

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
 Data File : BG049169.D
 Acq On : 2 Jul 2021 16:07
 Operator : CG/JU
 Sample : M2875-20
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
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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_G\METHODS\8270-BG063021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049169.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.133	9	16	25	rVV	110079	262573	8.33%	1.354%
2	3.209	25	29	39	rVB	58455	108375	3.44%	0.559%
3	5.184	355	365	376	rBV	1734663	2978245	94.52%	15.356%
4	5.642	436	443	454	rBV	166610	316256	10.04%	1.631%
5	7.240	708	715	722	rBV	84684	151670	4.81%	0.782%
6	7.622	771	780	787	rBV2	30423	58884	1.87%	0.304%
7	8.086	852	859	867	rBV2	123258	217869	6.91%	1.123%
8	9.255	1051	1058	1066	rVB	484079	867753	27.54%	4.474%
9	10.906	1332	1339	1349	rBV	151909	286875	9.10%	1.479%
10	13.351	1748	1755	1763	rBV	1092712	1803512	57.24%	9.299%
11	14.731	1983	1990	1997	rBV2	256108	419932	13.33%	2.165%
12	16.224	2238	2244	2259	rVB3	236979	566857	17.99%	2.923%
13	17.481	2452	2458	2465	rVB	313963	506378	16.07%	2.611%
14	19.608	2816	2820	2840	rVB3	391651	1338876	42.49%	6.903%
15	20.084	2895	2901	2907	rVB	2333675	3150754	100.00%	16.246%
16	20.172	2912	2916	2926	rVB7	48554	99299	3.15%	0.512%
17	20.542	2974	2979	2980	rBV5	20952	32076	1.02%	0.165%
18	20.601	2982	2989	2996	rVB	226786	471759	14.97%	2.432%
19	20.789	3014	3021	3034	rVB2	294874	648384	20.58%	3.343%
20	21.476	3131	3138	3147	rBV2	303400	655446	20.80%	3.380%
21	21.764	3181	3187	3194	rVB	346342	575905	18.28%	2.969%
22	22.328	3277	3283	3297	rVB2	72046	217218	6.89%	1.120%
23	22.504	3305	3313	3322	rVB2	232969	596386	18.93%	3.075%
24	23.709	3510	3518	3527	rVB2	215912	619053	19.65%	3.192%
