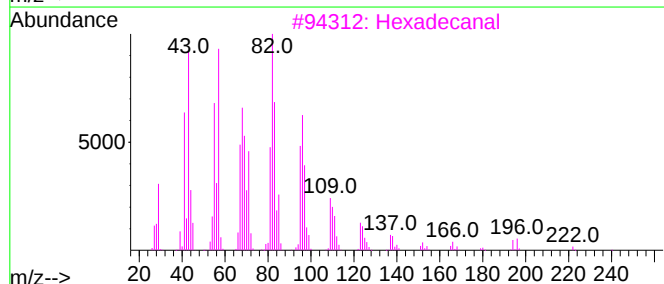
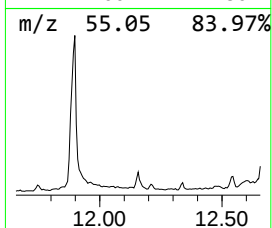
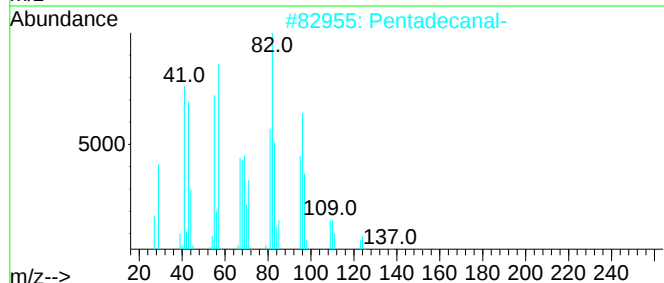
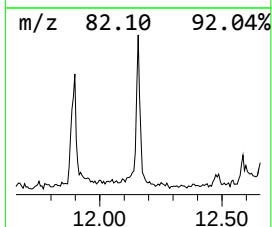
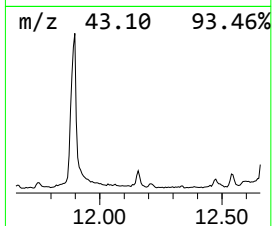
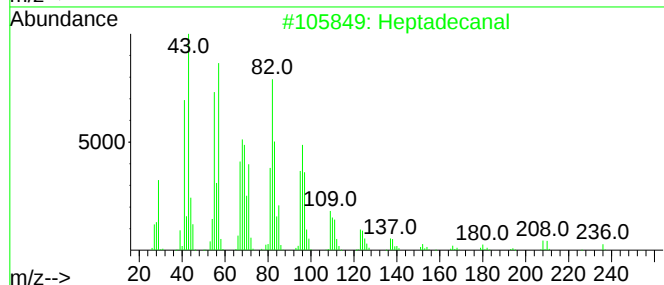
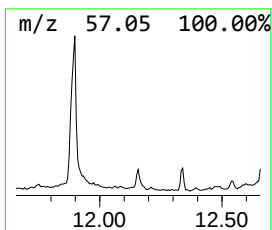
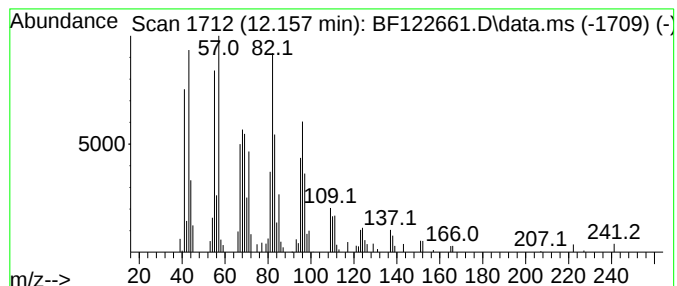
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Heptadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.157	2.27 ng	165242	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanal	254	C17H34O	1000376-70-0	94
2			Pentadecanal-	226	C15H30O	002765-11-9	94
3			Hexadecanal	240	C16H32O	000629-80-1	94
4			Tetradecanal	212	C14H28O	000124-25-4	91
5			17-Octadecenal	266	C18H34O	056554-86-0	91



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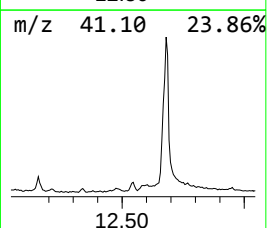
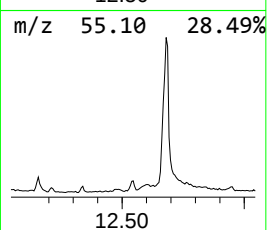
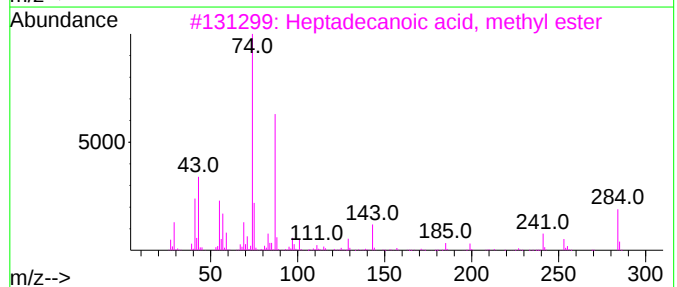
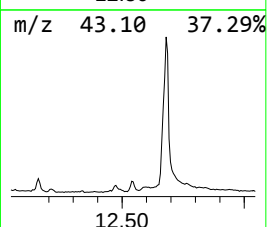
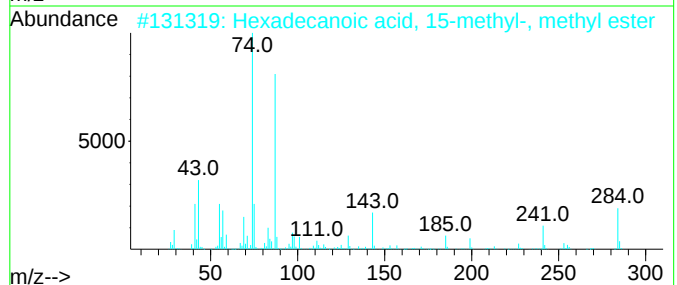
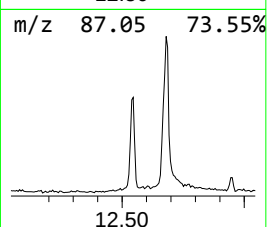
