

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123585.D
 Acq On : 16 Apr 2021 11:06
 Operator : JU/CG
 Sample : M2048-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-13.5-14.0

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-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123585.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	16	rBV	1792203	2461277	29.86%	3.986%
2	5.487	573	578	581	rBV	7050324	7241563	87.86%	11.728%
3	6.498	744	750	753	rBV	6810627	7335054	88.99%	11.879%
4	6.869	809	813	816	rBV	1577749	1336962	16.22%	2.165%
5	7.428	903	908	911	rBV	4553756	4901274	59.46%	7.937%
6	8.151	1027	1031	1034	rBV	2265272	1725614	20.94%	2.795%
7	9.233	1210	1215	1218	rBV	8866220	7649133	92.80%	12.388%
8	9.622	1278	1281	1285	rBV	306747	237631	2.88%	0.385%
9	9.910	1326	1330	1334	rVB	2209193	1927412	23.38%	3.121%
10	10.704	1460	1465	1468	rBV	6429056	5653077	68.59%	9.155%
11	11.398	1580	1583	1587	rBV	2266453	2054811	24.93%	3.328%
12	11.933	1668	1674	1682	rBV	927933	1203810	14.61%	1.950%
13	12.068	1694	1697	1701	rBV3	112225	125834	1.53%	0.204%
14	12.110	1701	1704	1710	rVV4	95784	150956	1.83%	0.244%
15	12.215	1714	1722	1737	rVB5	116825	548506	6.65%	0.888%
16	12.721	1804	1808	1815	rBV	125091	154252	1.87%	0.250%
17	12.874	1831	1834	1841	rVB3	104301	146704	1.78%	0.238%
18	12.998	1850	1855	1858	rBV	8796965	8242305	100.00%	13.348%
19	13.451	1924	1932	1943	rVB2	246744	670181	8.13%	1.085%
20	13.904	2005	2009	2018	rBV2	676770	1103820	13.39%	1.788%
21	14.051	2029	2034	2037	rBV	1826881	1673283	20.30%	2.710%
