

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012021\
 Data File : BG047942.D
 Acq On : 20 Jan 2021 18:14
 Operator : CG/JU
 Sample : M1160-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BASIN-6

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_G\METHODS\8270-BG012021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047942.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.106	293	301	306	rBV3	20449	39704	1.39%	0.259%
2	5.705	395	403	415	rVB	672645	1090530	38.27%	7.110%
3	6.534	531	544	551	rBV2	47370	133775	4.69%	0.872%
4	7.292	665	673	684	rBV	701257	1195024	41.94%	7.791%
5	8.149	813	819	826	rVB	172411	292057	10.25%	1.904%
6	8.901	940	947	952	rBV3	16707	29932	1.05%	0.195%
7	9.313	1007	1017	1024	rBV	403113	704242	24.72%	4.592%
8	10.964	1290	1298	1305	rBV	221742	397459	13.95%	2.591%
9	13.402	1703	1713	1719	rBV	1059663	1612789	56.60%	10.515%
10	14.213	1846	1851	1863	rVB	59340	88445	3.10%	0.577%
11	14.771	1937	1946	1954	rBV	381223	575697	20.20%	3.753%
12	16.252	2190	2198	2206	rBV	861113	1313870	46.11%	8.566%
13	17.515	2407	2413	2419	rBV	503756	764674	26.84%	4.986%
14	18.396	2557	2563	2570	rBV	140984	206387	7.24%	1.346%
15	19.659	2774	2778	2784	rBV3	49066	66973	2.35%	0.437%
16	20.024	2834	2840	2845	rVB	70950	86844	3.05%	0.566%