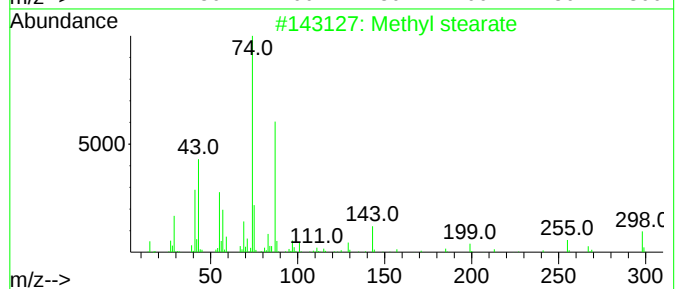
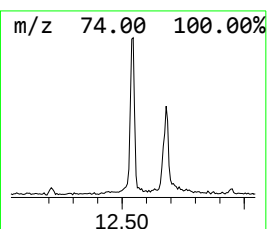
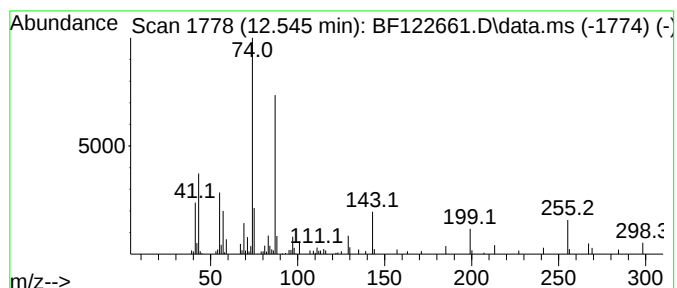
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Methyl stearate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	2.04 ng	148500	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90
3			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86



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ALS Vial : 6 Sample Multiplier: 1

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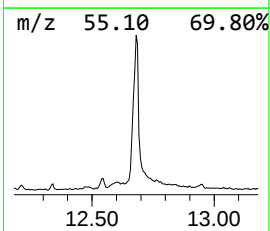
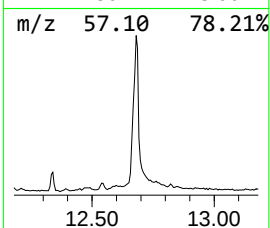
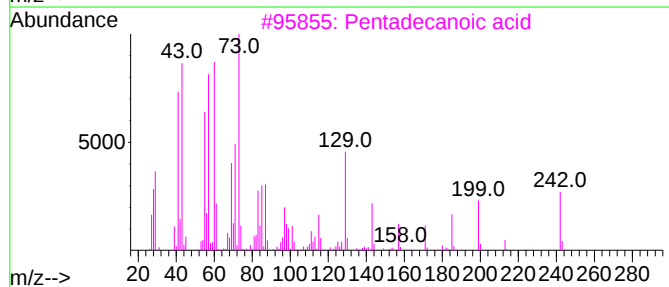
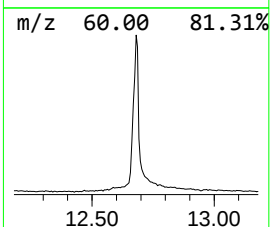
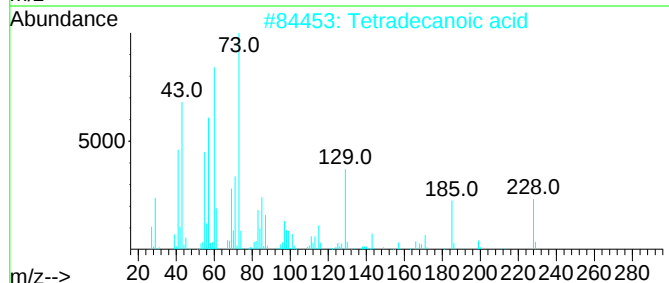
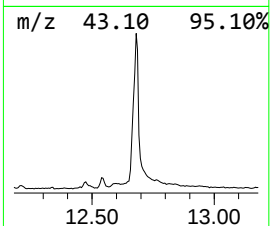
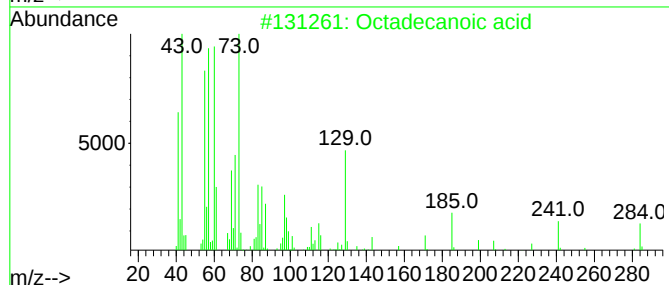
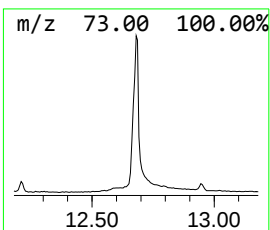
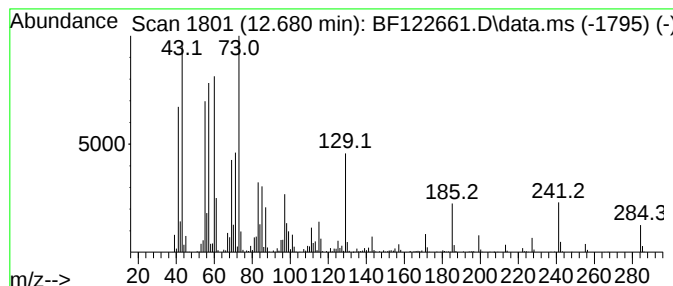
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	37.50 ng	2725720	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62