22	14.215	2055	2062	2067	rBV	382983	713776	8.66%	1.156%
23	14.527	2111	2115	2117	rBV	104539	98807	1.20%	0.160%
24	14.839	2160	2168	2175	rBV	382997	723547	8.78%	1.172%
25	15.186	2223	2227	2232	rVB	124769	147261	1.79%	0.238%
26	15.533	2276	2286	2291	rBV	1027195	1625949	19.73%	2.633%
27	15.580	2291	2294	2300	rVB	112433	159564	1.94%	0.258%
28	15.927	2346	2353	2365	rBV8	195730	680099	8.25%	1.101%
29	16.027	2366	2370	2375	rVB2	75560	132034	1.60%	0.214%
30	16.280	2408	2413	2427	rVB3	130803	357353	4.34%	0.579%
31	16.668	2474	2479	2490	rVB7	94307	233573	2.83%	0.378%
32	17.180	2559	2566	2567	rBV4	74655	146647	1.78%	0.237%
33	18.245	2741	2747	2758	rVB5	60751	186429	2.26%	0.302%

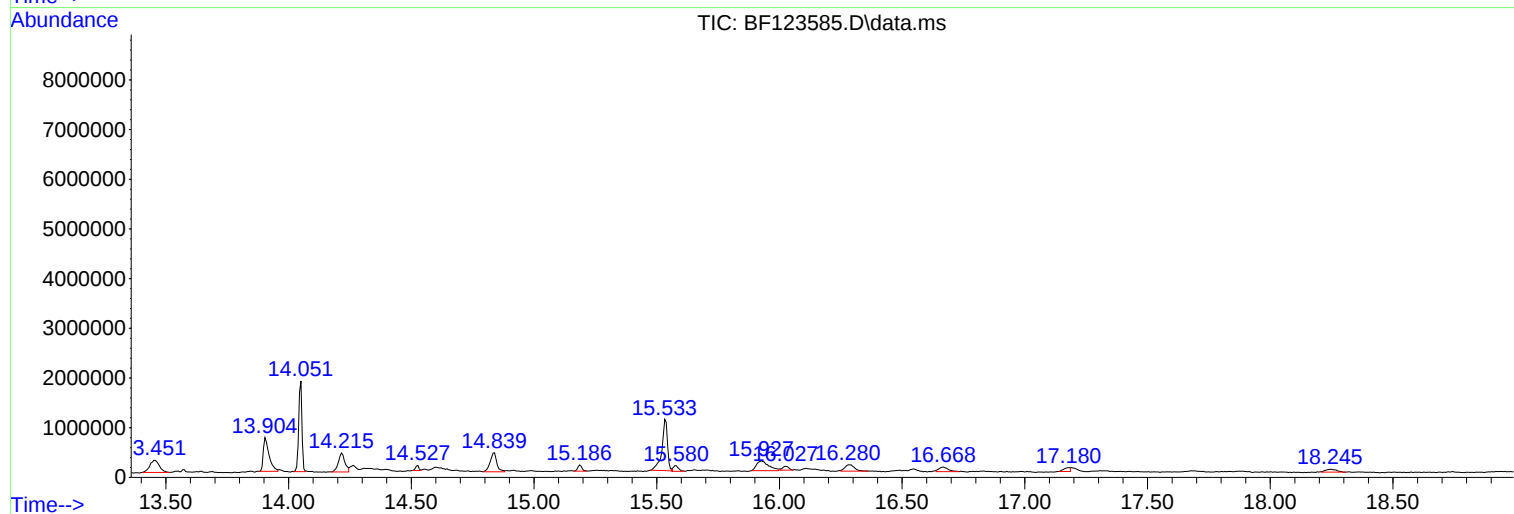
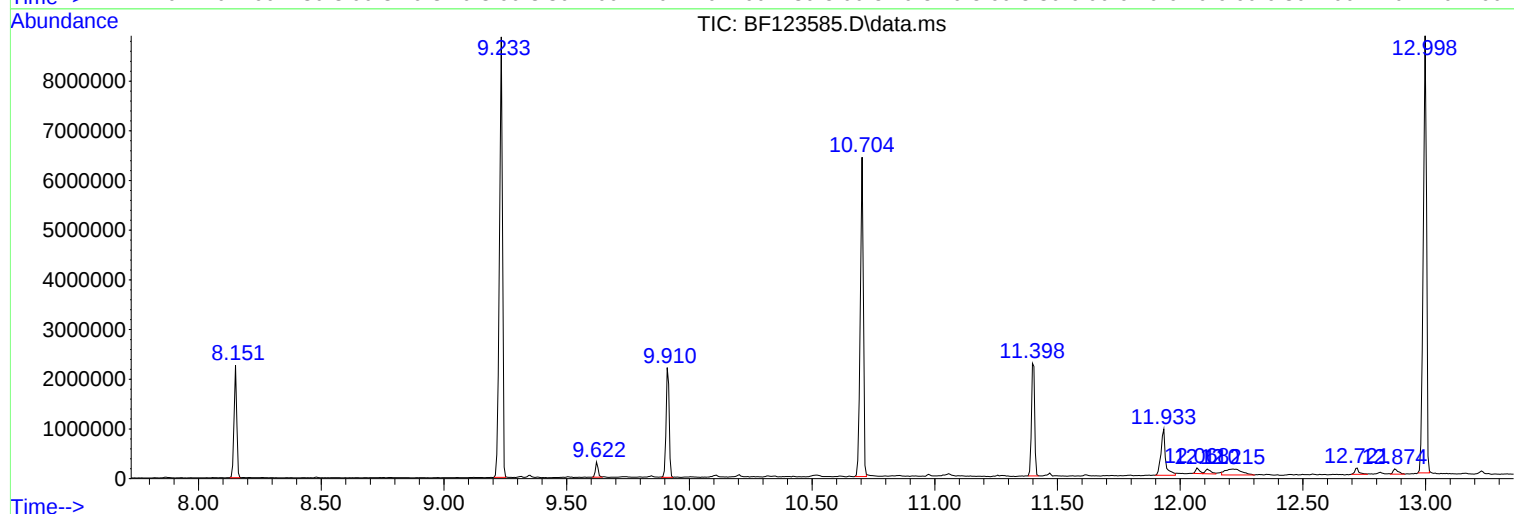
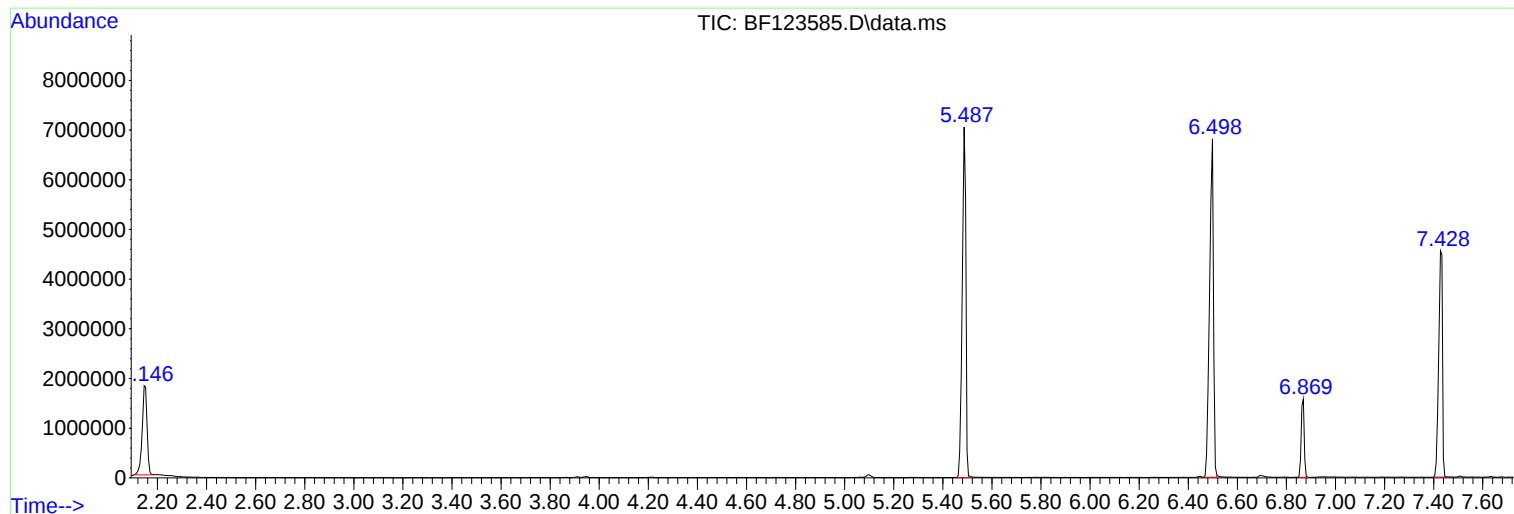
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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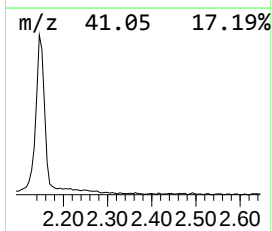
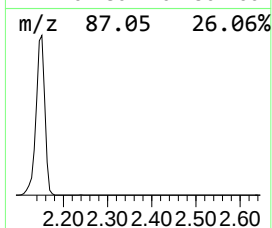
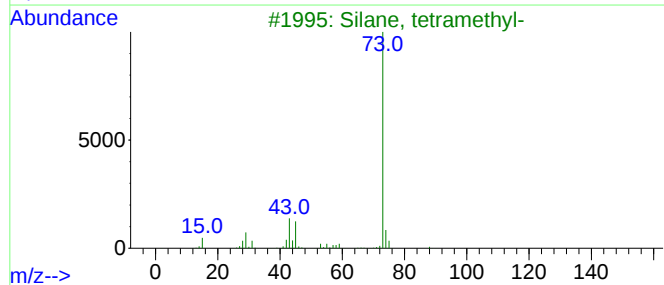
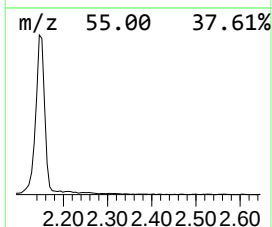
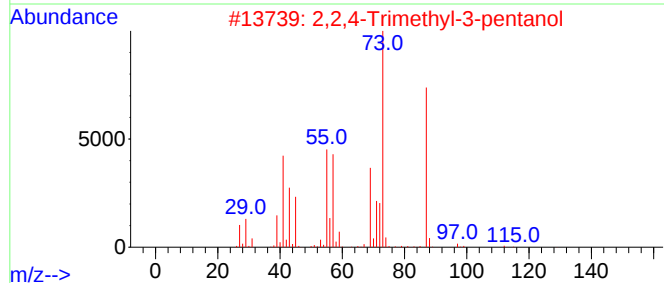
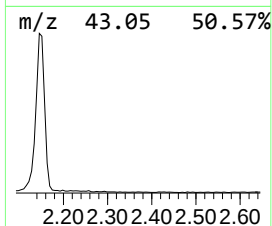
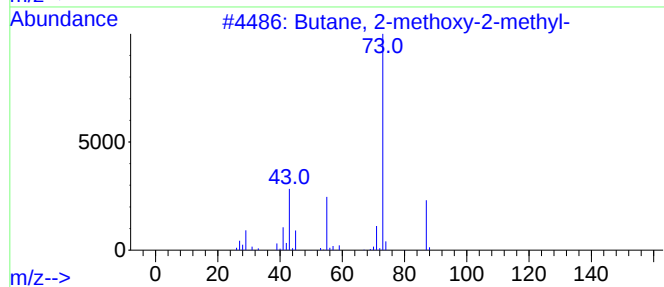
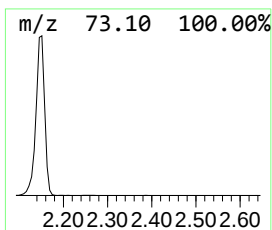
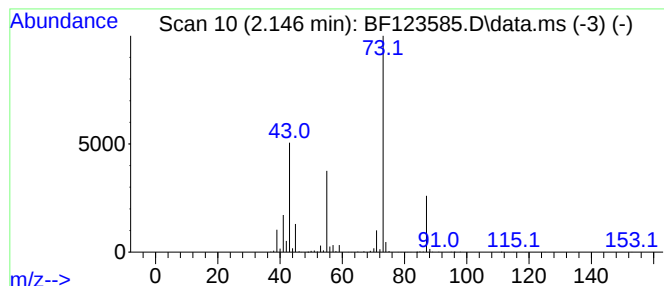
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	36.82 ng	2461280	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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	32
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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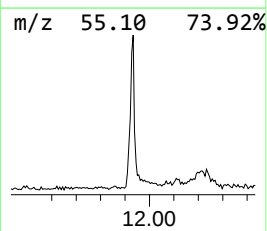