25	24.725	3684	3691	3706	rVB2	137597	546845	17.36%	2.820%
26	25.072	3741	3750	3756	rBV	198629	608339	19.31%	3.137%
27	26.846	4043	4052	4072	rVB6	93828	507943	16.12%	2.619%
28	28.022	4240	4252	4274	rVB6	134976	780908	24.78%	4.026%

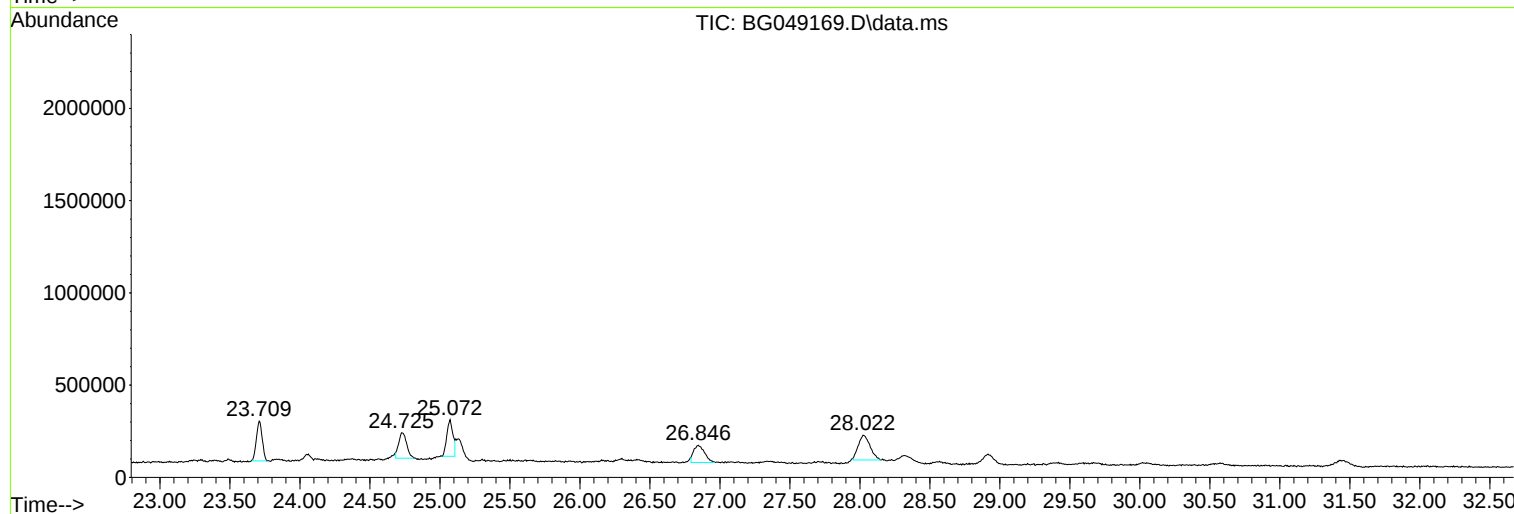
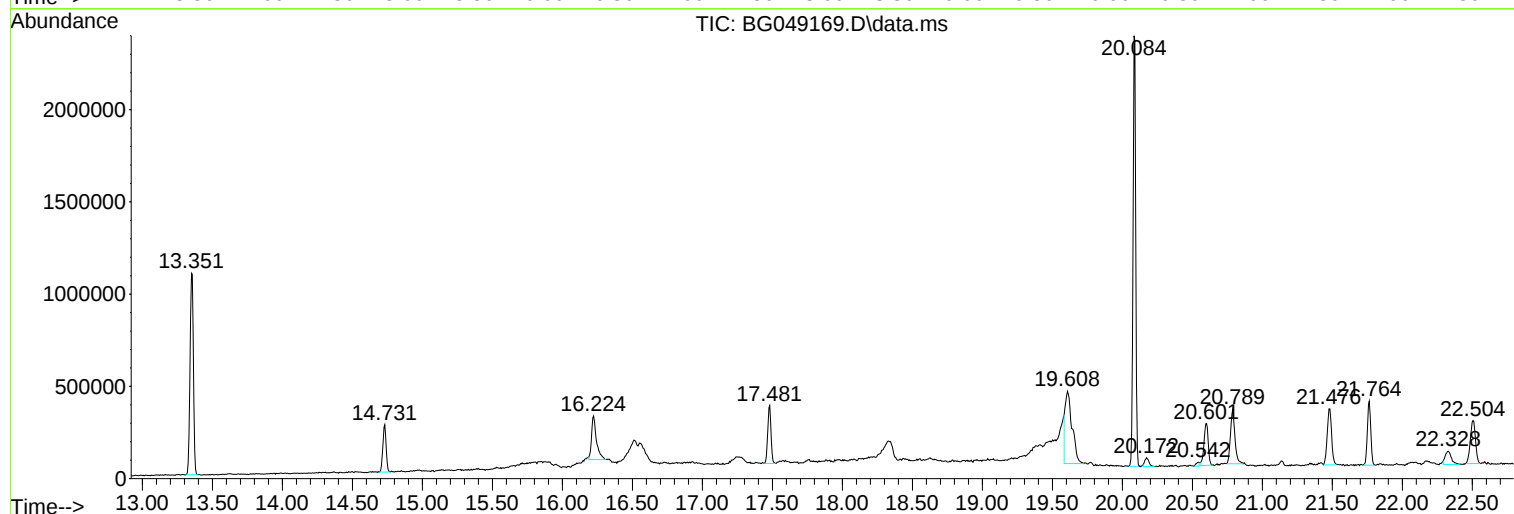
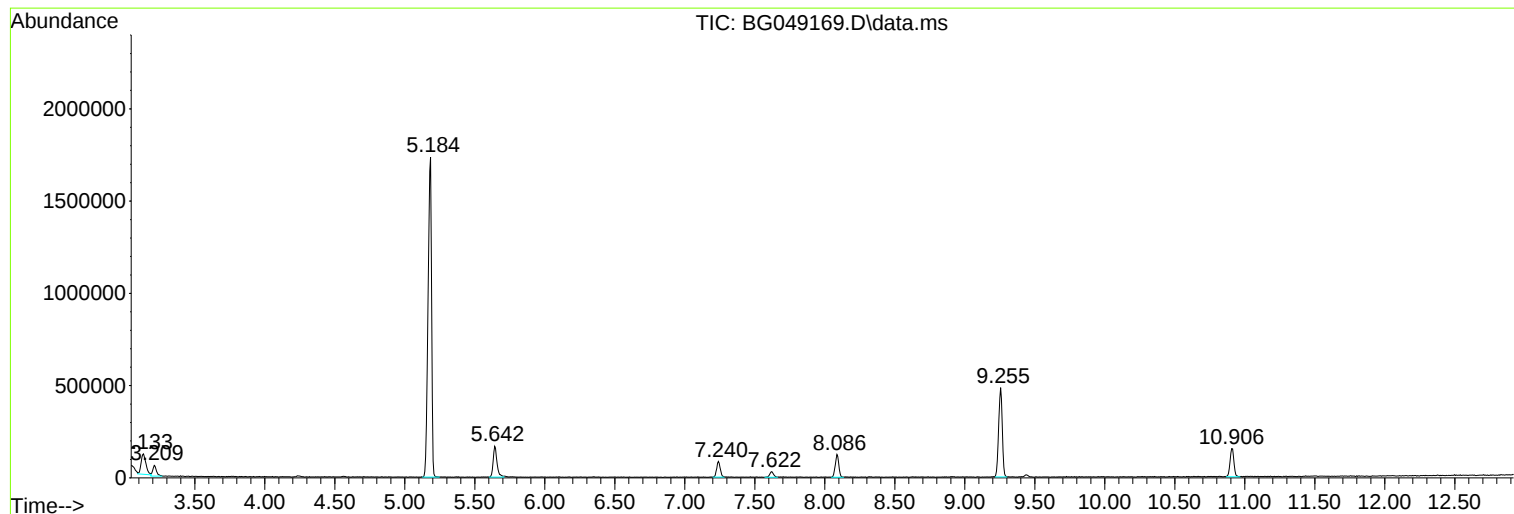
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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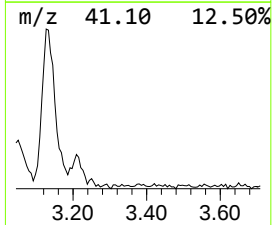
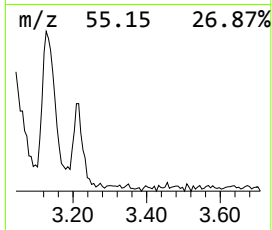
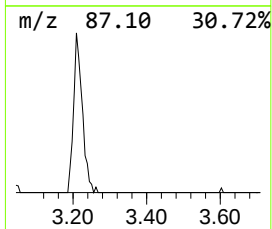
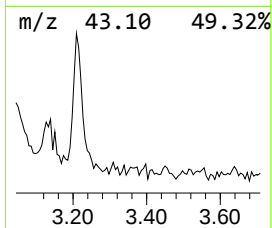
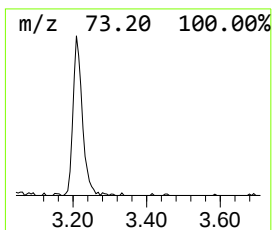
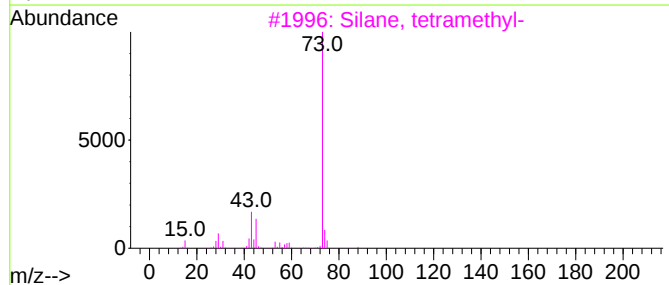
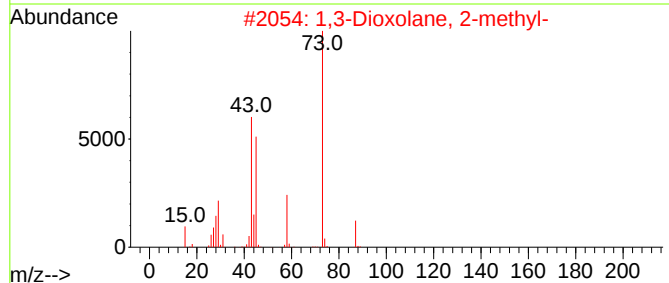
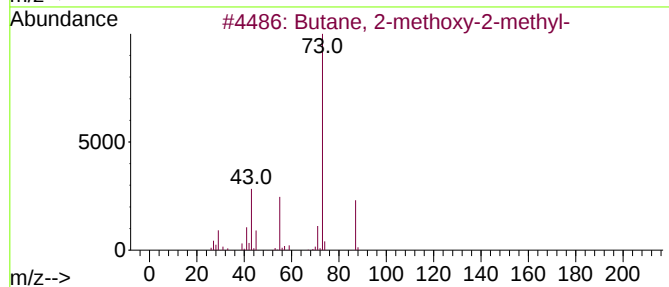
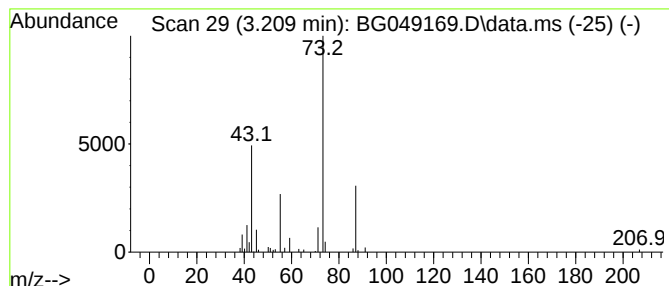
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Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.209	9.95 ng	108375	1,4-Dichlorobenzene-d4	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	17
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9



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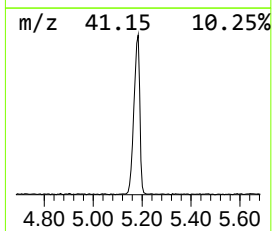
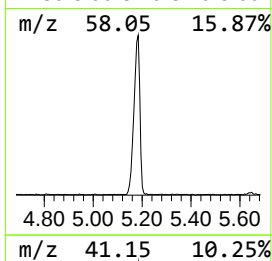
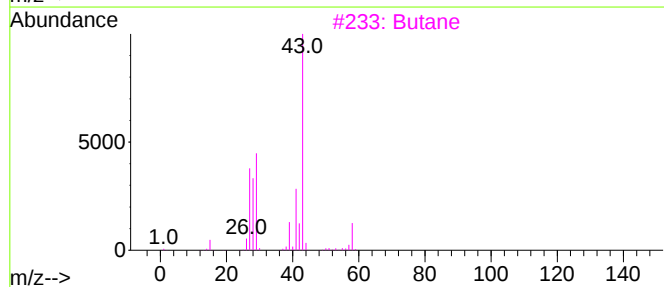
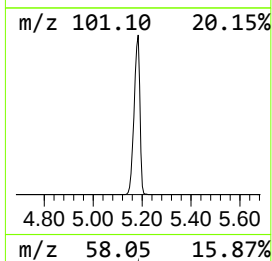
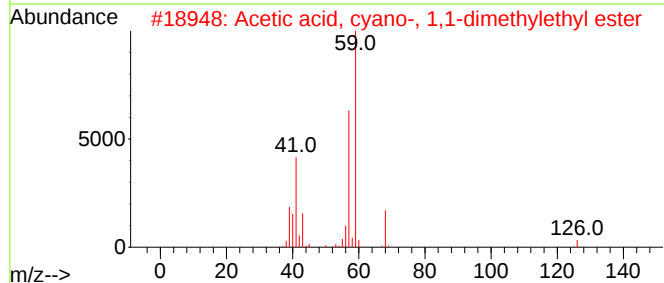
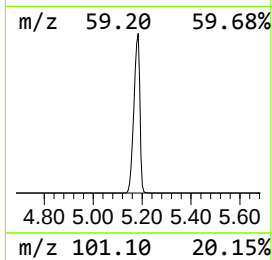
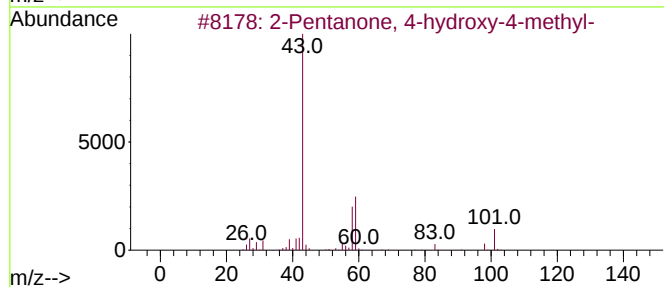
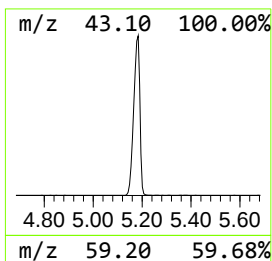
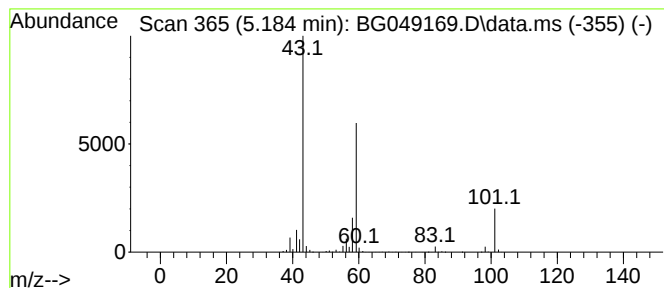
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.184	273.40 ng	2978250	1,4-Dichlorobenzene-d4	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Butane	58	C4H10	000106-97-8	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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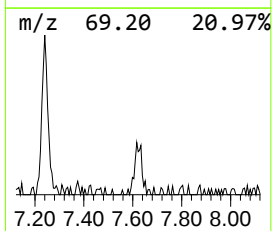