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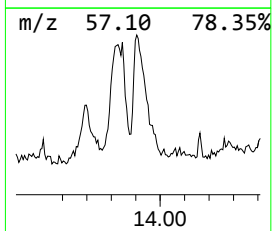
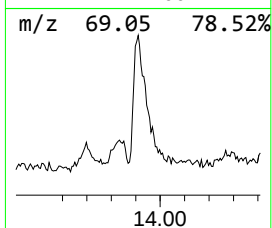
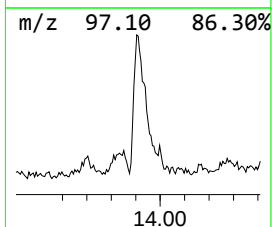
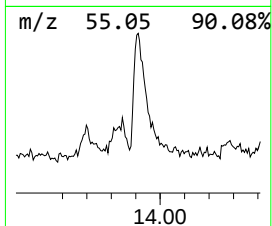
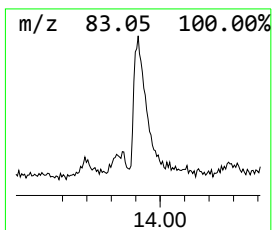
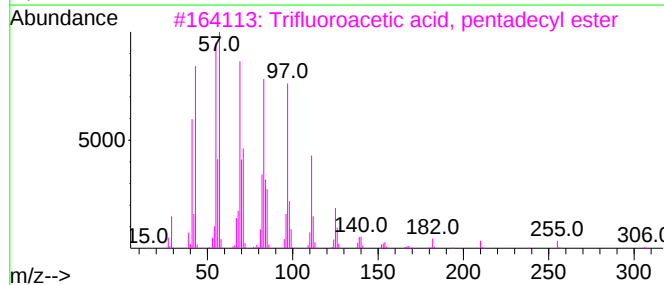
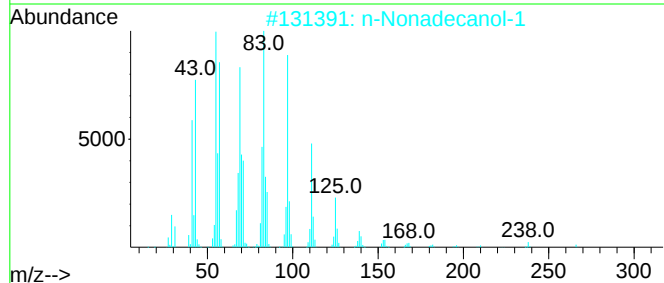
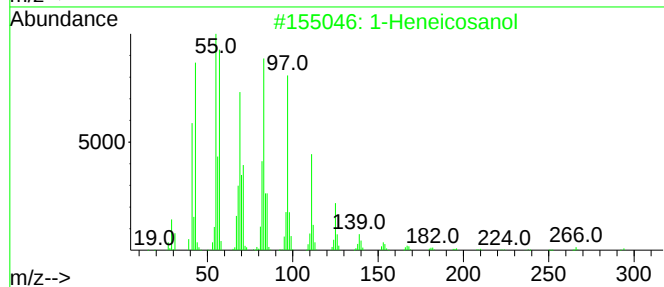
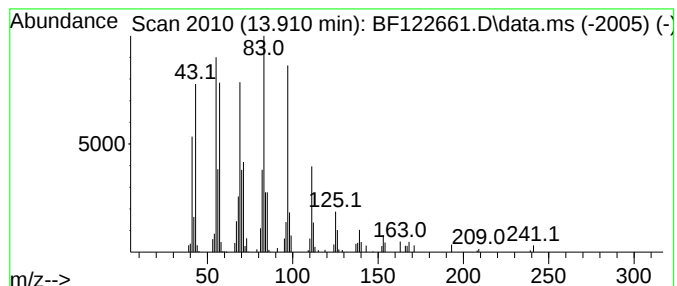
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	4.51 ng	324966	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
4			Behenic alcohol	326	C22H46O	000661-19-8	93
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93



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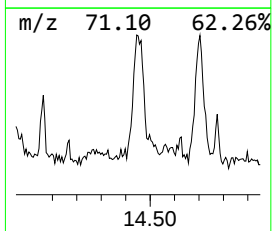
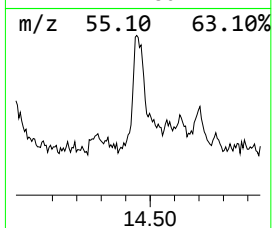
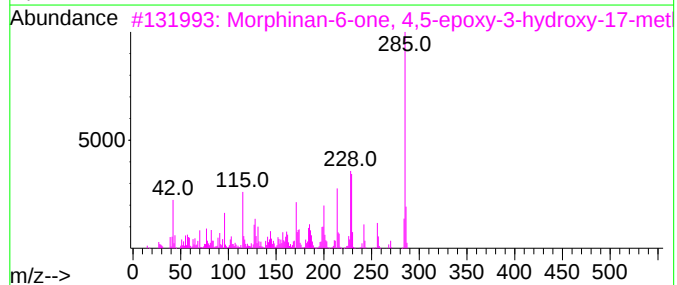
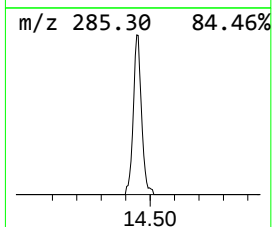
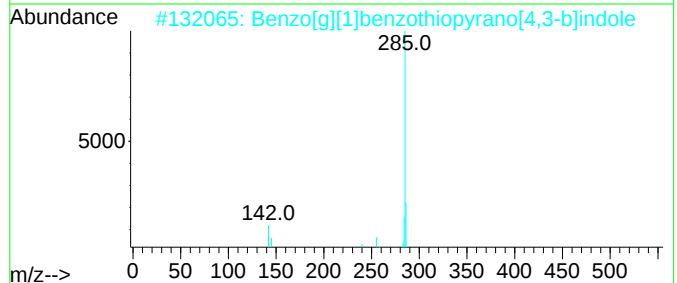
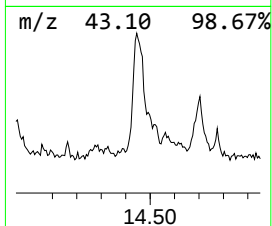
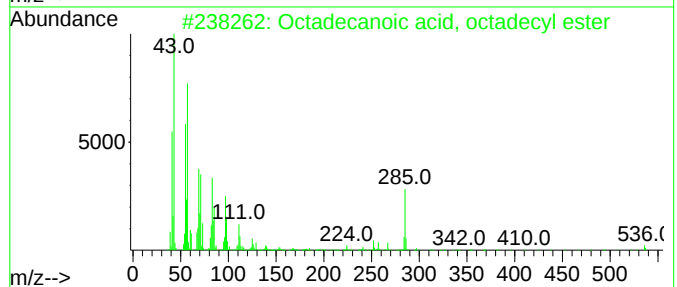
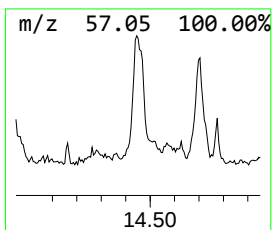
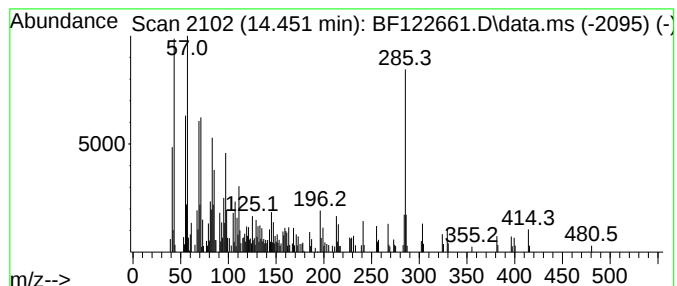