17	20.118	2849	2856	2862	rBV	2253365	2849418	100.00%	18.578%
18	20.970	2997	3001	3006	rBV4	21799	32103	1.13%	0.209%
19	21.434	3074	3080	3097	rBV	156794	280466	9.84%	1.829%
20	21.792	3135	3141	3149	rBV2	569973	939827	32.98%	6.128%
21	22.656	3282	3288	3296	rBV4	77221	169485	5.95%	1.105%
22	23.725	3464	3470	3478	rVB7	23874	49834	1.75%	0.325%
23	24.213	3545	3553	3570	rBV	253175	641781	22.52%	4.184%
24	25.100	3692	3704	3715	rBV2	308628	905592	31.78%	5.904%
25	25.200	3717	3721	3728	rVB6	12024	28751	1.01%	0.187%
26	25.741	3805	3813	3821	rVB9	28661	76991	2.70%	0.502%
27	26.393	3912	3924	3935	rVV3	97548	314763	11.05%	2.052%
28	26.498	3935	3942	3954	rVB9	26165	93452	3.28%	0.609%
29	28.625	4298	4304	4318	rVB10	19152	66406	2.33%	0.433%
30	30.664	4636	4651	4667	rBV10	56708	290543	10.20%	1.894%

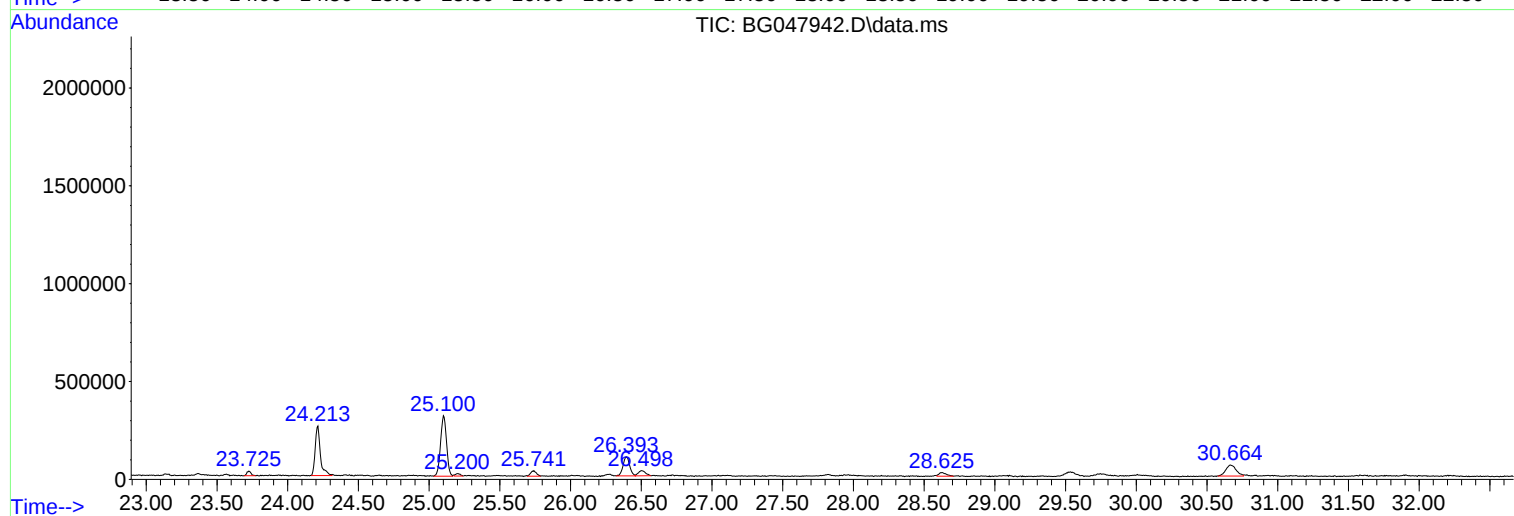
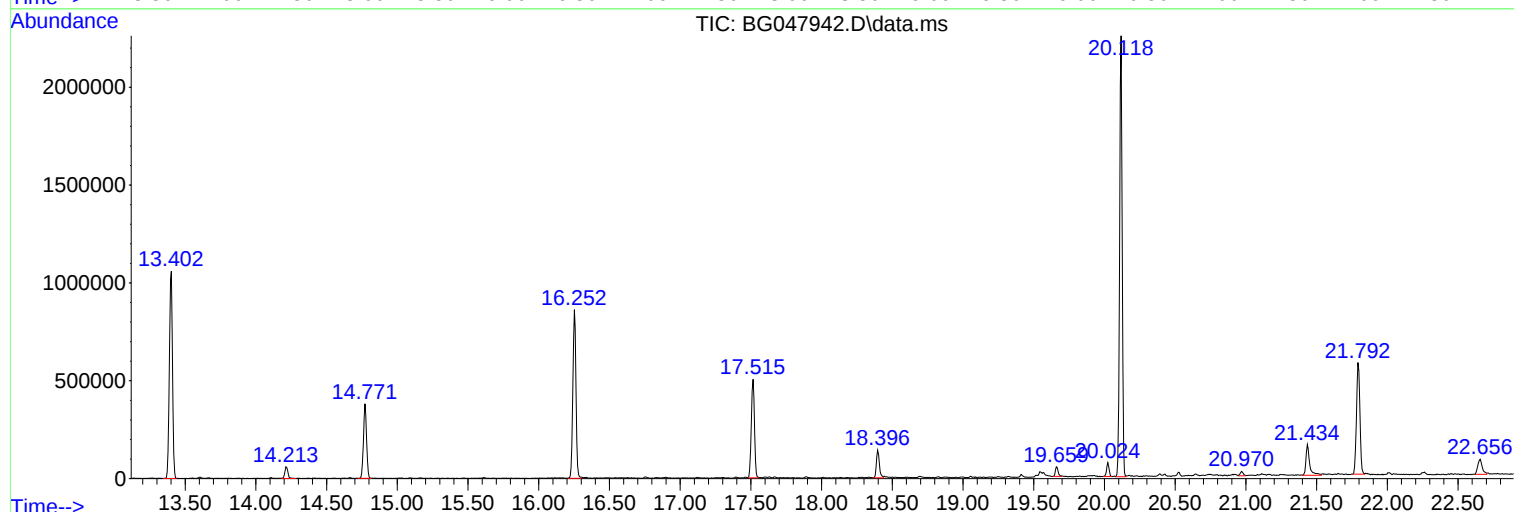
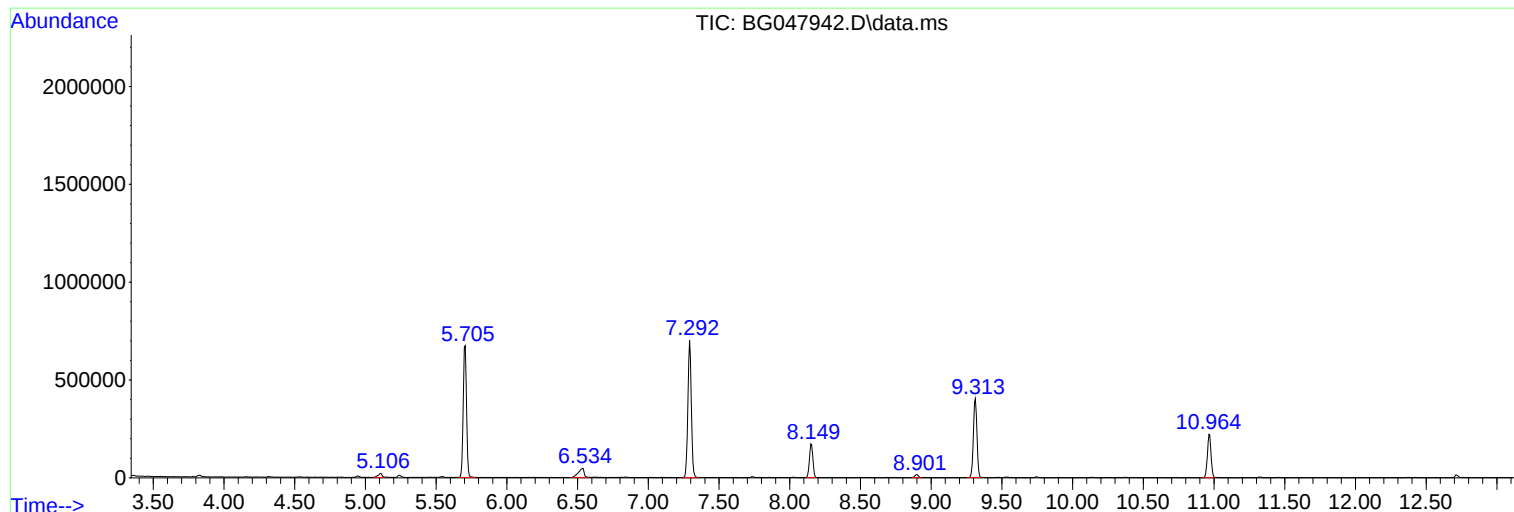
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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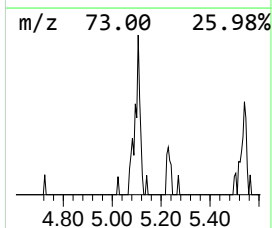
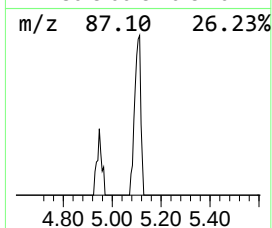
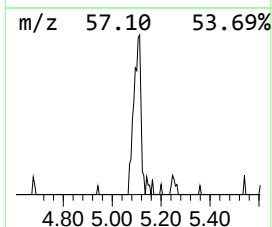
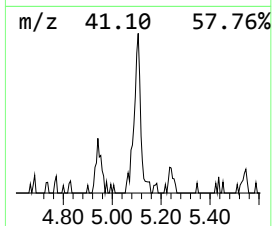
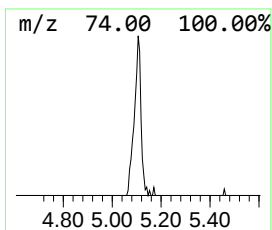
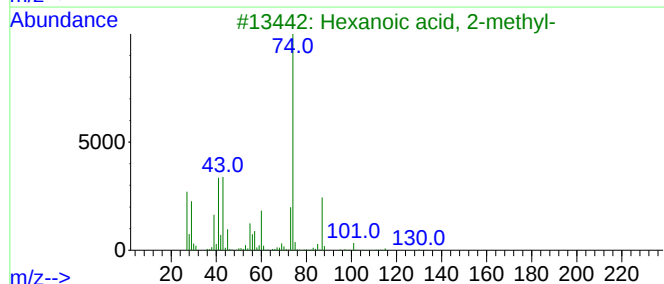
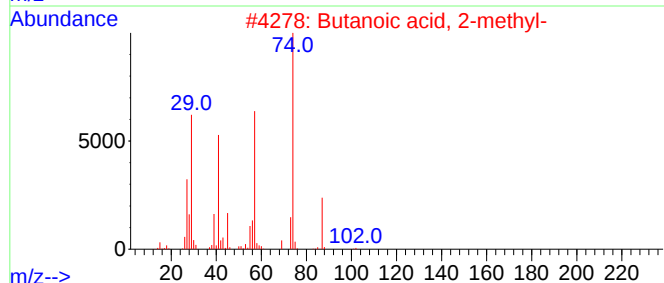
