

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
 Data File : BG055538.D
 Acq On : 10 Nov 2022 13:48
 Operator : CG/JU
 Sample : N5378-08
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EB-20221028

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055538.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.331	3	7	22	rVB	599054	1036968	26.07%	6.099%
2	5.329	339	347	355	rBV	88799	138848	3.49%	0.817%
3	5.799	420	427	437	rBV	411345	670333	16.85%	3.943%
4	7.403	688	700	711	rBV	232510	400384	10.06%	2.355%
5	8.272	841	848	855	rBV	192386	325081	8.17%	1.912%
6	9.442	1038	1047	1054	rBV	629432	1119117	28.13%	6.582%
7	11.099	1322	1329	1338	rBV	242346	440783	11.08%	2.592%
8	13.519	1733	1741	1748	rVB	1642285	2588524	65.07%	15.225%
9	13.889	1787	1804	1805	rBV3	61818	193477	4.86%	1.138%
10	14.888	1968	1974	1981	rVB	370782	597847	15.03%	3.516%
11	16.369	2219	2226	2236	rBV	1377020	2079013	52.26%	12.228%
12	16.774	2281	2295	2296	rBV4	159663	509498	12.81%	2.997%
13	17.626	2434	2440	2448	rVB	493969	735304	18.48%	4.325%
14	17.738	2455	2459	2463	rVB5	32981	41808	1.05%	0.246%
15	18.490	2584	2587	2595	rVB3	49888	92537	2.33%	0.544%
16	20.217	2875	2881	2886	rBV	3041785	3978037	100.00%	23.397%
17	21.927	3165	3172	3181	rVB	501663	894736	22.49%	5.262%