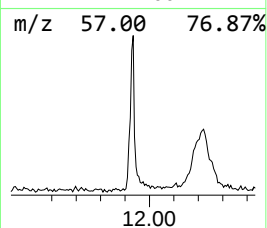
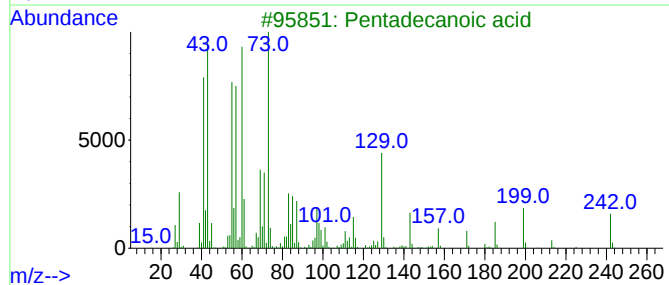
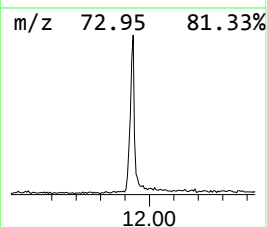
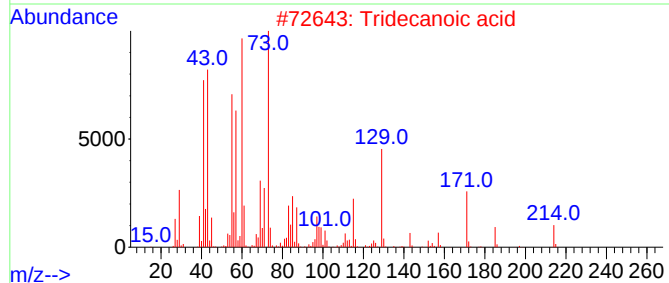
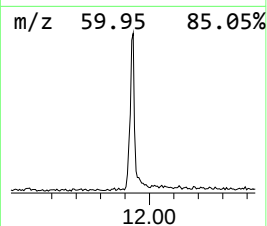
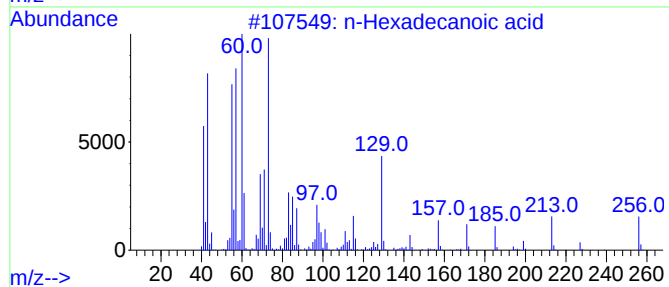
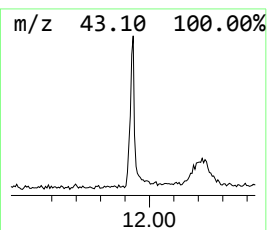
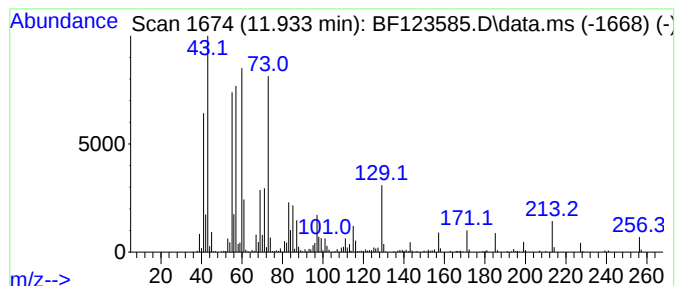
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.933	11.72 ng	1203810	Phenanthrene-d10		11.404	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	96
2	Tridecanoic acid		214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Undecanoic acid		186	C11H22O2	000112-37-8	64
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	64



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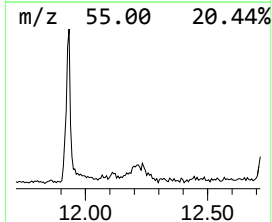
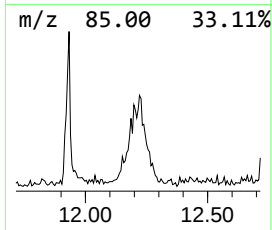
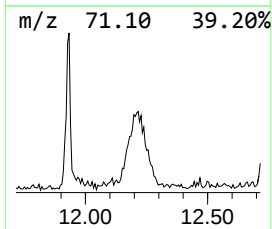
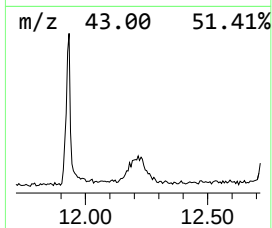
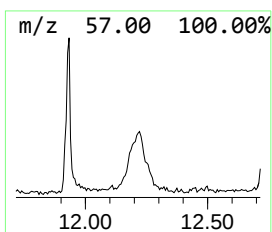
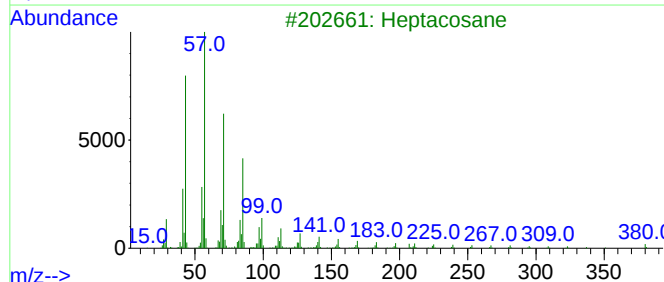
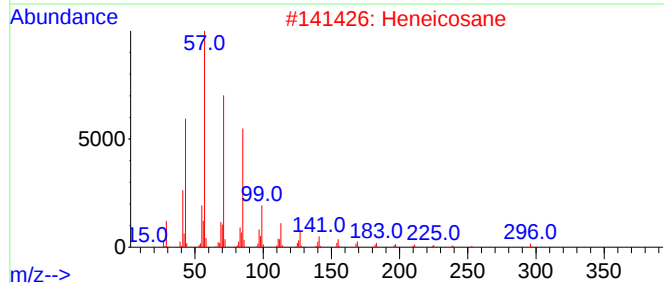
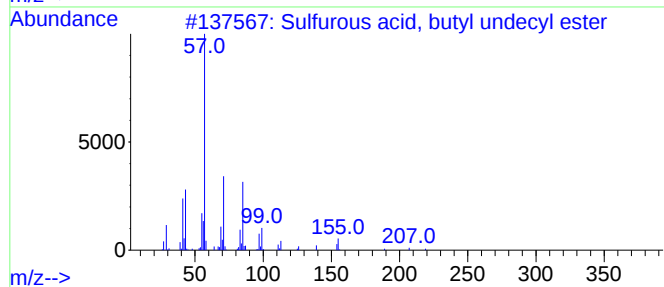
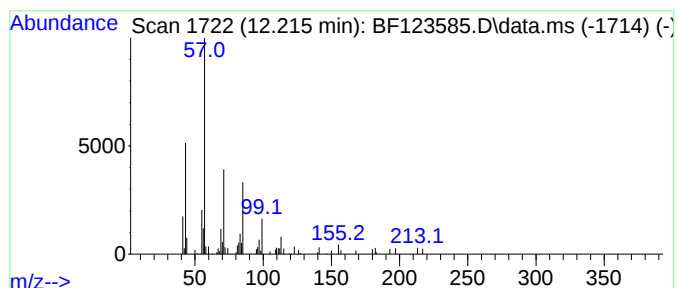
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Sulfurous acid, butyl undec... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.216	5.34 ng	548506	Phenanthrene-d10		11.404	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl undecyl ester		292	C15H32O3S	1000309-17-8	90
2	Heneicosane		296	C21H44	000629-94-7	80
3	Heptacosane		380	C27H56	000593-49-7	80
4	2-methyloctacosane		408	C29H60	1000376-72-8	72