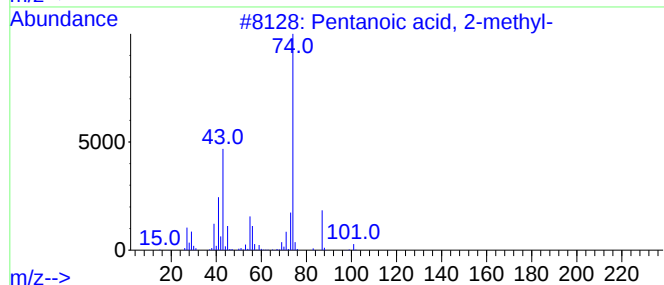
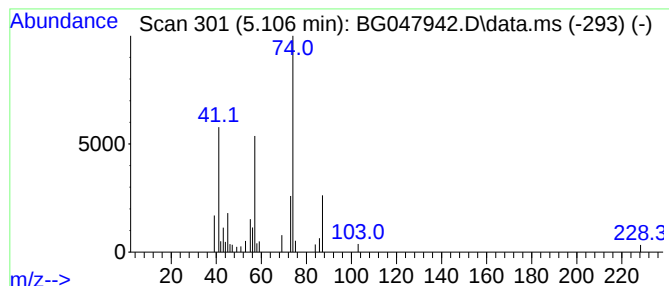
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butanoic acid, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.106	2.72 ng	39704	1,4-Dichlorobenzene-d4	8.149

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	64
2			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	64
3			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	56
4			Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	45
5			Methyl valerate	116	C6H12O2	000624-24-8	38



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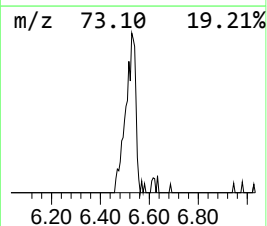
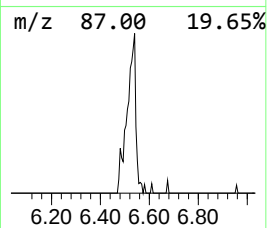
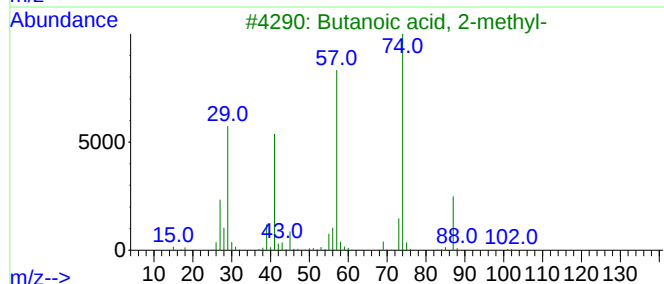
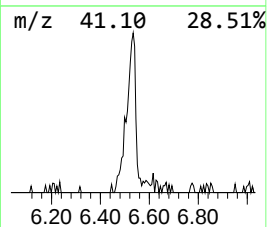
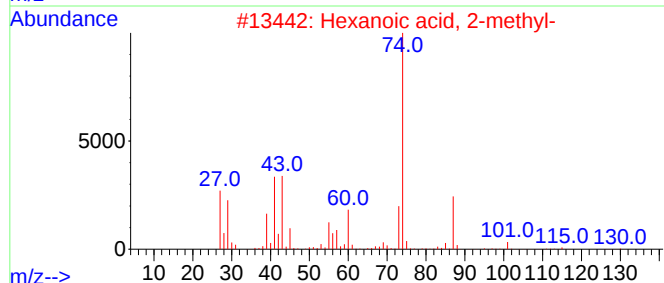
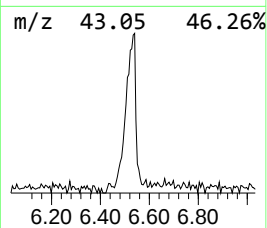
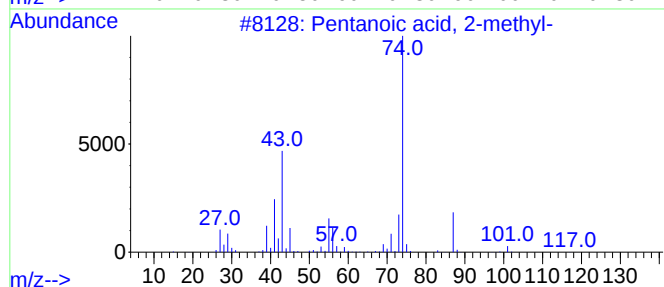
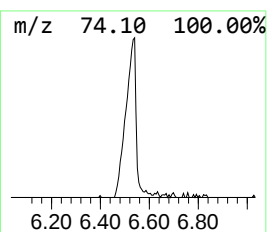
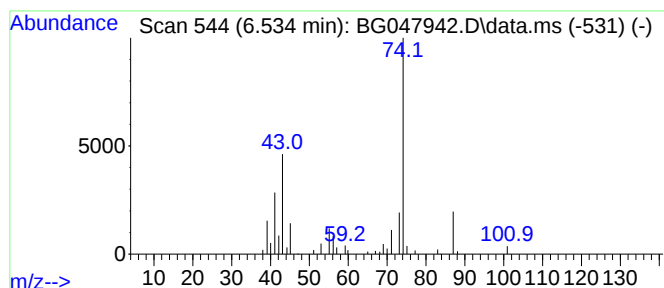
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentanoic acid, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.534	9.16 ng	133775	1,4-Dichlorobenzene-d4	8.149

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	83
2			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72
3			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	45