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid, octadecy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	12.15 ng	876078	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, octadecyl ester	537	C36H72O2	002778-96-3	58
2			Benzo[g][1]benzothiopyrano[4,3-b...	285	C19H11NS	010023-23-1	50
3			Morphinan-6-one, 4,5-epoxy-3-hyd...	285	C17H19NO3	000466-99-9	42
4			Benz[a]acridine, 8,10-diethyl-	285	C21H19N	003518-07-8	41
5			Morphine	285	C17H19NO3	000057-27-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
Data File : BF122661.D
Acq On : 11 Dec 2020 14:04
Operator : JU/CG
Sample : L5033-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
CS-48

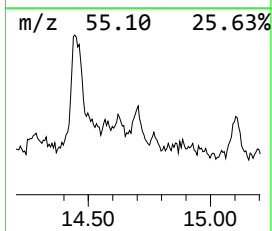
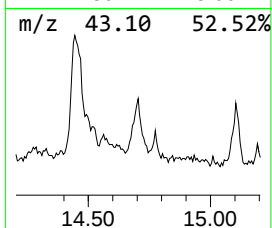
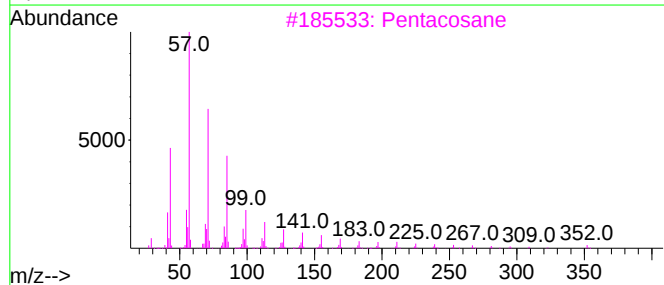
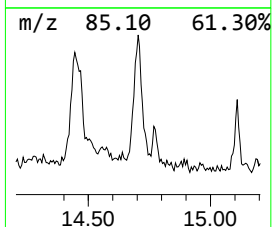
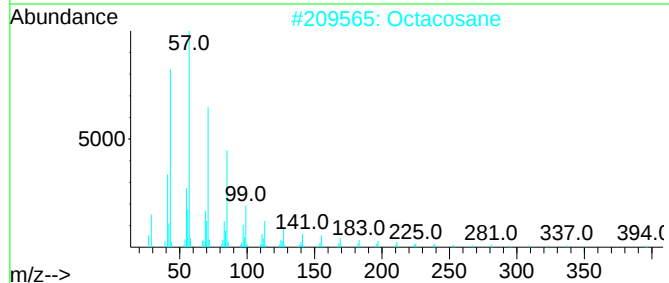
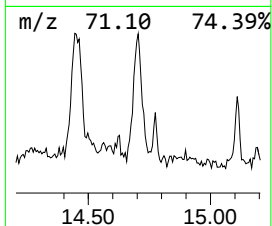
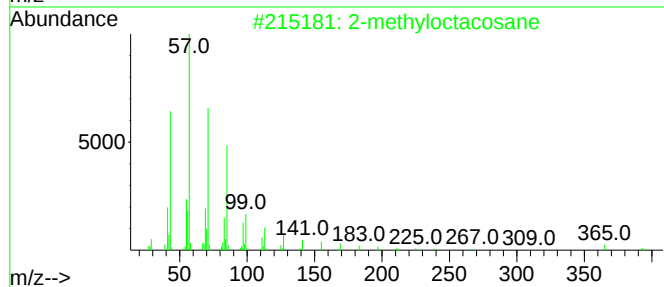
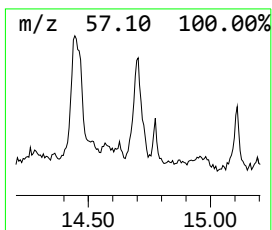
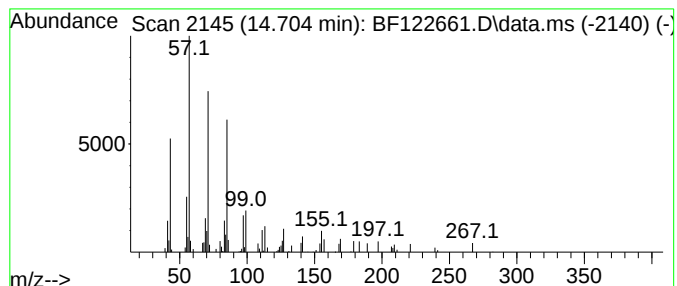