5	Tetradecane, 6,9-dimethyl-		226	C16H34	055045-13-1	72



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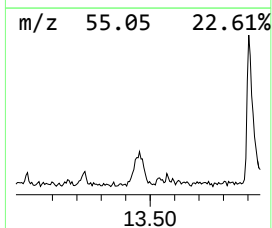
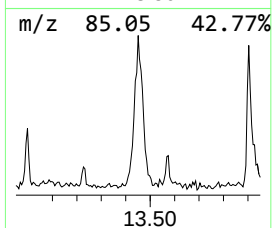
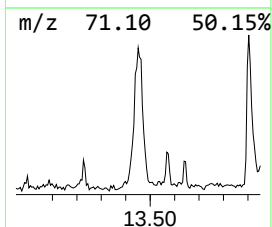
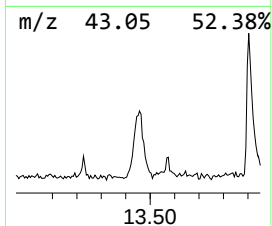
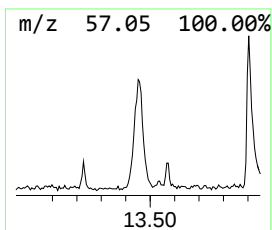
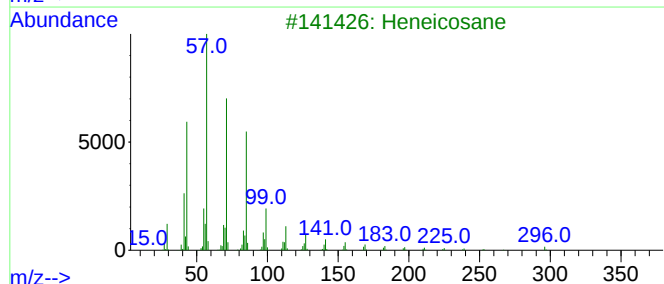
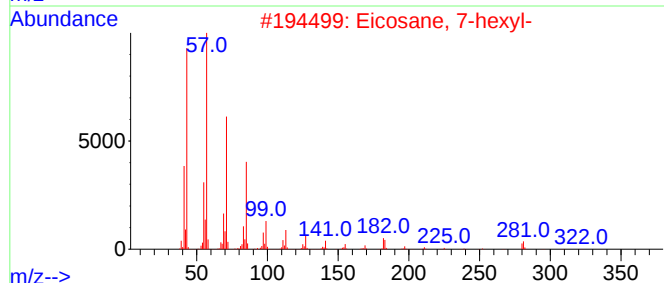
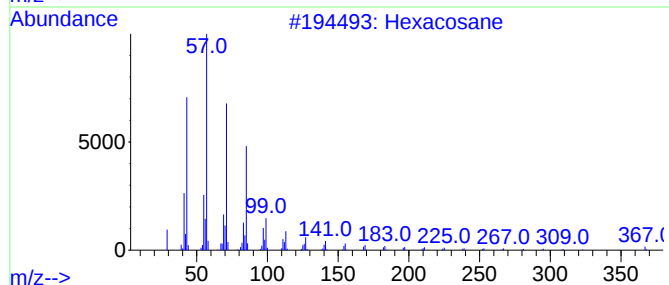
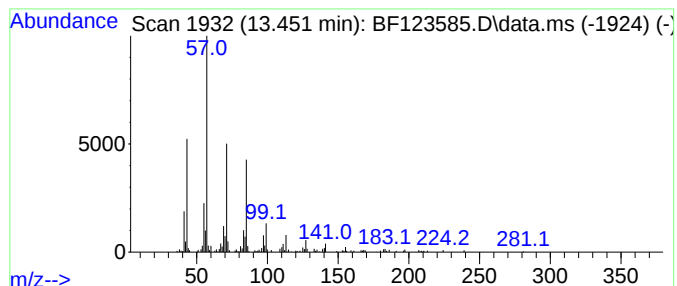
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Peak Number 4 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.451	8.01 ng	670181	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3			Heneicosane	296	C21H44	000629-94-7	87
4			Hexadecane	226	C16H34	000544-76-3	86
5			Heptadecane	240	C17H36	000629-78-7	80



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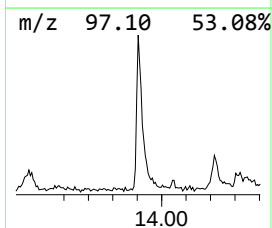
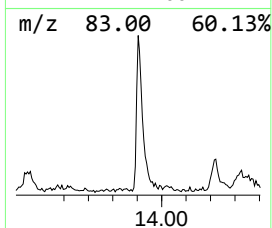
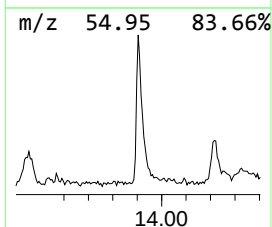
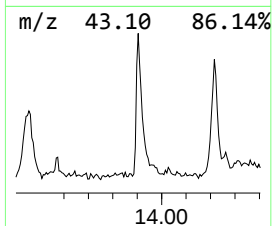
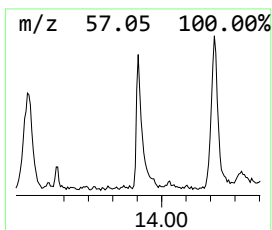
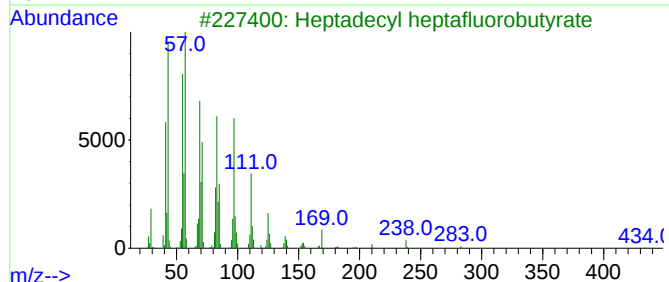
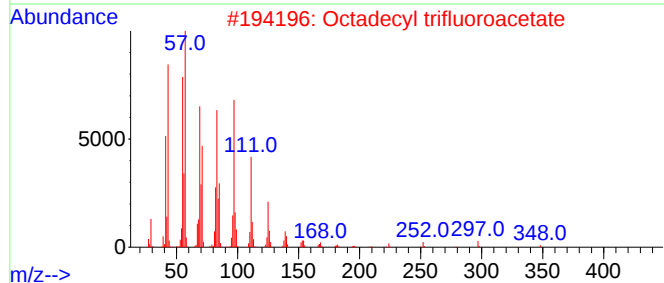
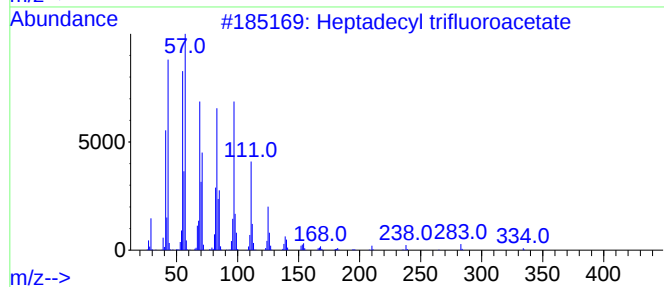
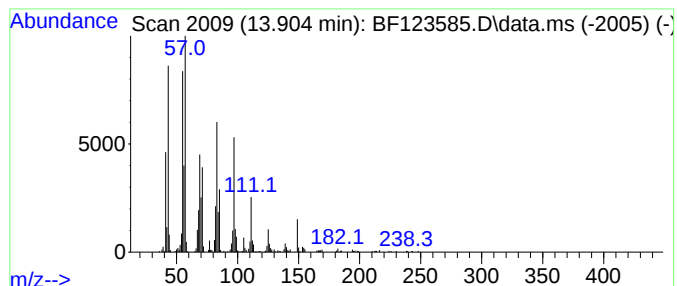
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Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.904	13.19 ng	1103820	Chrysene-d12		14.051	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate		352	C19H35F3O2	1000351-87-0	91
2	Octadecyl trifluoroacetate		366	C20H37F3O2	079392-43-1	91
3	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	91