4			2-Methylheptanoic acid	144	C8H16O2	001188-02-9	38
5			Propanoic acid	74	C3H6O2	000079-09-4	9



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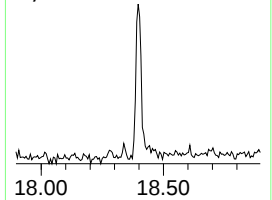
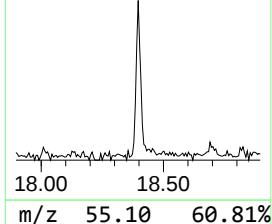
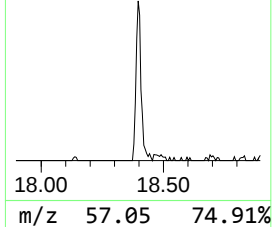
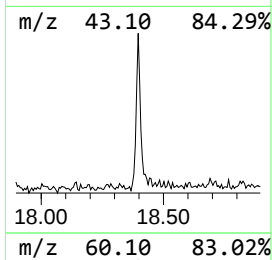
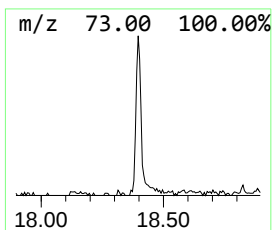
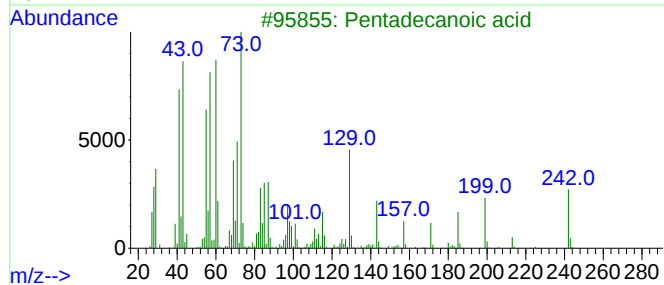
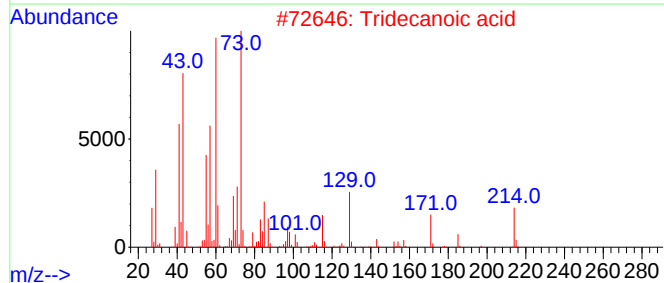
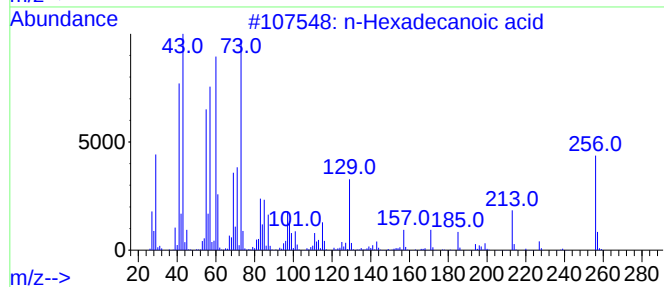
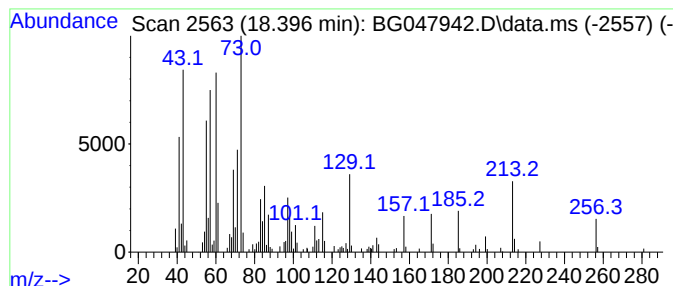
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.396	5.40 ng	206387	Phenanthrene-d10	17.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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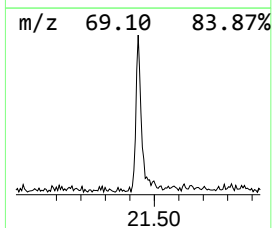
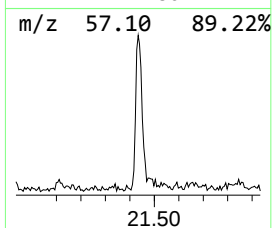
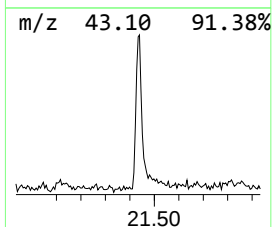
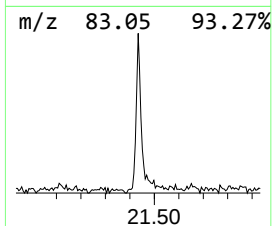
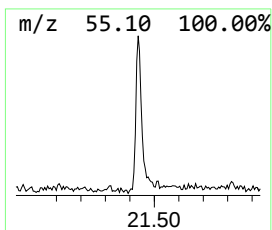
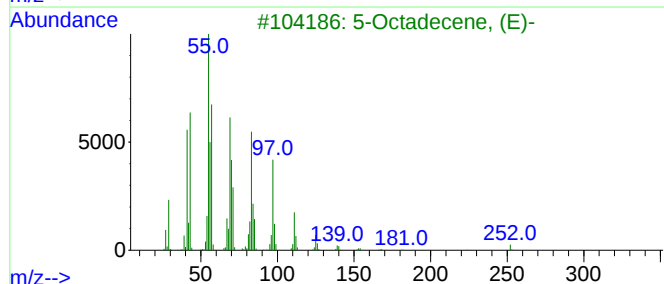
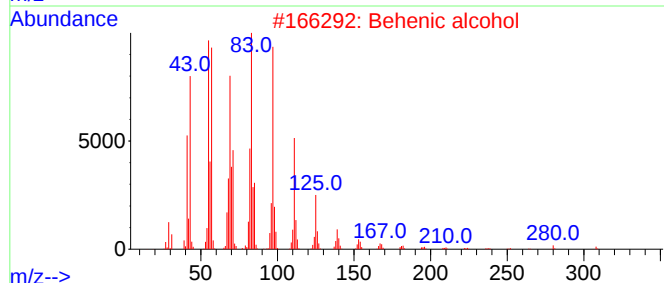
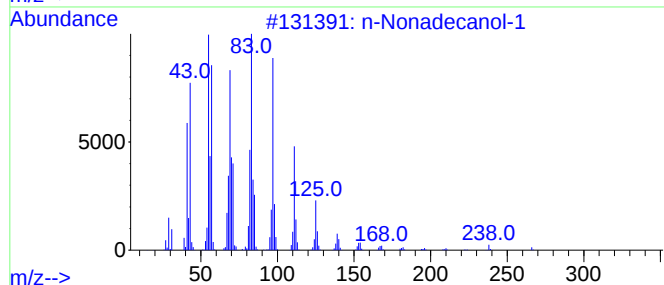
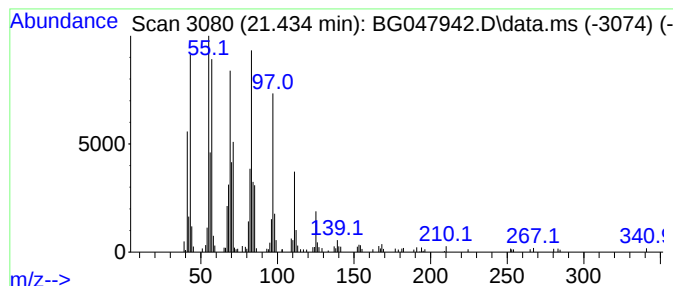
Instrument :
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.434	5.97 ng	280466	Chrysene-d12	21.792	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	1-Nonadecene	266	C19H38	018435-45-5	91