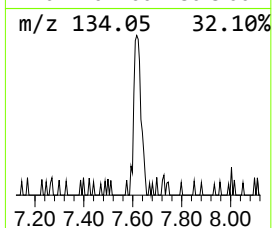
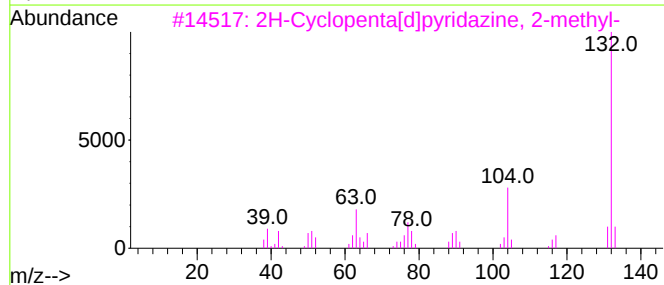
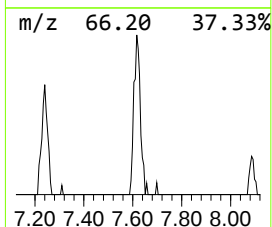
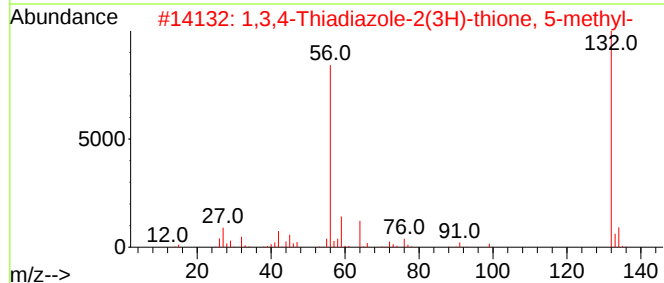
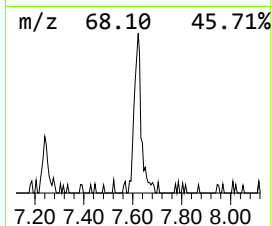
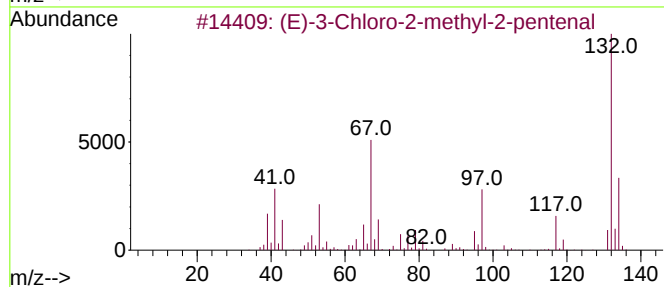
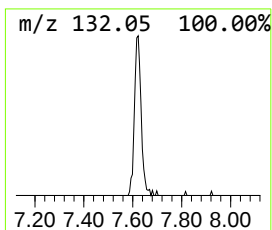
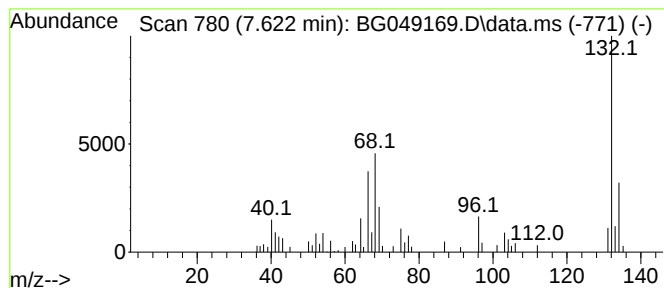
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.622 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.622	5.41 ng	58884	1,4-Dichlorobenzene-d4	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27		
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27		
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	27		
4	1H-Indazole, 3-methyl-	132	C8H8N2	1000316-00-2	22		
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22		



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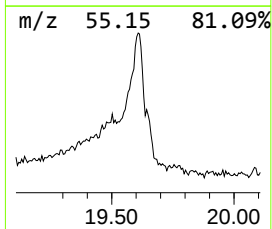
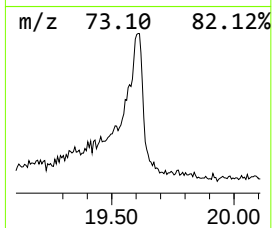
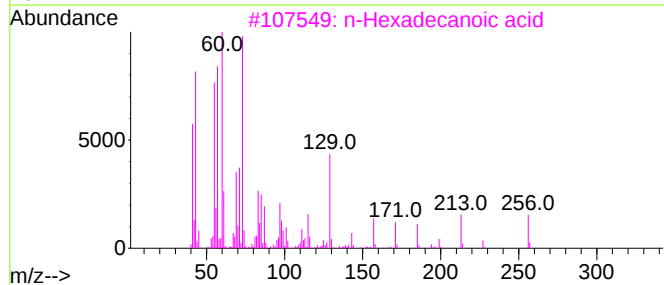
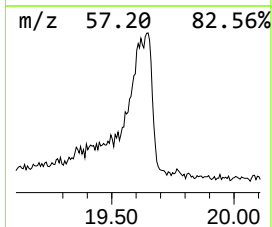
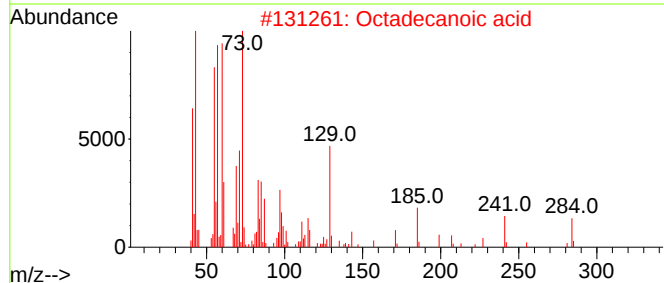
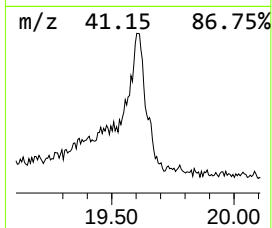
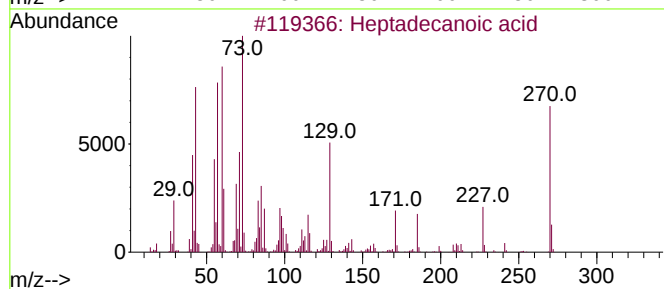
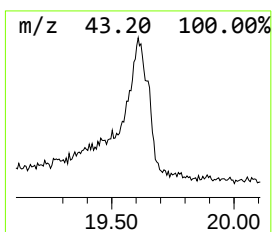
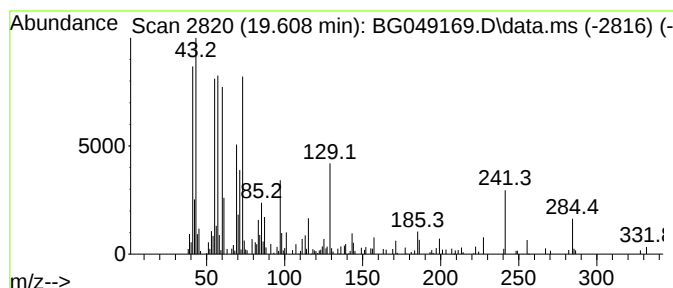
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Peak Number 5 Heptadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.608	52.88 ng	1338880	Phenanthrene-d10		17.481	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecanoic acid		270	C17H34O2	000506-12-7	90
2	Octadecanoic acid		284	C18H36O2	000057-11-4	83
3	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	64
4	Undecanoic acid		186	C11H22O2	000112-37-8	62
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	53