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.704	2.05 ng	147879	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Pentacosane	352	C25H52	000629-99-2	90
4			Tetratetracontane	619	C44H90	007098-22-8	90
5			triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
Data File : BF122661.D
Acq On : 11 Dec 2020 14:04
Operator : JU/CG
Sample : L5033-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CS-48

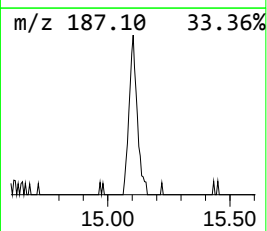
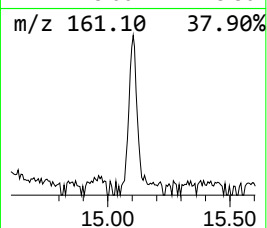
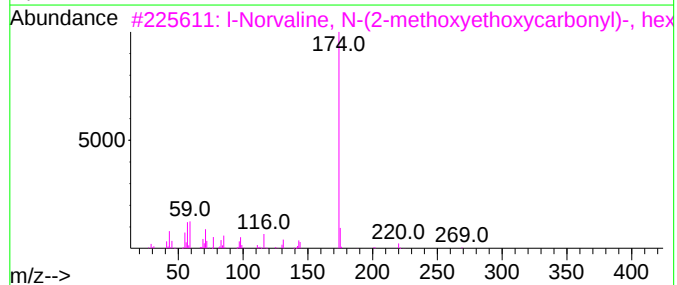
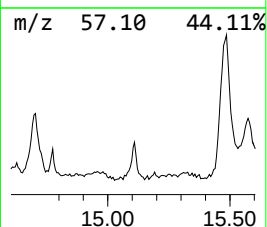
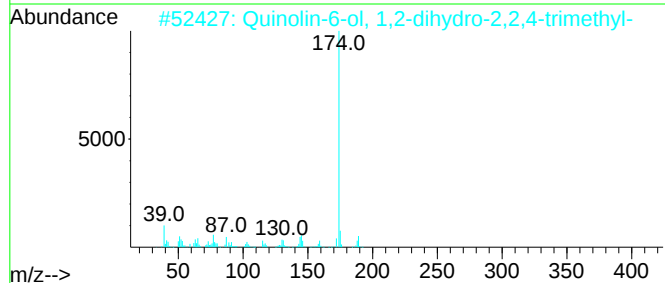
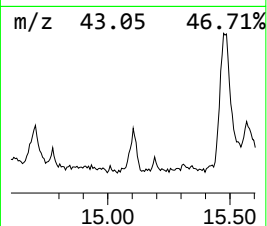
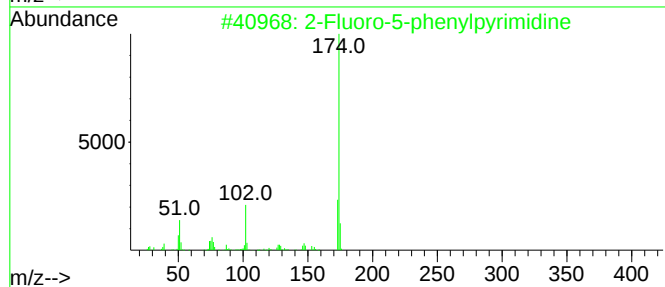
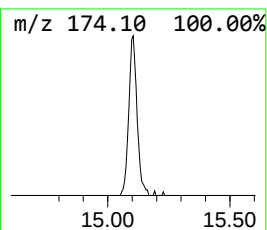
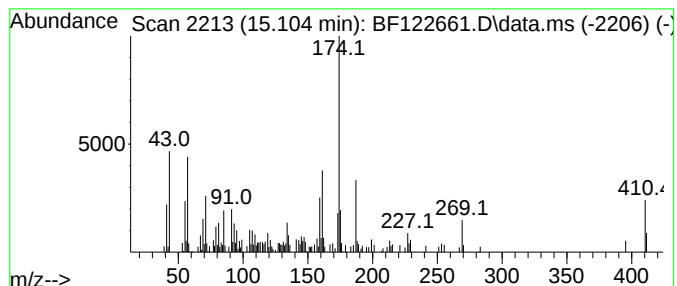
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.10 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	2.70 ng	278389	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Fluoro-5-phenylpyrimidine	174	C10H7FN2	062850-13-9	27
2			Quinolin-6-ol, 1,2-dihydro-2,2,4...	189	C12H15NO	072107-05-2	27