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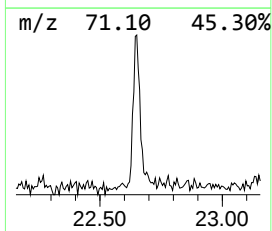
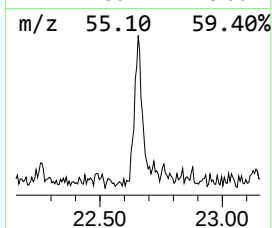
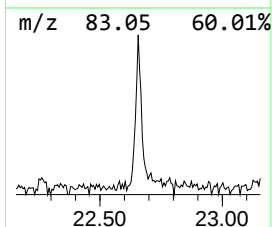
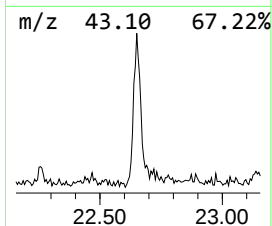
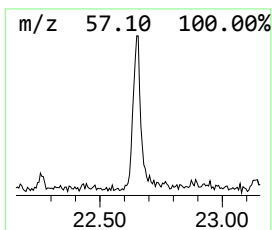
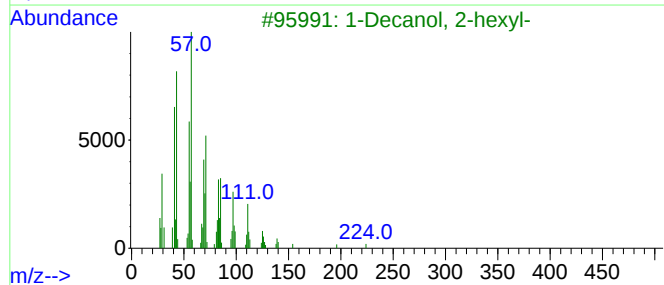
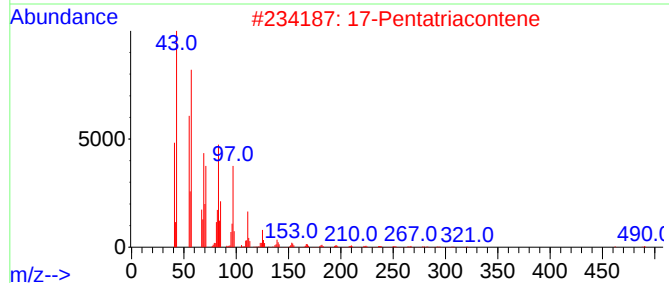
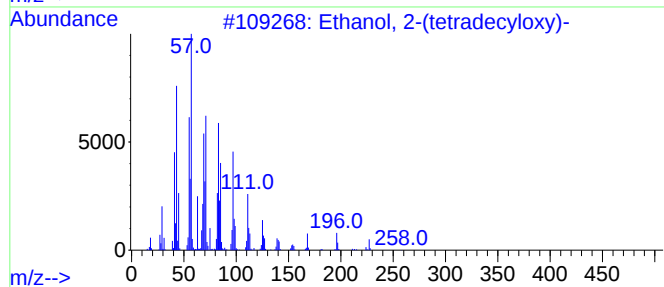
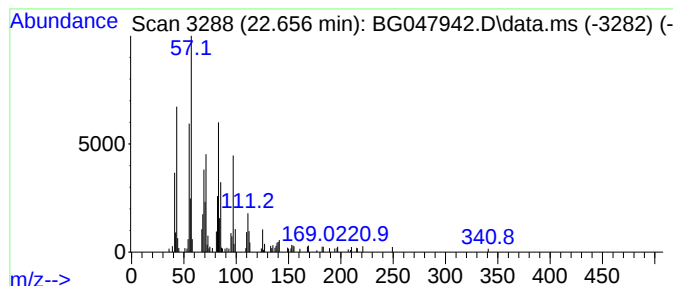
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.656	3.61 ng	169485	Chrysene-d12	21.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2			17-Pentatriacontene	491	C35H70	006971-40-0	80
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	74
4			1-Tricosene	322	C23H46	018835-32-0	68
5			2-Hexyl-1-octanol	214	C14H30O	019780-79-1	68



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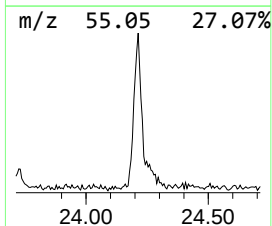
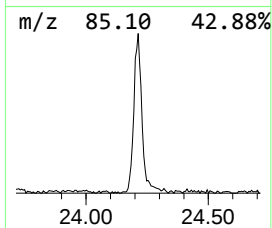
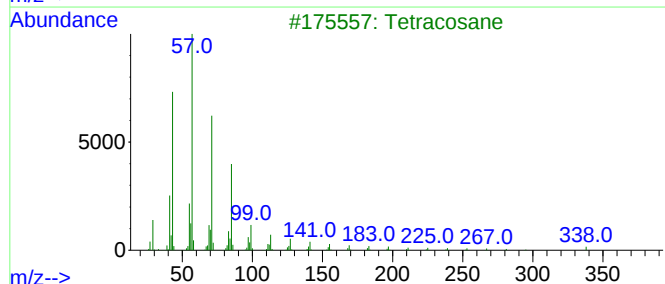
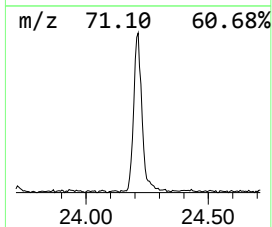
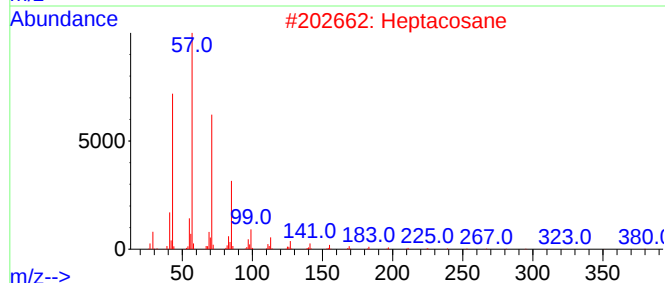
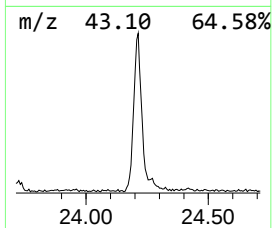
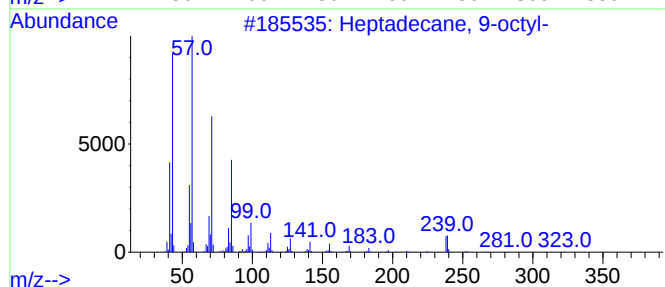
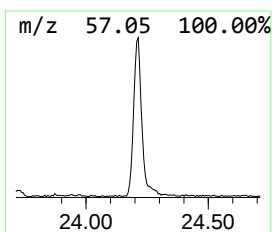
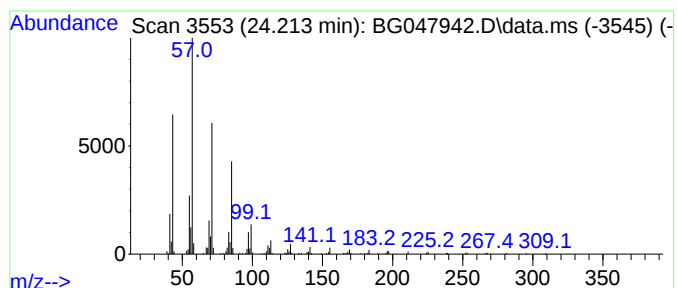
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.213	14.17 ng	641781	Perylene-d12	25.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Tetracosane	338	C24H50	000646-31-1	90