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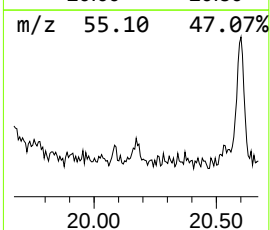
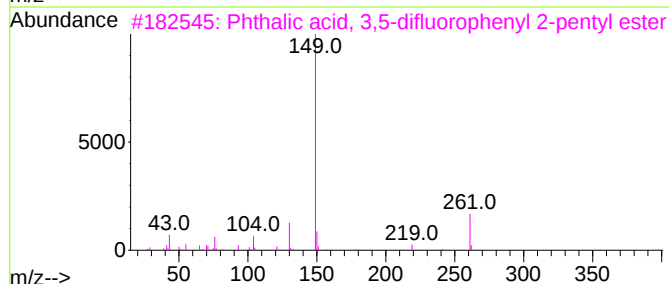
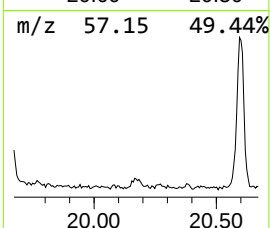
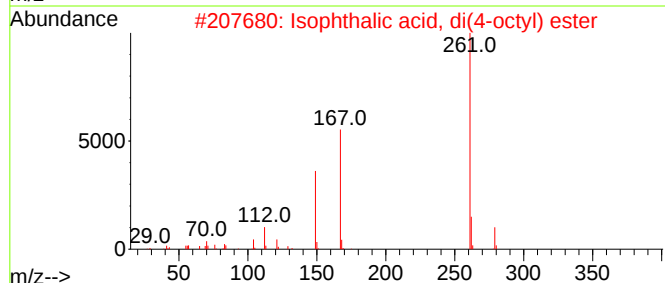
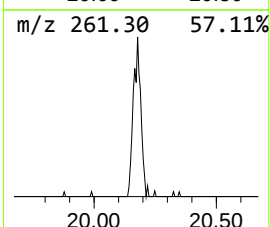
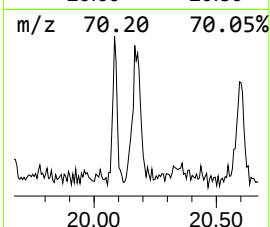
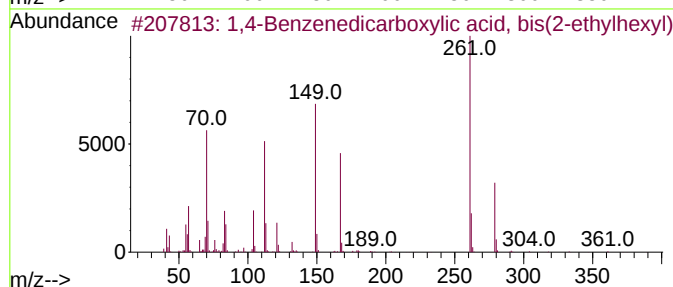
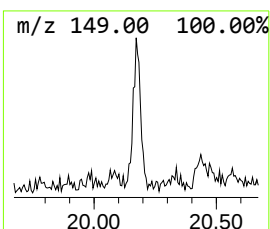
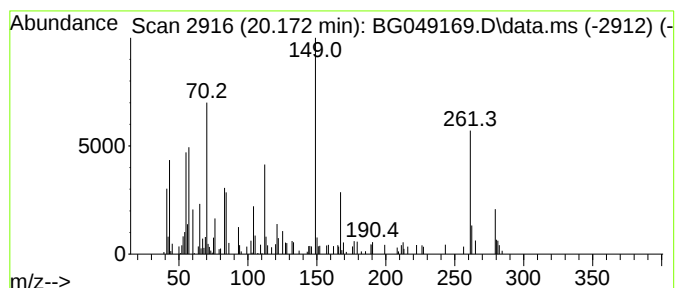
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Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.172	3.45 ng	99299	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	50
2			Isophthalic acid, di(4-octyl) ester	390	C24H3804	1000344-04-3	47
3			Phthalic acid, 3,5-difluoropheny...	348	C19H18F2O4	1000315-55-2	38
4			Phthalic acid, 3,5-difluoropheny...	348	C19H18F2O4	1000315-54-1	35
5			2-(Nonyloxycarbonyl)benzoic acid	292	C17H24O4	1000373-89-9	25



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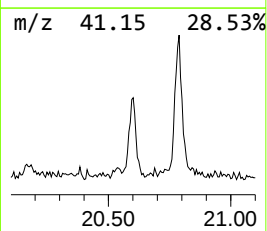
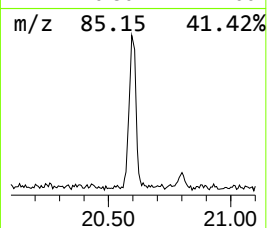
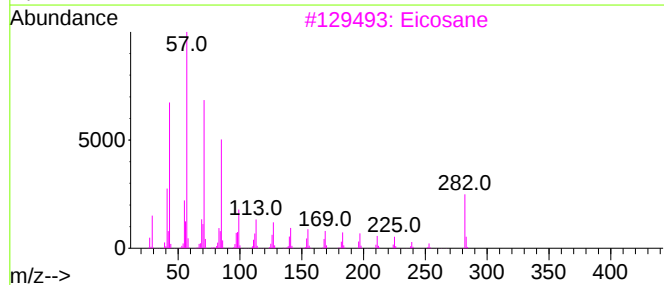
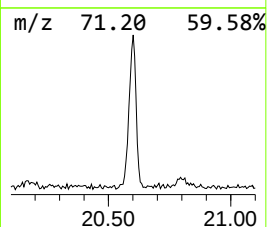
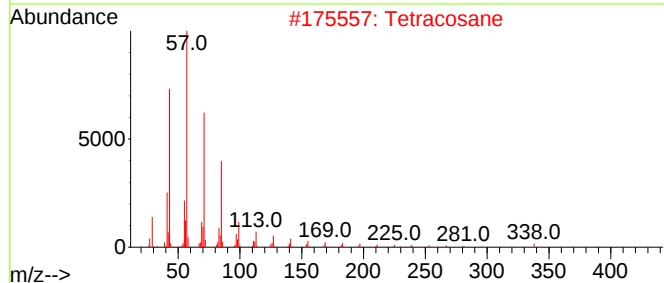
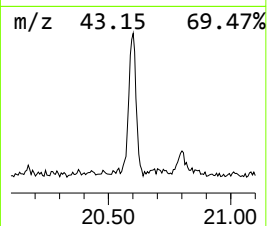
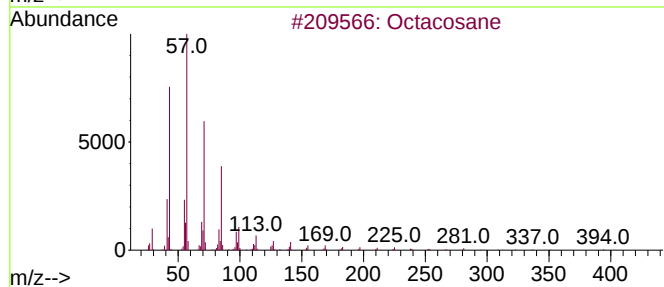
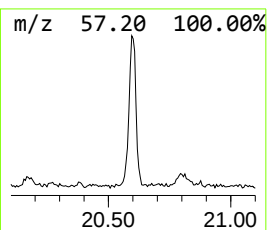
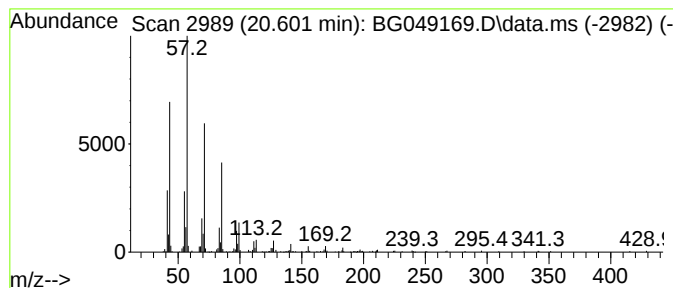
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.601	16.38 ng	471759	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Eicosane	282	C20H42	000112-95-8	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049169.D
Acq On : 2 Jul 2021 16:07
Operator : CG/JU
Sample : M2875-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

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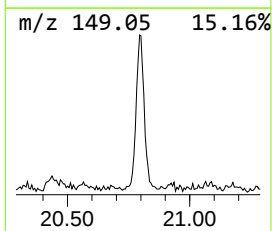
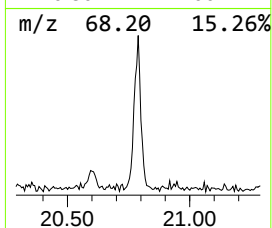
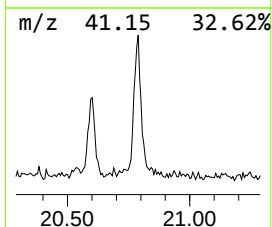