3			l-Norvaline, N-(2-methoxyethoxyc...	443	C25H49NO5	1000328-64-7	27
4			1-(Prop-2-enyl)-1-phenylaminocyc...	215	C15H21N	127934-37-6	27
5			1,4-Naphthalenediol, 2-methyl-, ...	258	C15H14O4	000573-20-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
Data File : BF122661.D
Acq On : 11 Dec 2020 14:04
Operator : JU/CG
Sample : L5033-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CS-48

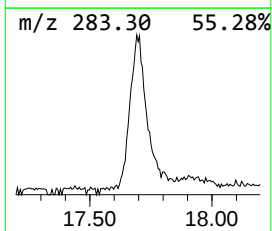
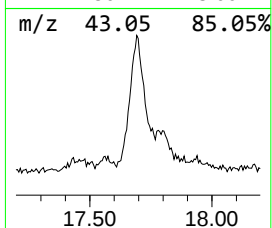
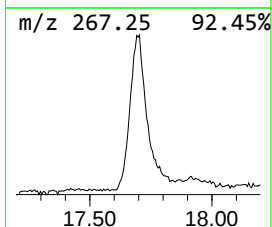
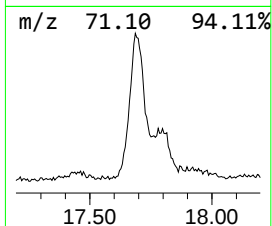
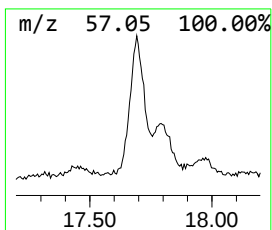
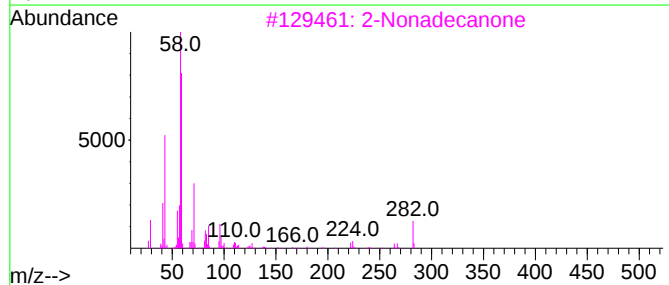
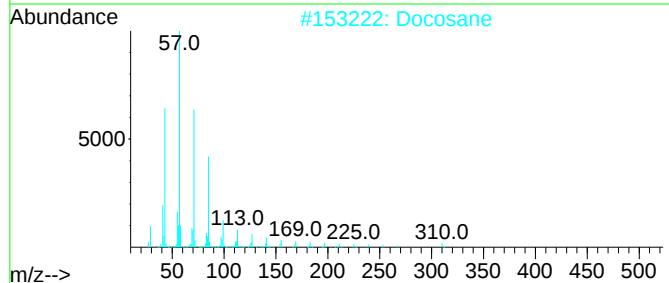
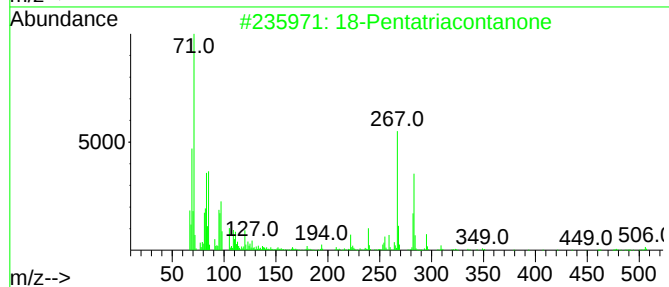
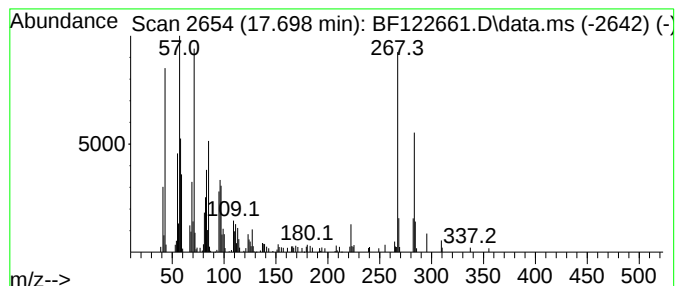
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 18-Pentatriacontanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.698	8.65 ng	891755	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			18-Pentatriacontanone	507	C35H70O	000504-53-0	58