4			Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90
5			Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012021\
Data File : BG047942.D
Acq On : 20 Jan 2021 18:14
Operator : CG/JU
Sample : M1160-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BASIN-6

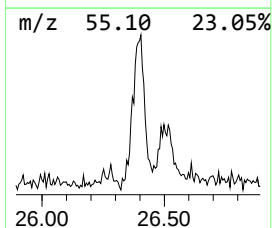
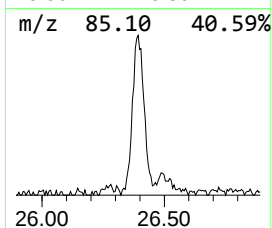
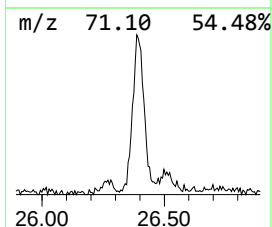
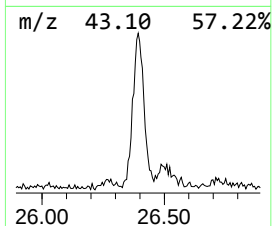
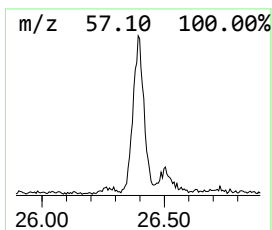
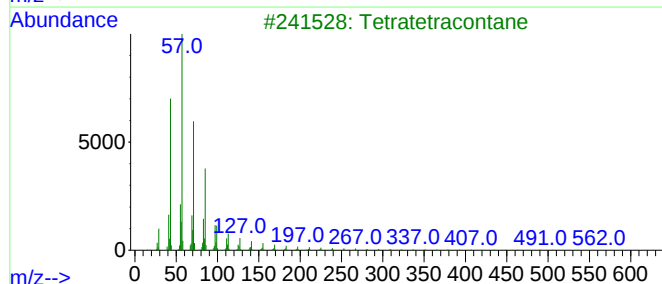
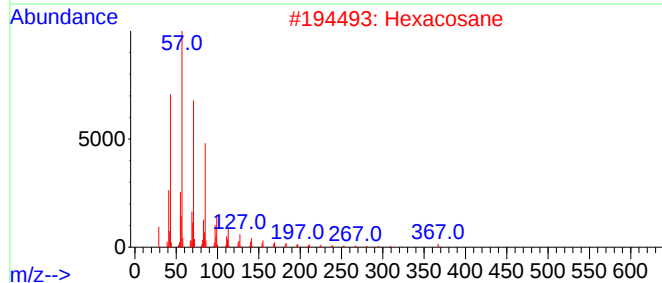
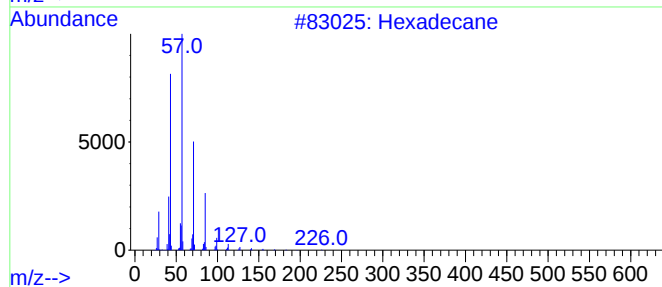
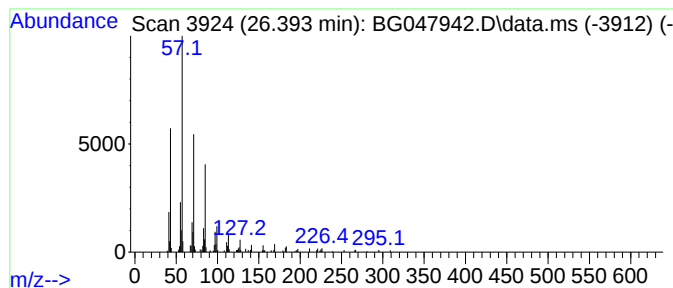
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.393	6.95 ng	314763	Perylene-d12	25.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	95
2			Hexacosane	366	C26H54	000630-01-3	93
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Tetracosane	338	C24H50	000646-31-1	90
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012021\
Data File : BG047942.D
Acq On : 20 Jan 2021 18:14
Operator : CG/JU
Sample : M1160-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BASIN-6

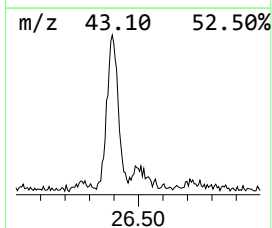
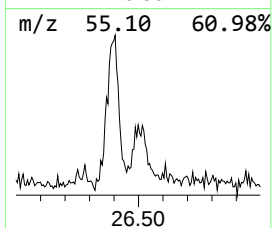