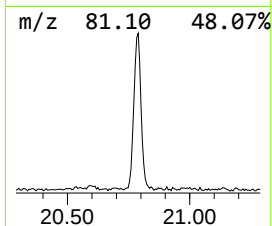
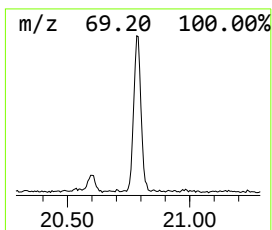
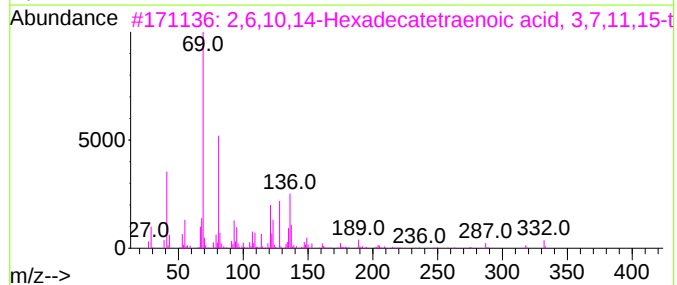
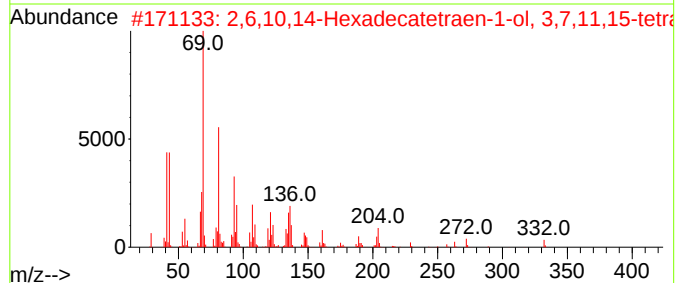
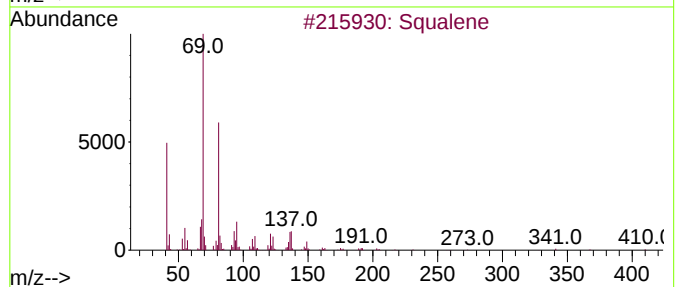
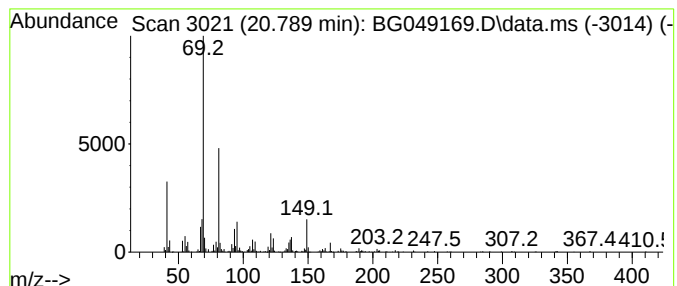
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.789	22.52 ng	648384	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	93
2			2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5			4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049169.D
Acq On : 2 Jul 2021 16:07
Operator : CG/JU
Sample : M2875-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

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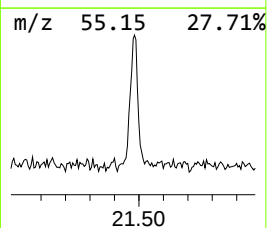
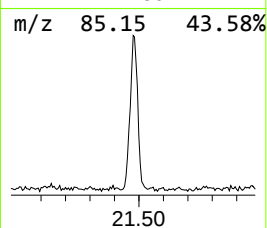
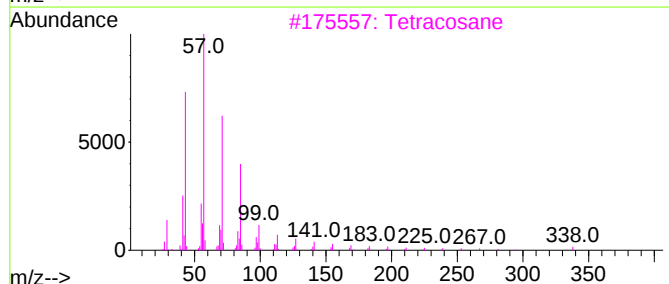
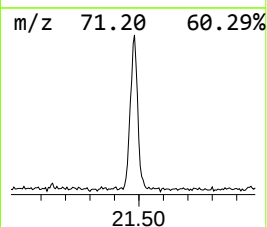
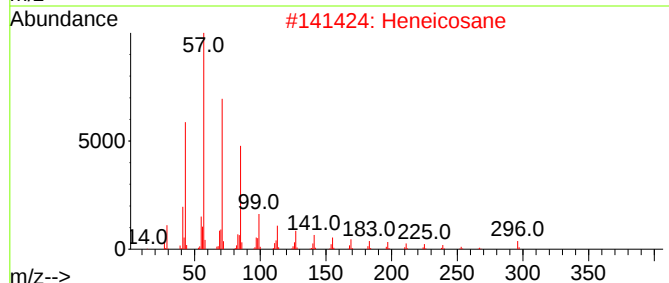
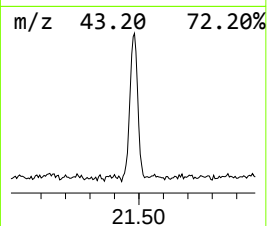
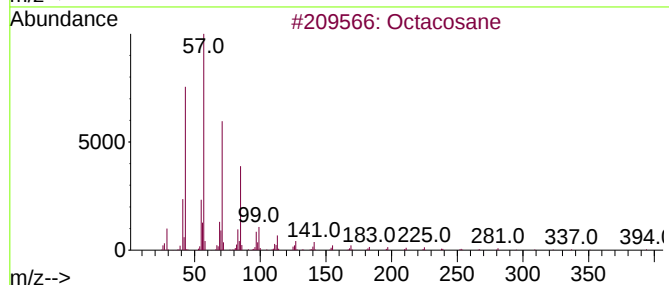
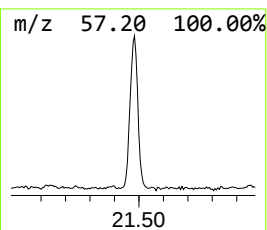
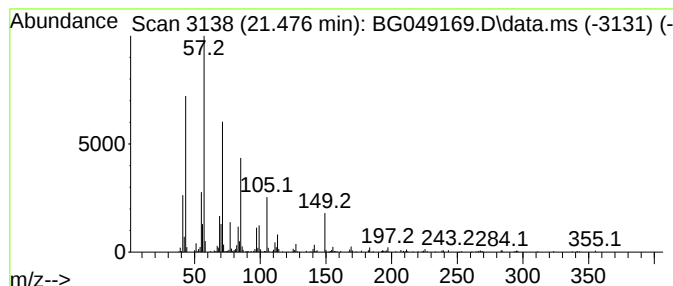
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.476	22.76 ng	655446	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	81
2			Heneicosane	296	C21H44	000629-94-7	70
3			Tetracosane	338	C24H50	000646-31-1	68
4			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	68
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049169.D
Acq On : 2 Jul 2021 16:07
Operator : CG/JU
Sample : M2875-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

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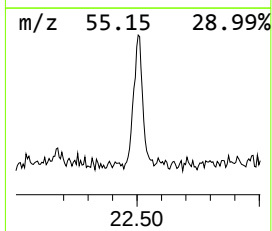
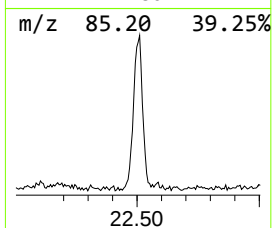
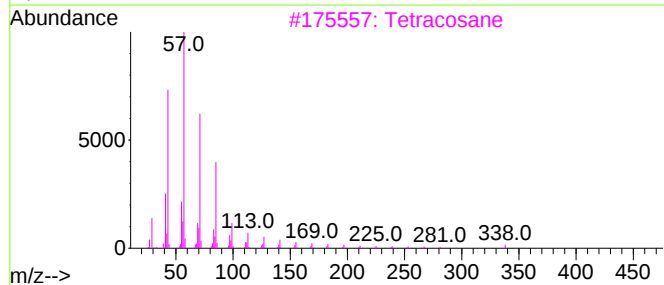
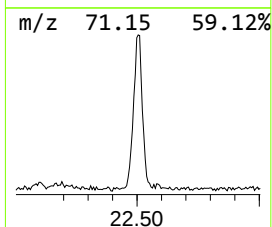
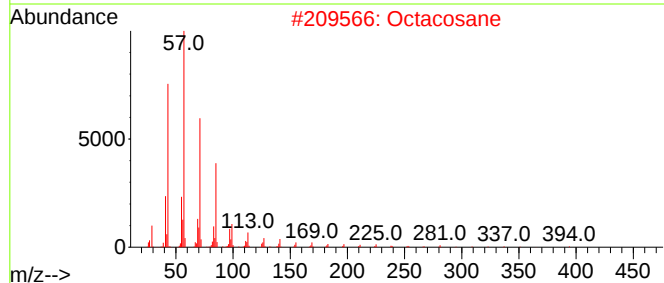