2			Docosane	310	C22H46	000629-97-0	55
3			2-Nonadecanone	282	C19H38O	000629-66-3	35
4			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	35
5			Nonadecane	268	C19H40	000629-92-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
Data File : BF122661.D
Acq On : 11 Dec 2020 14:04
Operator : JU/CG
Sample : L5033-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CS-48

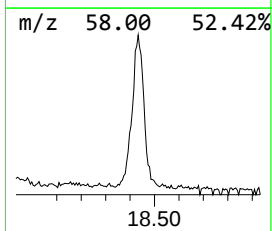
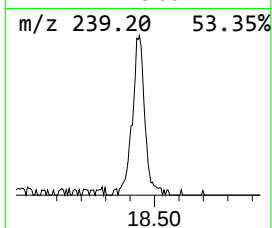
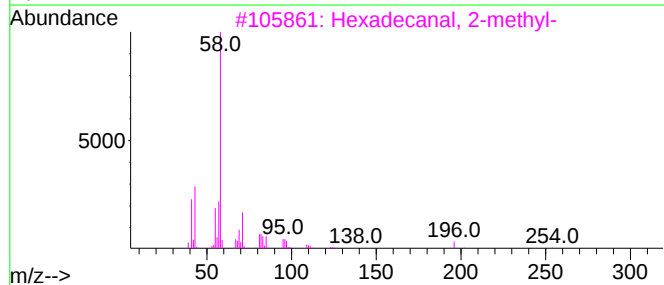
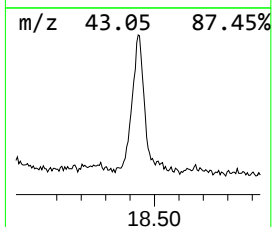
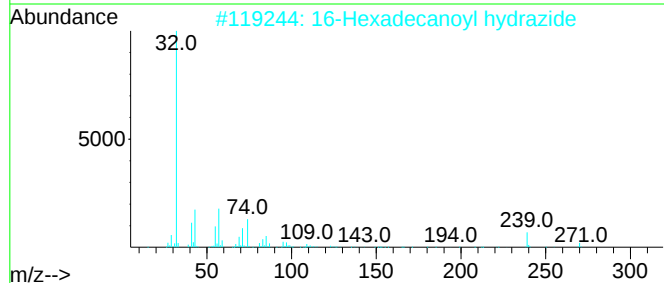
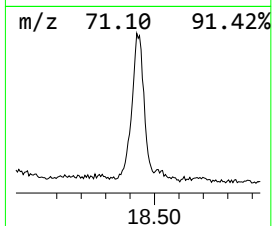
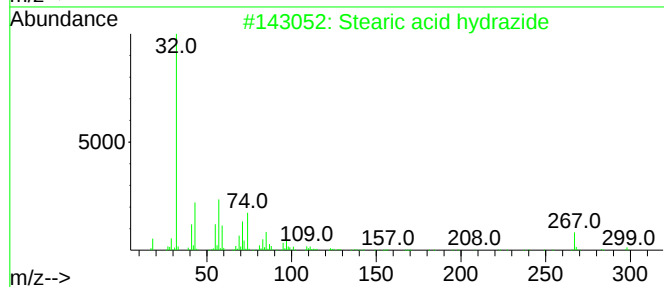
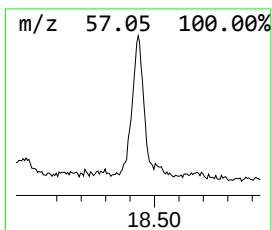
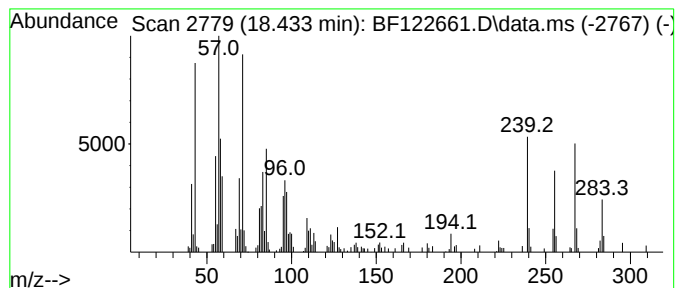
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Stearic acid hydrazide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.433	7.21 ng	743259	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Stearic acid hydrazide	298	C18H38N2O	004130-54-5	50
2			16-Hexadecanoyl hydrazide	270	C16H34N2O	002619-88-7	49