18	22.115	3197	3204	3210	rVB4	52545	148184	3.73%	0.872%
19	22.991	3348	3353	3359	rBV2	40372	90022	2.26%	0.529%
20	25.347	3746	3754	3772	rVB3	279859	921838	23.17%	5.422%

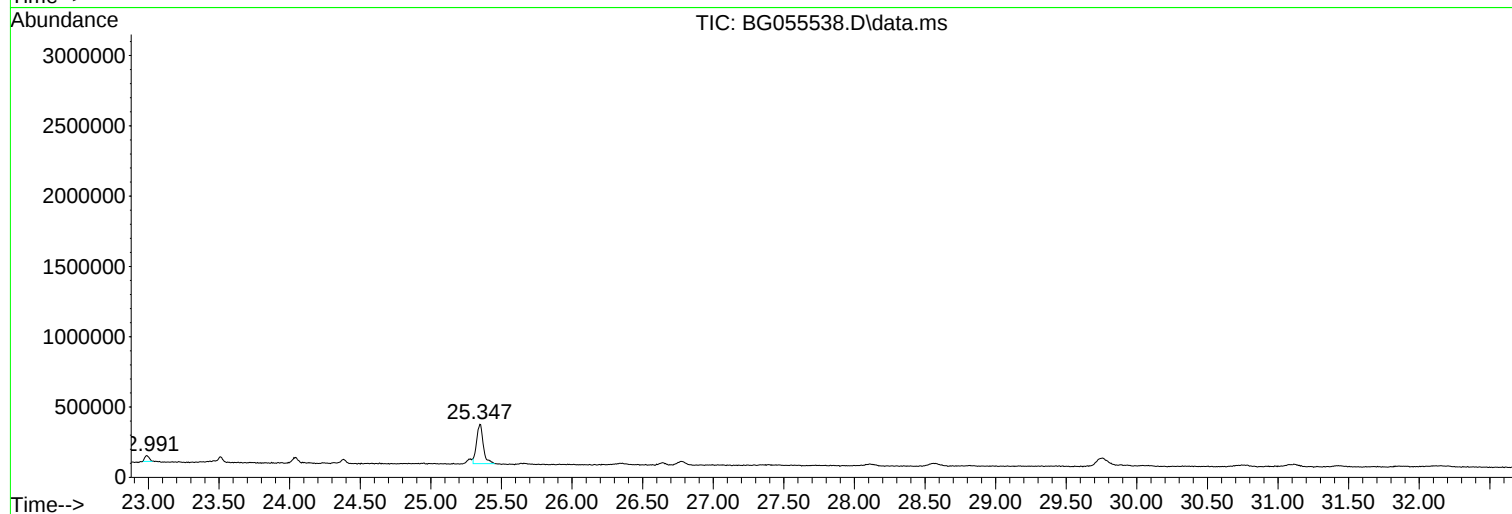
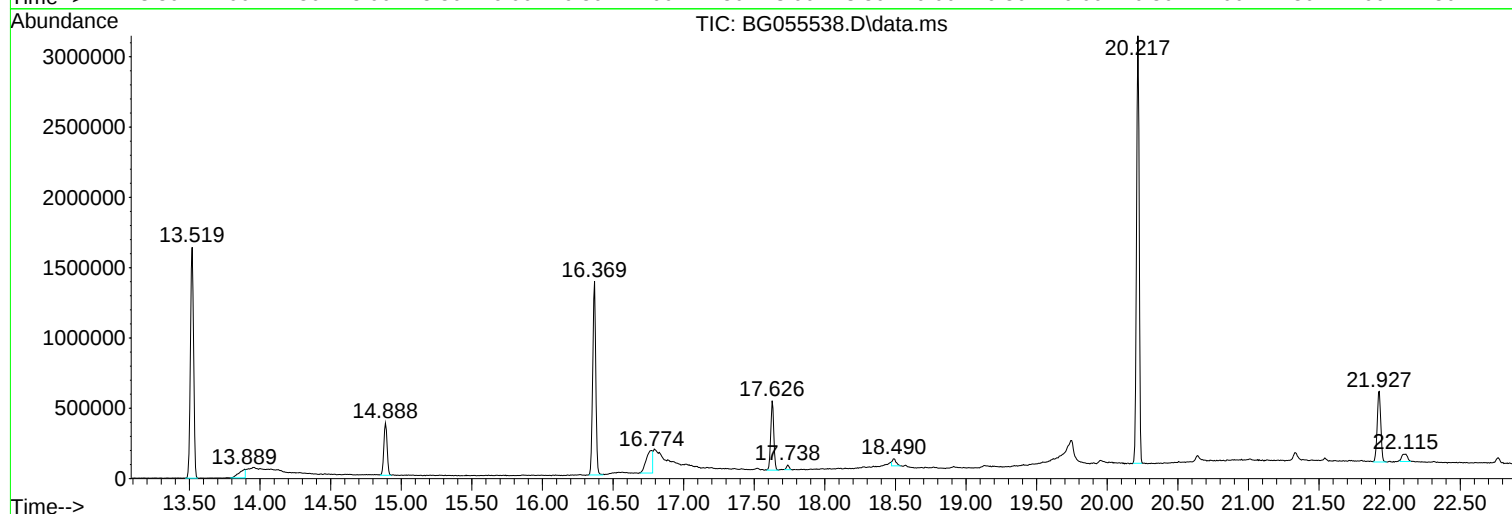
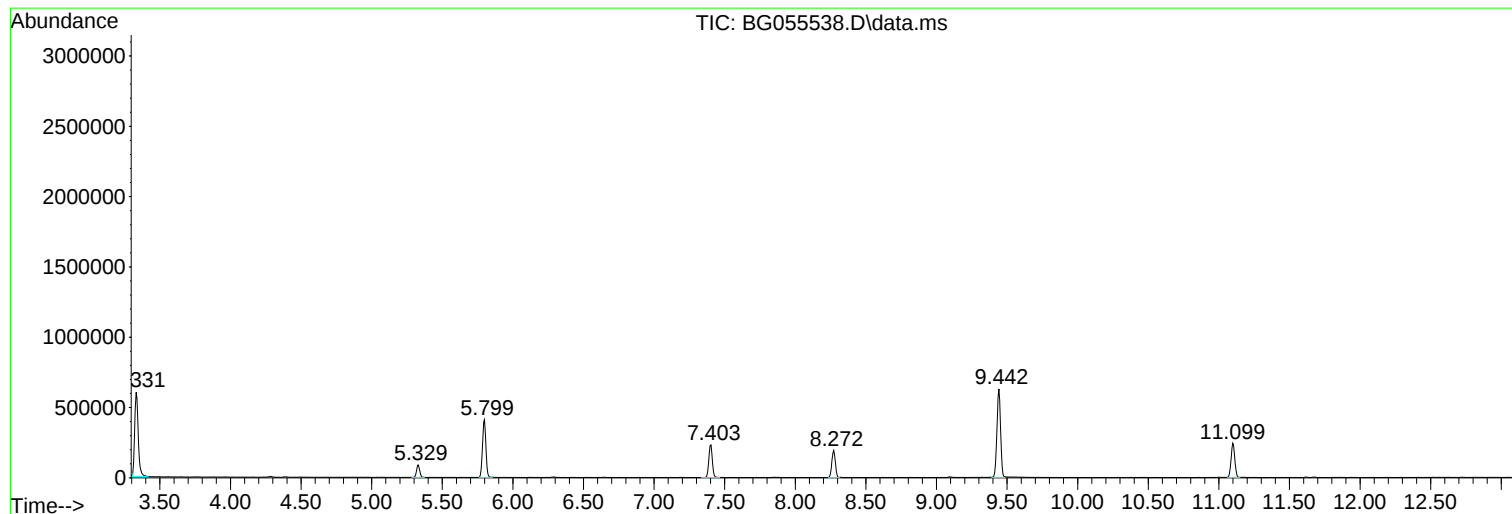
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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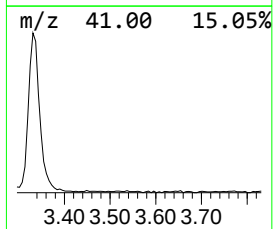
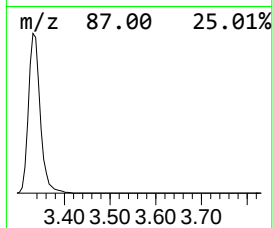
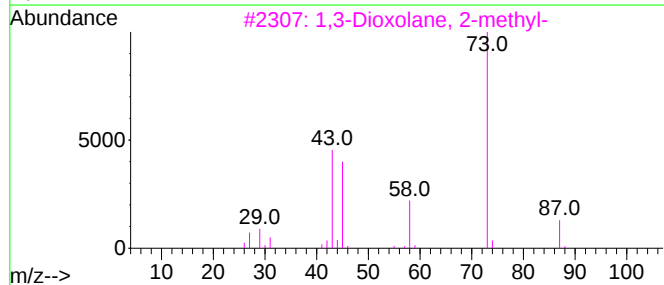
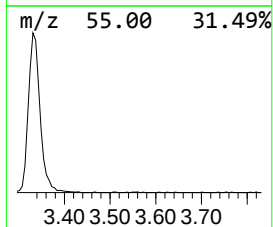
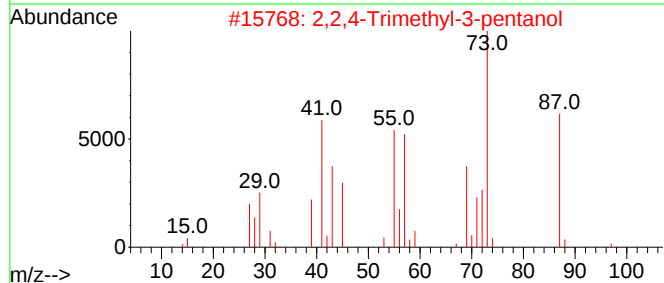
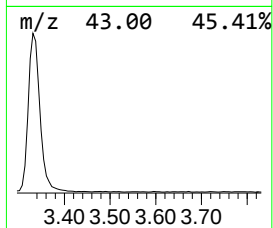
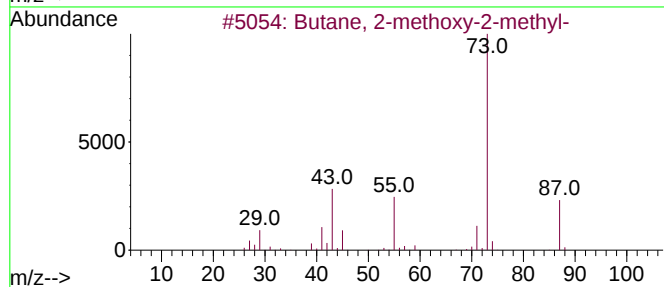