4	17-Pentatriacontene		491	C35H70	006971-40-0	90
5	Heneicosyl heptafluorobutyrate		508	C25H43F7O2	1000351-83-8	87



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ClientSampleId :
SB-02-13.5-14.0

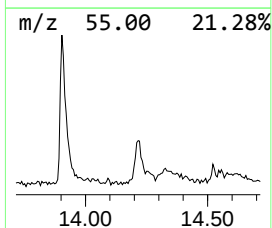
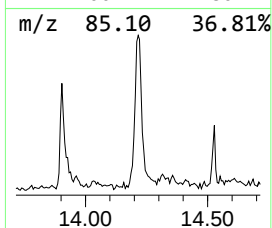
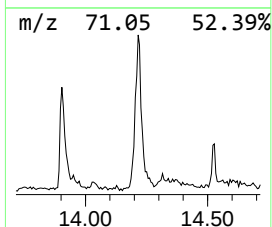
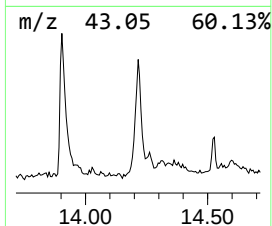
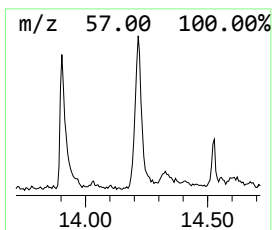
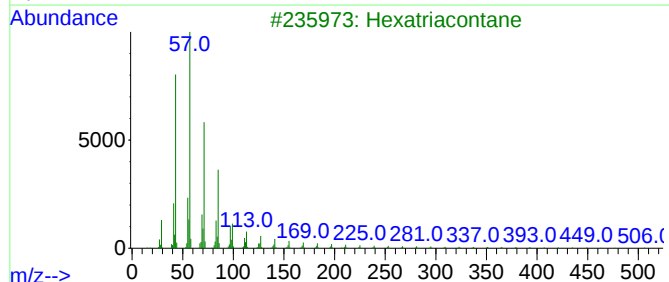
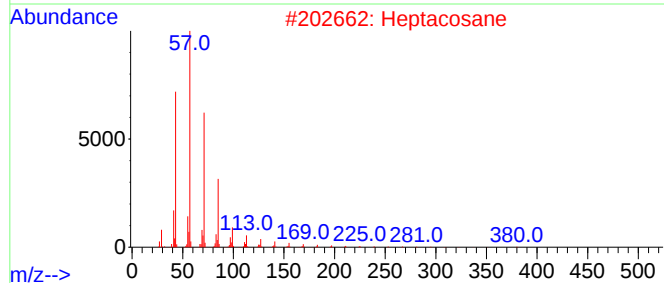
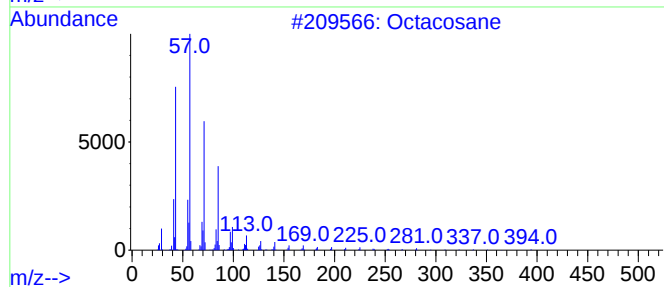
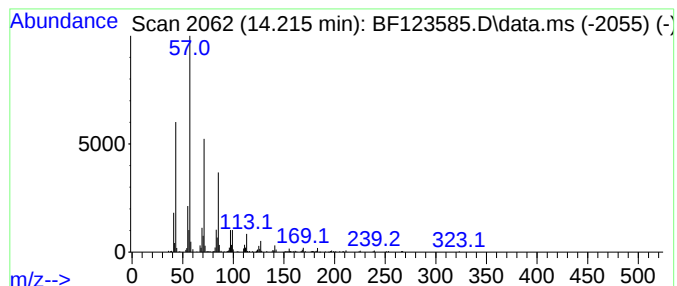
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.215	8.53 ng	713776	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Hexatriacontane	507	C36H74	000630-06-8	91
4			Heneicosane	296	C21H44	000629-94-7	90
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123585.D
Acq On : 16 Apr 2021 11:06
Operator : JU/CG
Sample : M2048-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-13.5-14.0

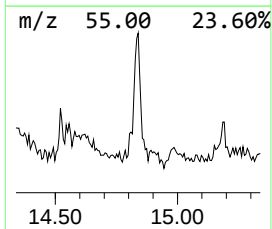
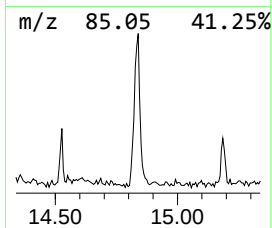
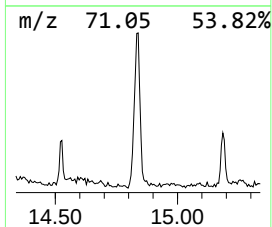
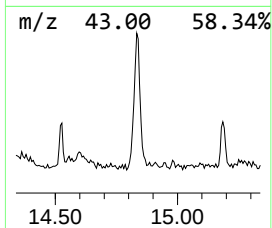
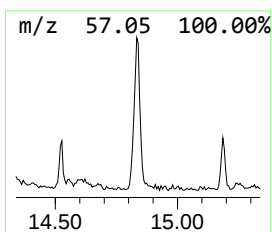
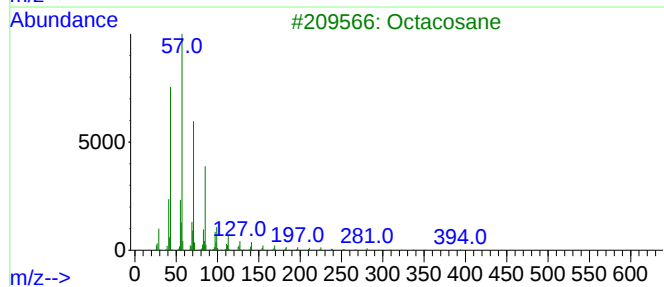
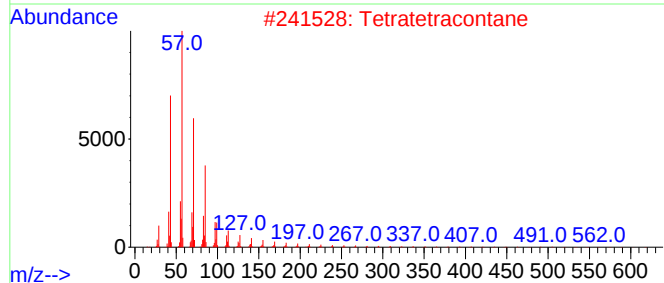
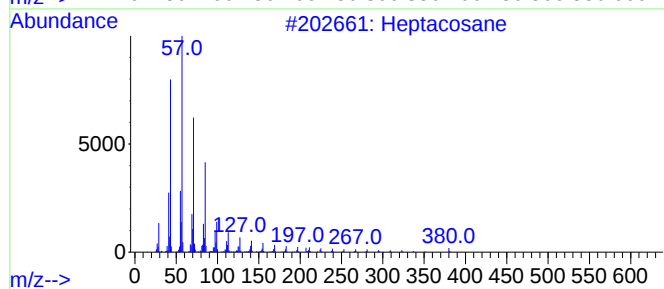
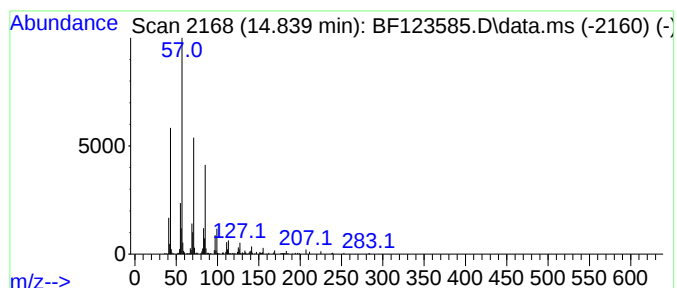
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	8.90 ng	723547	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123585.D
Acq On : 16 Apr 2021 11:06
Operator : JU/CG