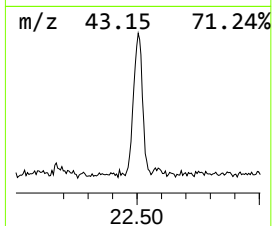
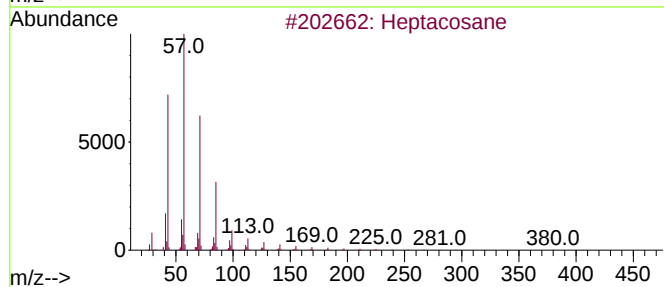
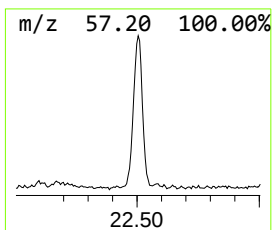
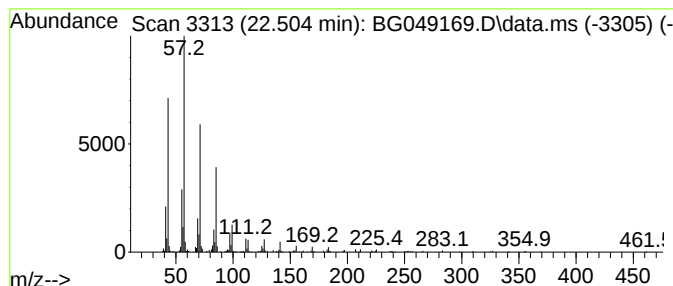
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.505	20.71 ng	596386	Chrysene-d12	21.764

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Hexatriacontane	507	C36H74	000630-06-8	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049169.D
Acq On : 2 Jul 2021 16:07
Operator : CG/JU
Sample : M2875-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

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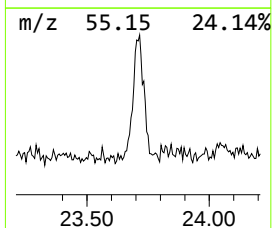
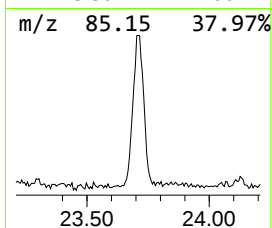
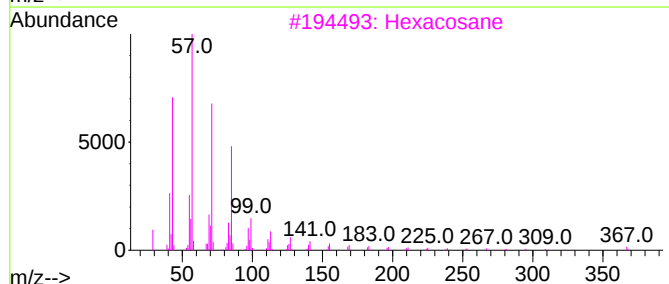
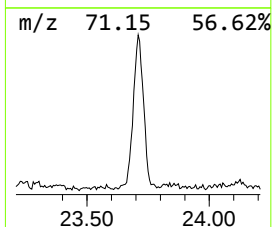
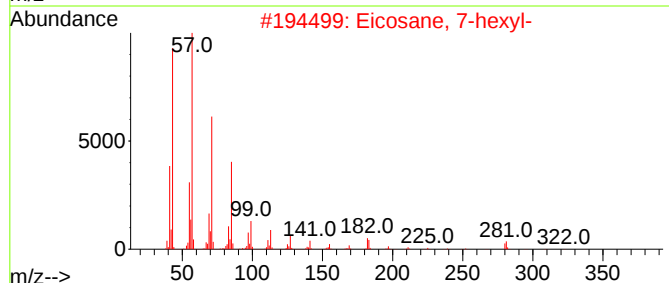
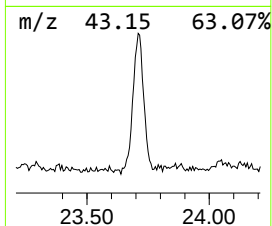
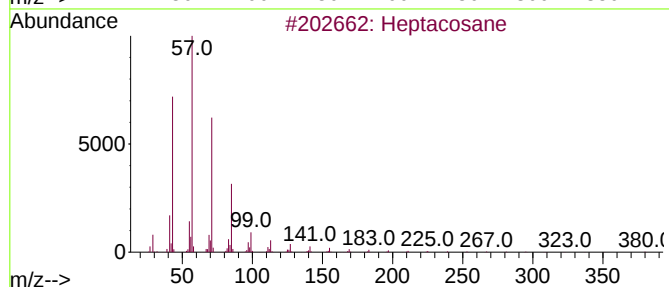
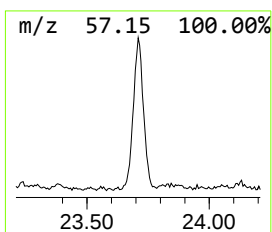
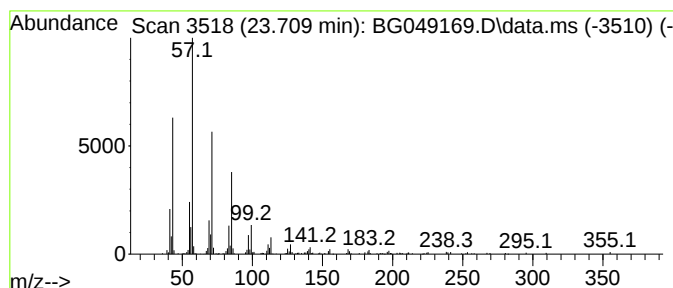
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane, 7-hexyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.709	20.35 ng	619053	Perylene-d12	25.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Tridecane, 2-methyl-	198	C14H30	001560-96-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049169.D
Acq On : 2 Jul 2021 16:07
Operator : CG/JU
Sample : M2875-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

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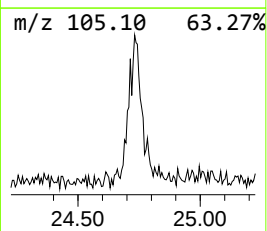
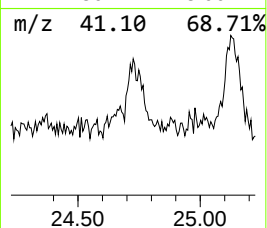
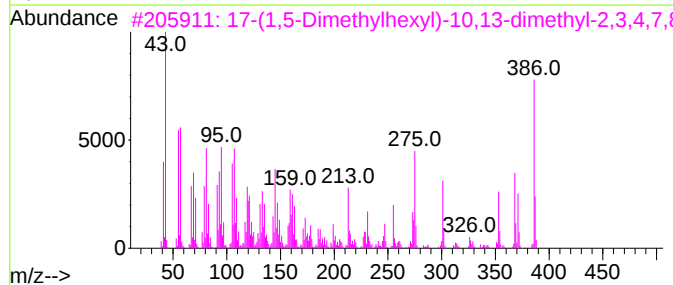
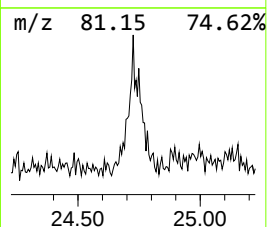
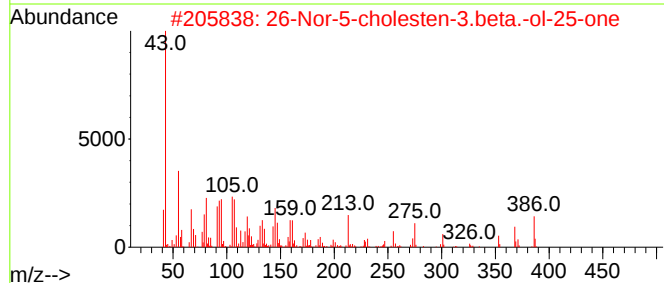
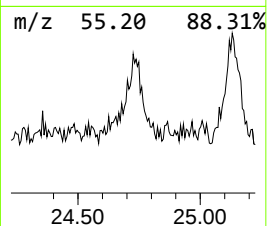
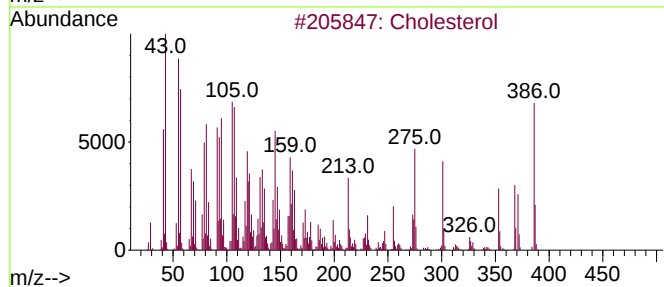
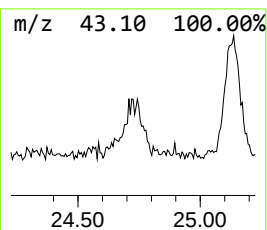
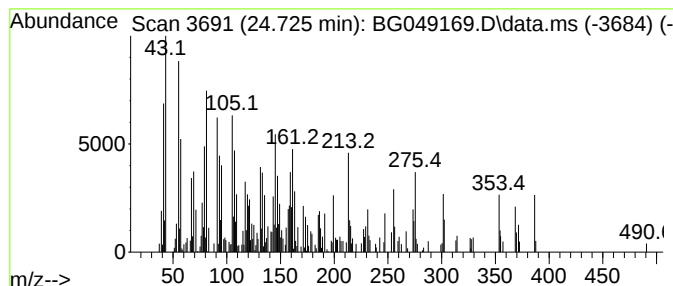