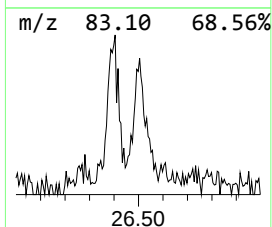
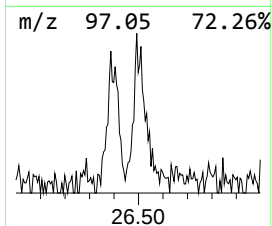
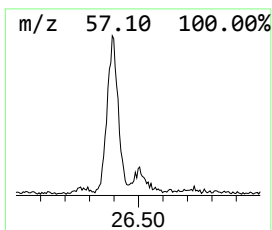
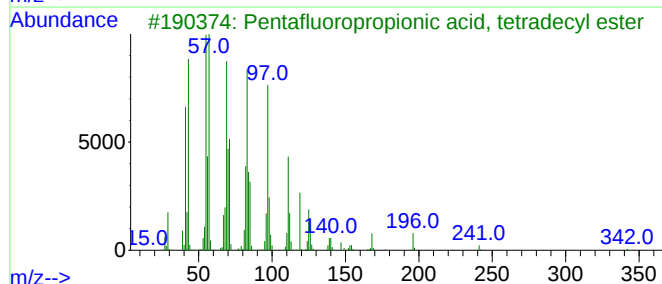
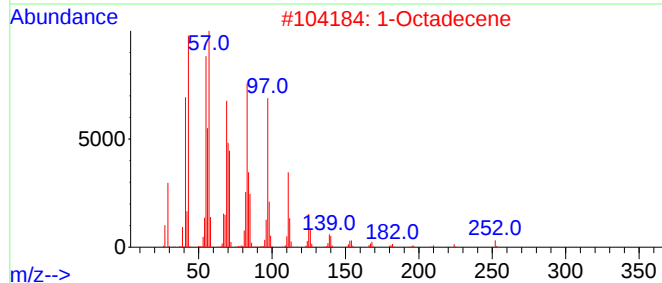
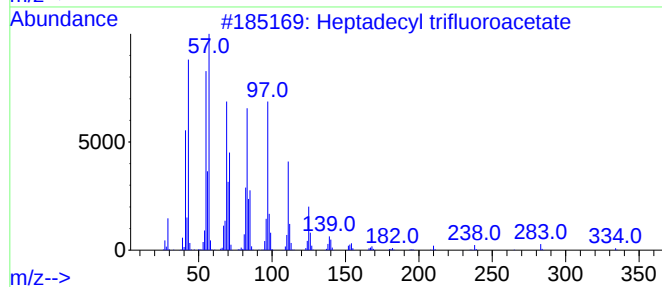
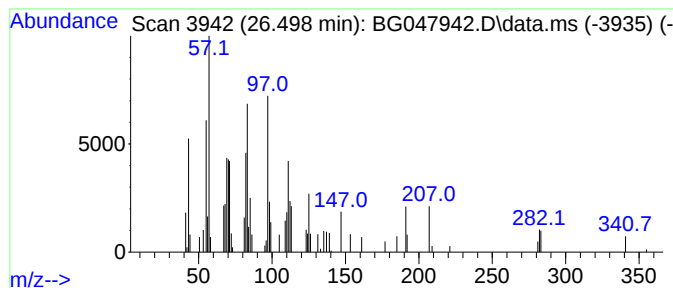
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown26.49 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.499	2.06 ng	93452	Perylene-d12	25.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	49
2			1-Octadecene	252	C18H36	000112-88-9	49
3			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	47
4			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	47
5			n-Pentadecanol	228	C15H32O	000629-76-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012021\
Data File : BG047942.D
Acq On : 20 Jan 2021 18:14
Operator : CG/JU
Sample : M1160-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

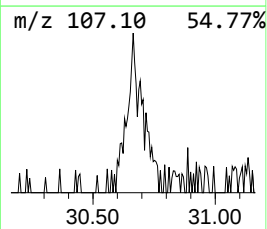
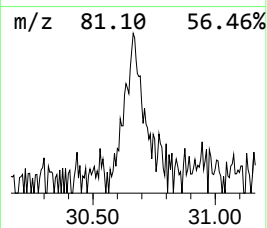
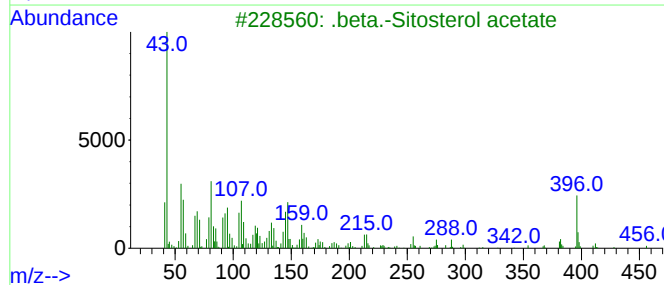
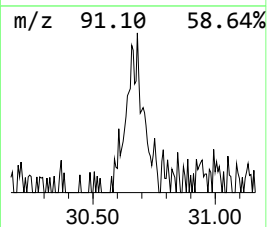
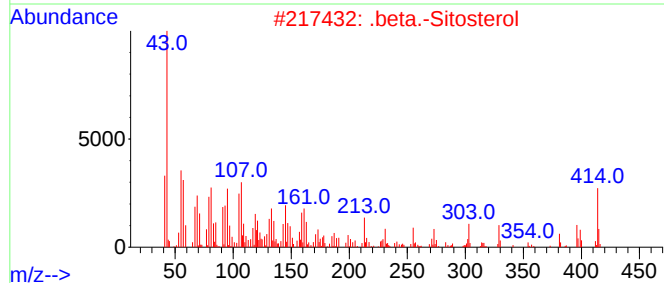
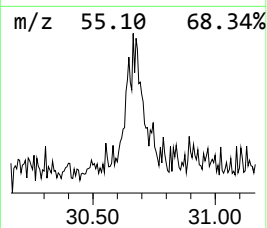
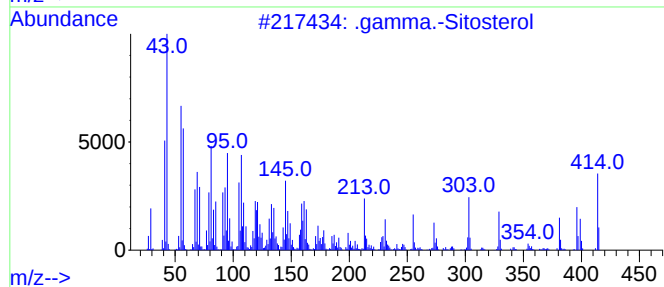
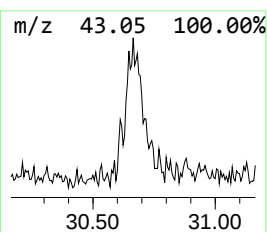
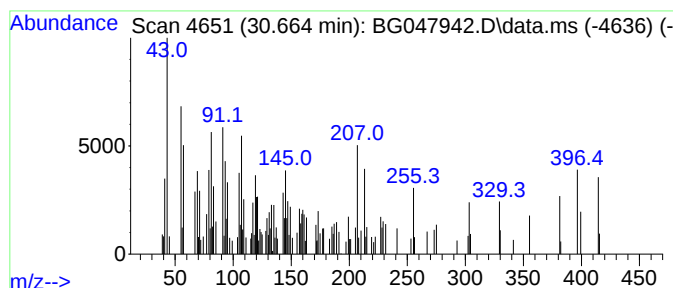
Instrument :
BNA_G
ClientSampleId :