Sample : M2048-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-02-13.5-14.0

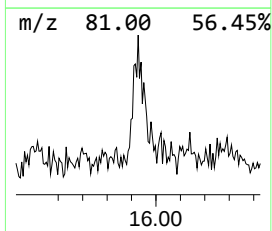
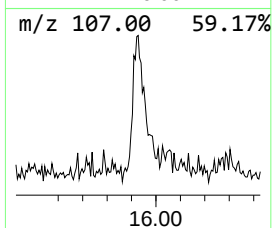
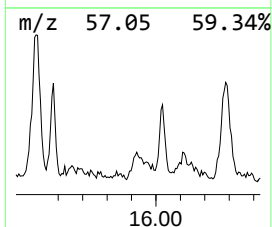
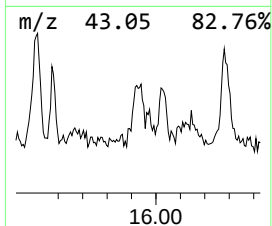
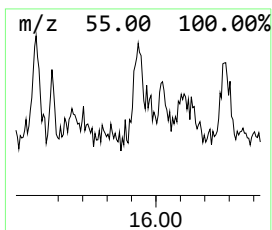
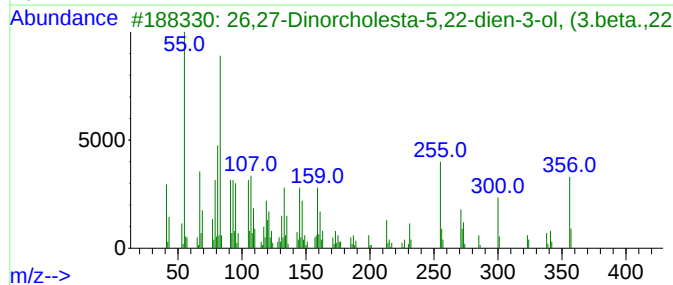
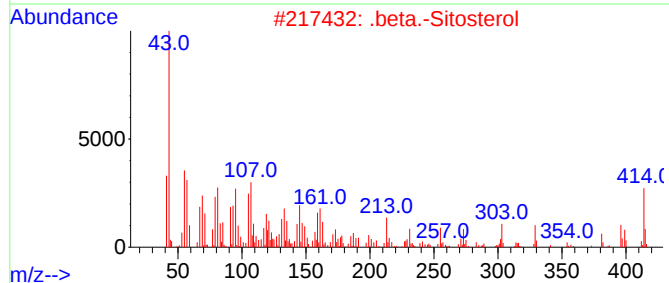
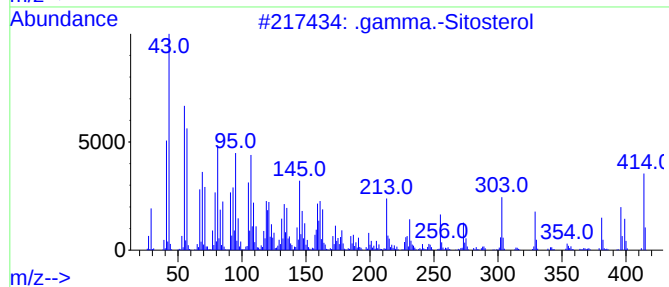
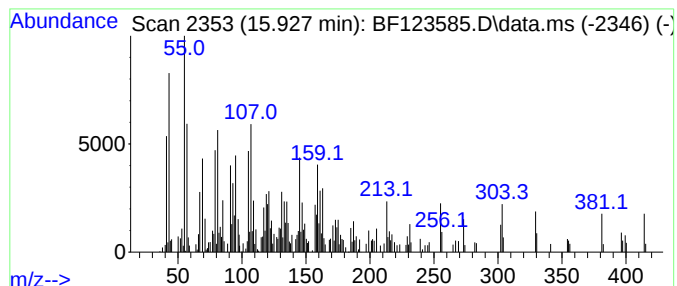
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .gamma.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.927	8.37 ng	680099	Perylene-d12	15.533

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	55
3		26,27-Dinorcholesta-5,22-dien-3-...	356	C25H40O	057597-10-1	53
4		5-Cholestene-3-ol, 24-methyl-	400	C28H48O	1000214-17-4	47
5		Isocholesteryl methyl ether	400	C28H48O	029944-53-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123585.D
Acq On : 16 Apr 2021 11:06
Operator : JU/CG
Sample : M2048-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

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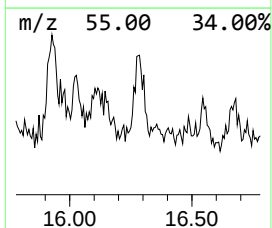
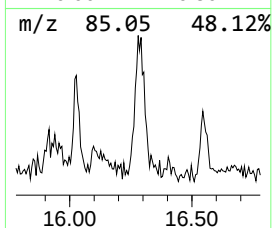
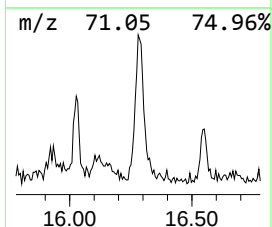
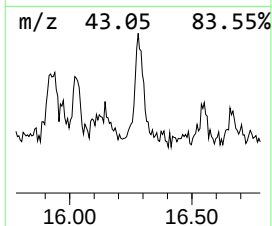
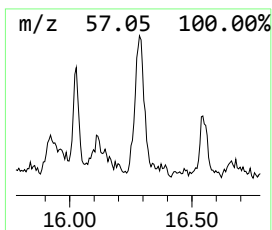
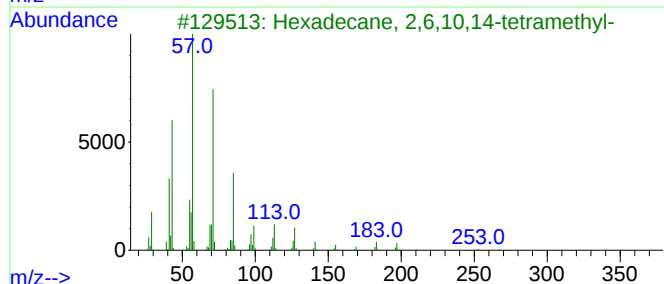
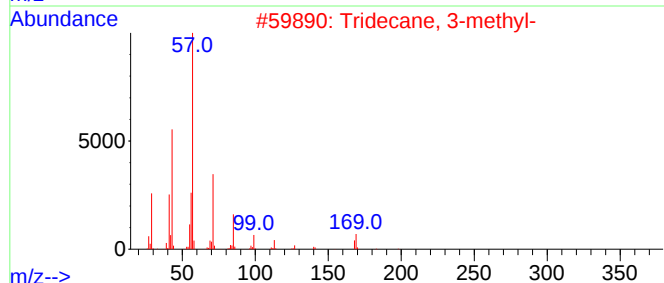
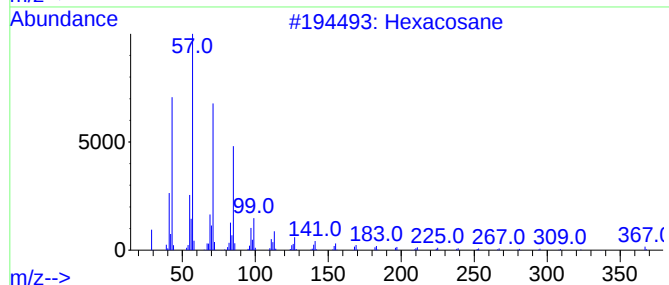
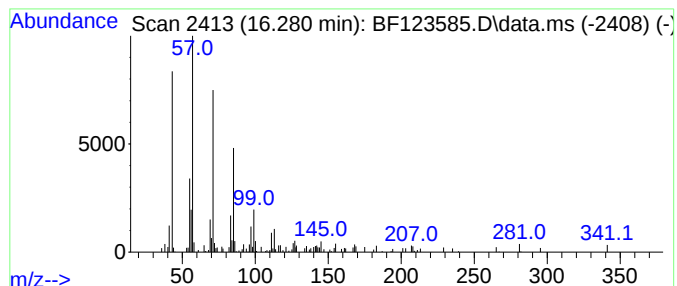
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.280	4.40 ng	357353	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Tridecane, 3-methyl-	198	C14H30	006418-41-3	87