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Cholesterol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.725	17.98 ng	546845	Perylene-d12	25.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholesterol	386	C27H46O	000057-88-5	64
2			26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	55
3			17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	53
4			Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	49
5			Cholest-5-en-3-ol, (3.alpha.)-	386	C27H46O	000474-77-1	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049169.D
Acq On : 2 Jul 2021 16:07
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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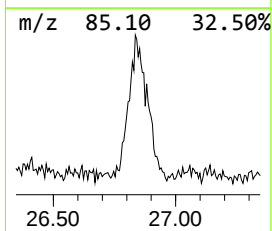
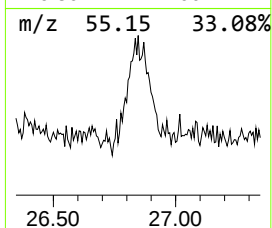
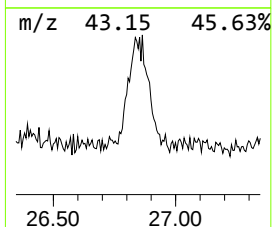
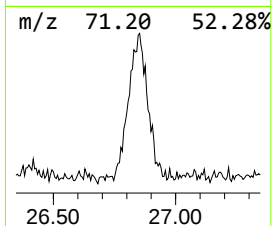
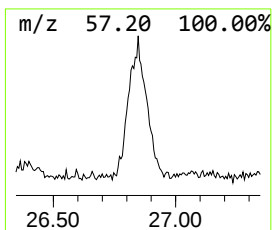
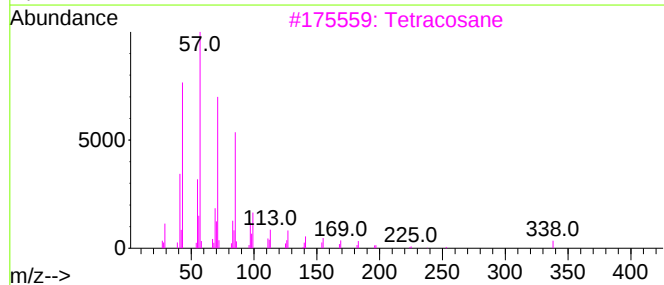
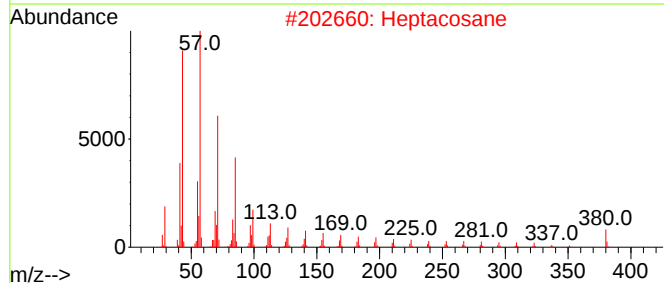
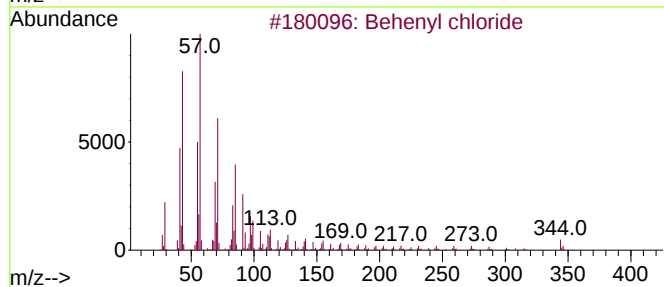
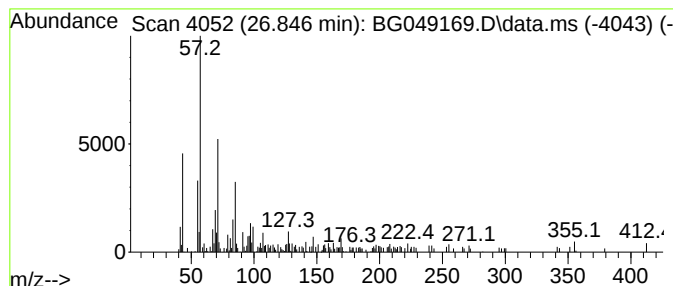
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Behenyl chloride Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.846	16.70 ng	507943	Perylene-d12	25.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenyl chloride	344	C22H45Cl	042217-03-8	64
2			Heptacosane	380	C27H56	000593-49-7	64
3			Tetracosane	338	C24H50	000646-31-1	64
4			Hentriacontane	437	C31H64	000630-04-6	59
5			Tricosane	324	C23H48	000638-67-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049169.D
Acq On : 2 Jul 2021 16:07
Operator : CG/JU
Sample : M2875-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

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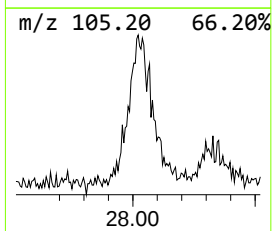