3			Hexadecanal, 2-methyl-	254	C17H34O	055019-46-0	43
4			Octadecane	254	C18H38	000593-45-3	38
5			Nonadecane	268	C19H40	000629-92-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
Data File : BF122661.D
Acq On : 11 Dec 2020 14:04
Operator : JU/CG
Sample : L5033-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CS-48

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.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
n-Hexadecanoic ...	11.898	32.2	ng	2340700	4	11.363	1453760	20.0
Heptadecanal	12.157	2.3	ng	165242	4	11.363	1453760	20.0
Methyl stearate	12.545	2.0	ng	148500	4	11.363	1453760	20.0
Octadecanoic acid	12.680	37.5	ng	2725720	4	11.363	1453760	20.0
1-Heneicosanol	13.910	4.5	ng	324966	5	14.004	1441800	20.0
Octadecanoic ac...	14.451	12.2	ng	876078	5	14.004	1441800	20.0
2-methyloctacosane	14.704	2.0	ng	147879	5	14.004	1441800	20.0
unknown15.10	15.104	2.7	ng	278389	6	15.468	2060980	20.0
18-Pentatriacon...	17.698	8.7	ng	891755	6	15.468	2060980	20.0
Stearic acid hy...	18.433	7.2	ng	743259	6	15.468	2060980	20.0