BASIN-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .gamma.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
30.664	6.42 ng	290543	Perylene-d12	25.100	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	55
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	38
3	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	14
4	22,26-Oxido-4,17-cholestadien-3...	414	C27H42O3	1000252-80-4	11
5	Piperidine, 4-butoxy-4-[4-(ethox...	381	C25H35NO2	1000115-53-7	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012021\
Data File : BG047942.D
Acq On : 20 Jan 2021 18:14
Operator : CG/JU
Sample : M1160-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BASIN-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012021.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
Butanoic acid, ...	5.106	2.7	ng	39704	1	8.149	292057	20.0
Pentanoic acid,...	6.534	9.2	ng	133775	1	8.149	292057	20.0
n-Hexadecanoic ...	18.396	5.4	ng	206387	4	17.515	764674	20.0
n-Nonadecanol-1	21.434	6.0	ng	280466	5	21.792	939827	20.0
Ethanol, 2-(tet...	22.656	3.6	ng	169485	5	21.792	939827	20.0
Heptadecane, 9-...	24.213	14.2	ng	641781	6	25.100	905592	20.0
Hexadecane	26.393	7.0	ng	314763	6	25.100	905592	20.0
unknown26.49	26.499	2.1	ng	93452	6	25.100	905592	20.0
.gamma.-Sitosterol	30.664	6.4	ng	290543	6	25.100	905592	20.0