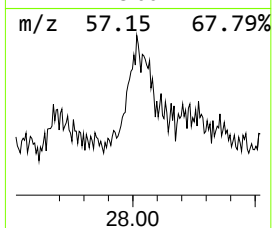
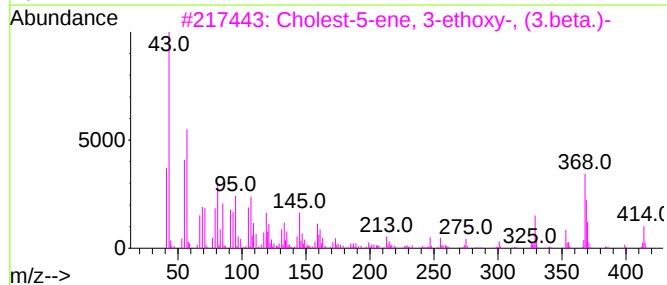
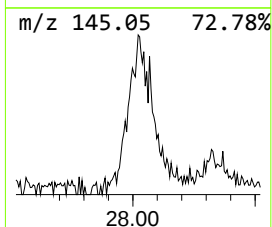
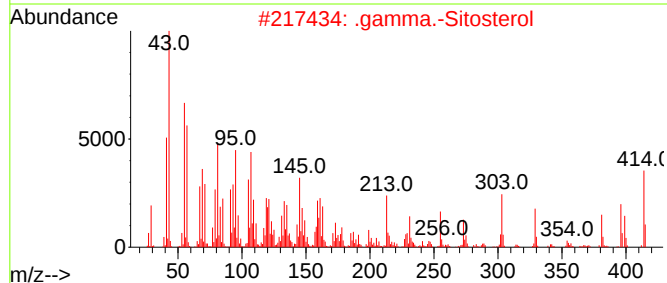
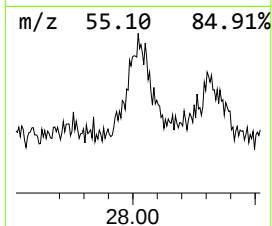
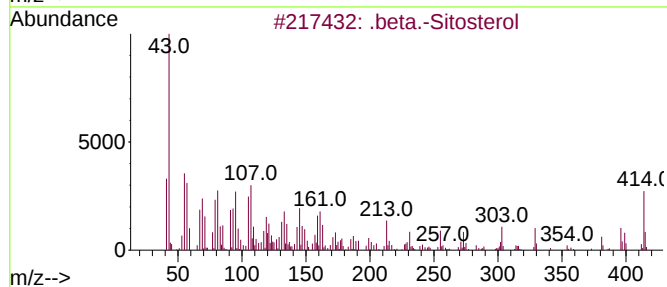
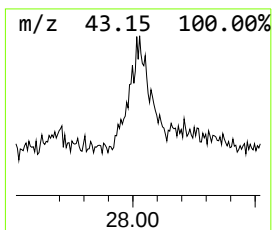
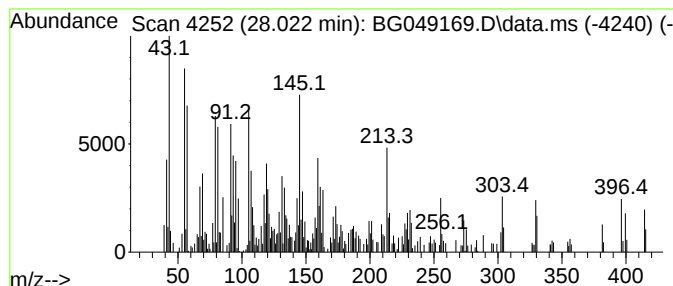
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 .beta.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.022	25.67 ng	780908	Perylene-d12	25.072

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Sitosterol	414	C29H50O	000083-46-5	89
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	83
3		Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	38
4		Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	16
5		Cholest-5-ene, 3-methoxy-, (3.be...	400	C28H48O	001174-92-1	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049169.D
Acq On : 2 Jul 2021 16:07
Operator : CG/JU
Sample : M2875-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FIELD-BLANK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.209	9.9	ng	108375	1	8.086	217869	20.0
2-Pentanone, 4-...	5.184	273.4	ng	2978250	1	8.086	217869	20.0
unknown7.622	7.622	5.4	ng	58884	1	8.086	217869	20.0
Heptadecanoic acid	19.608	52.9	ng	1338880	4	17.481	506378	20.0
1,4-Benzenedica...	20.172	3.5	ng	99299	5	21.764	575905	20.0
Octacosane	20.601	16.4	ng	471759	5	21.764	575905	20.0
Squalene	20.789	22.5	ng	648384	5	21.764	575905	20.0
Heneicosane	21.476	22.8	ng	655446	5	21.764	575905	20.0
Heptacosane	22.505	20.7	ng	596386	5	21.764	575905	20.0
Eicosane, 7-hexyl-	23.709	20.4	ng	619053	6	25.072	608339	20.0
Cholesterol	24.725	18.0	ng	546845	6	25.072	608339	20.0
Behenyl chloride	26.846	16.7	ng	507943	6	25.072	608339	20.0
.beta.-Sitosterol	28.022	25.7	ng	780908	6	25.072	608339	20.0