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
4			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	80
5			Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123585.D
Acq On : 16 Apr 2021 11:06
Operator : JU/CG
Sample : M2048-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

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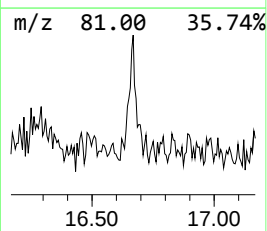
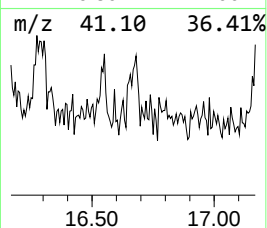
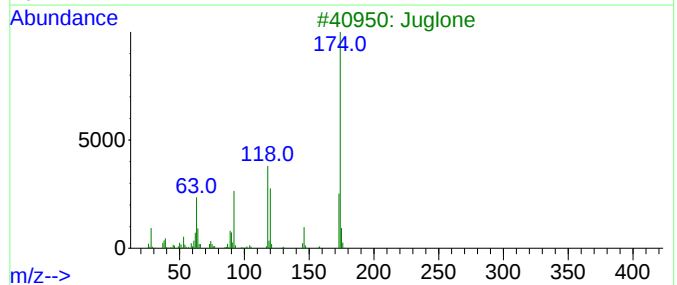
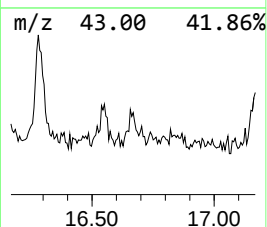
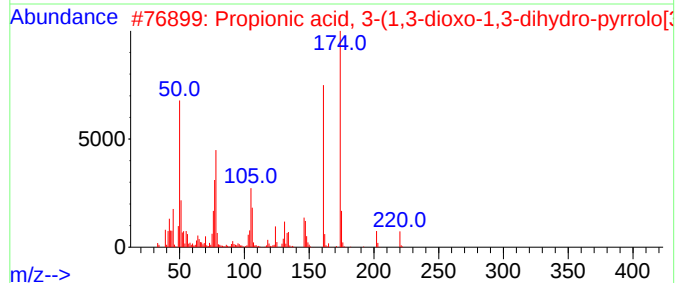
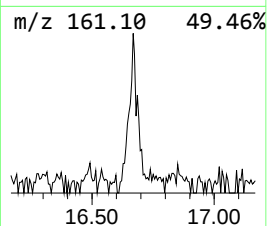
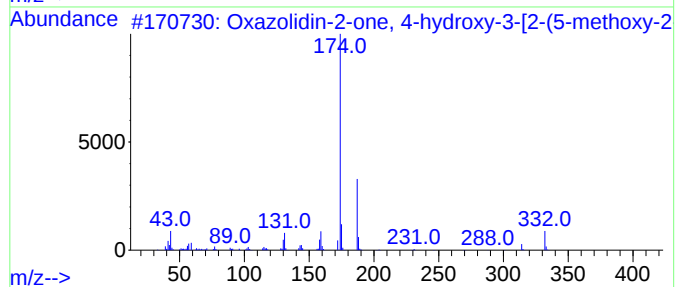
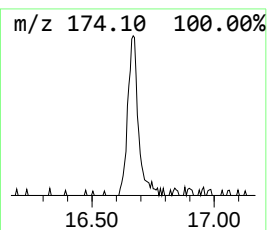
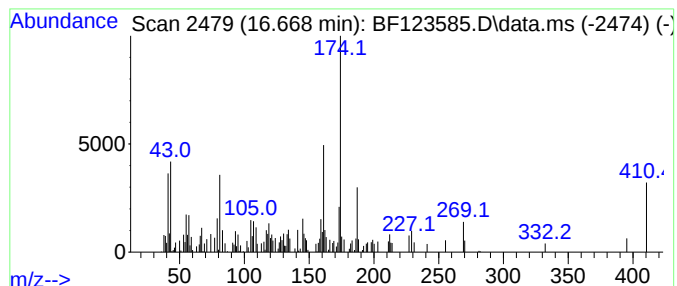
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.668 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.668	2.87 ng	233573	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxazolidin-2-one, 4-hydroxy-3-[2...	332	C18H24N2O4	1000310-03-3	41
2			Propionic acid, 3-(1,3-dioxo-1,3...	220	C10H8N2O4	1000310-02-2	37
3			Juglone	174	C10H6O3	000481-39-0	35
4			8-Quinolinol, 2-(aminomethyl)-	174	C10H10N2O	017018-81-4	35
5			2-(5-Amino-[1,3,4]thiadiazol-2-y...	314	C11H11ClN4O5	328281-60-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
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Acq On : 16 Apr 2021 11:06
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Sample : M2048-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

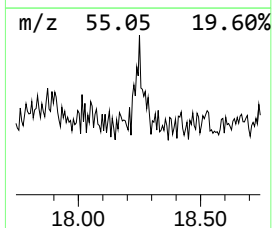
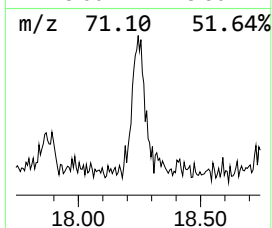
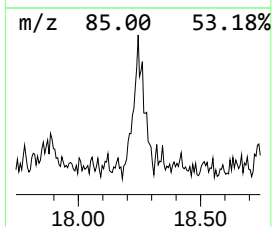
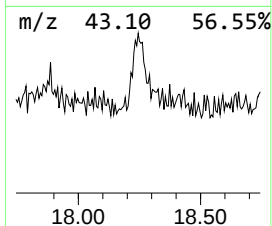
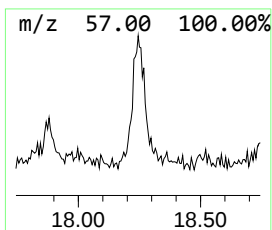
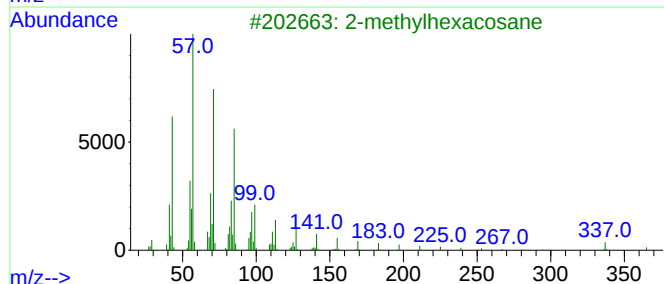
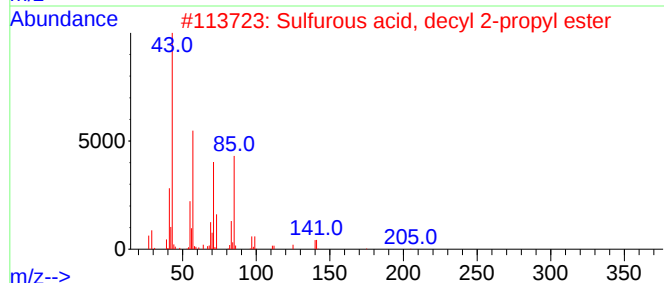
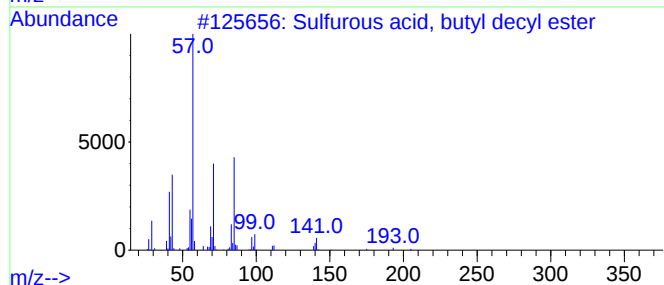
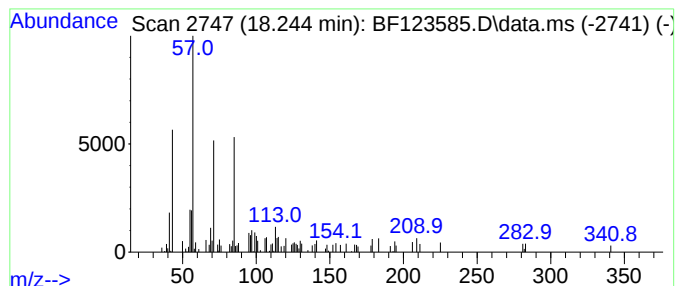
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Sulfurous acid, butyl decyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.244	2.29 ng	186429	Perylene-d12	15.533	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	72
2	Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	53
3	2-methylhexacosane	380	C27H56	1000376-72-7	53
4	Eicosane	282	C20H42	000112-95-8	52
5	2-methyloctacosane	408	C29H60	1000376-72-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123585.D
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 Operator : JU/CG
 Sample : M2048-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	36.8	ng	2461280	1	6.869	1336960	20.0
n-Hexadecanoic ...	11.933	11.7	ng	1203810	4	11.404	2054810	20.0
Sulfurous acid,...	12.216	5.3	ng	548506	4	11.404	2054810	20.0
Hexacosane	13.451	8.0	ng	670181	5	14.051	1673280	20.0
Heptadecyl trif...	13.904	13.2	ng	1103820	5	14.051	1673280	20.0
Octacosane	14.215	8.5	ng	713776	5	14.051	1673280	20.0
Heptacosane	14.839	8.9	ng	723547	6	15.533	1625950	20.0
.gamma.-Sitosterol	15.927	8.4	ng	680099	6	15.533	1625950	20.0
Tridecane, 3-me...	16.280	4.4	ng	357353	6	15.533	1625950	20.0
unknown16.668	16.668	2.9	ng	233573	6	15.533	1625950	20.0
Sulfurous acid,...	18.244	2.3	ng	186429	6	15.533	1625950	20.0