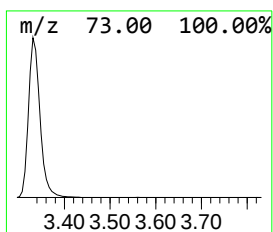
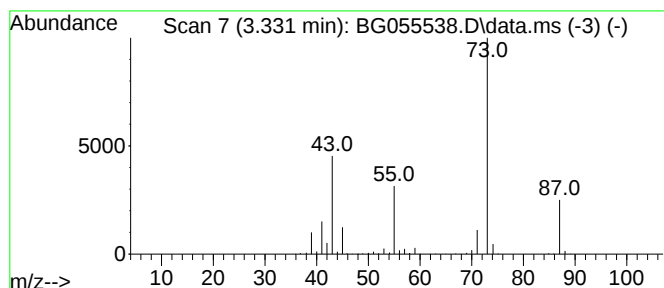
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
3.331	63.80 ng	1036970	1,4-Dichlorobenzene-d4	8.272

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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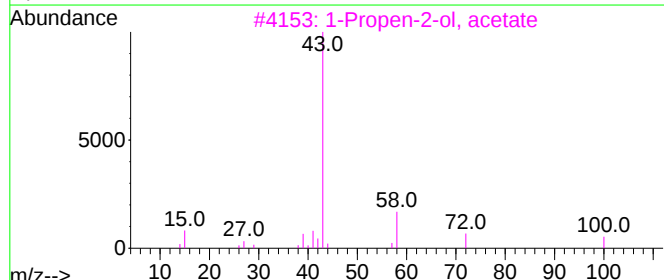
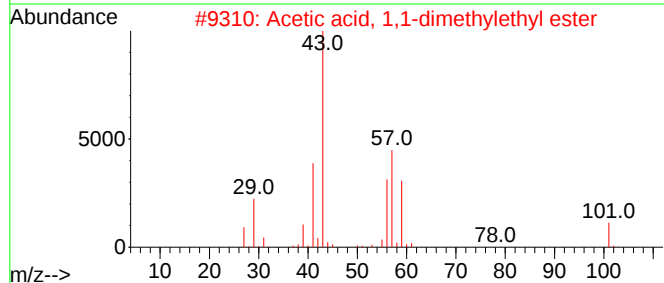
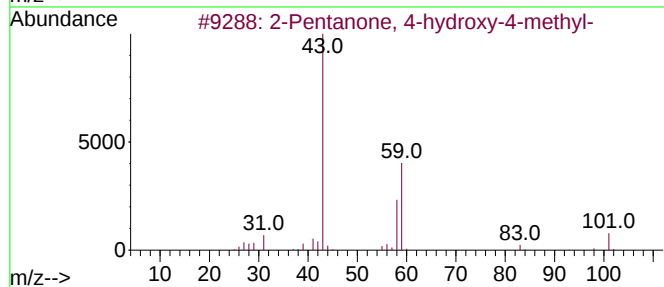
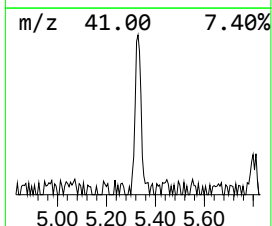
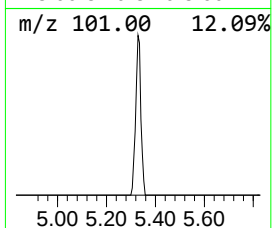
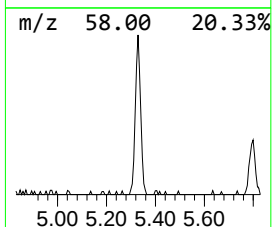
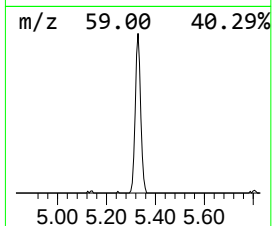
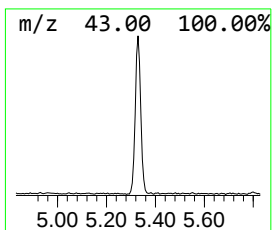
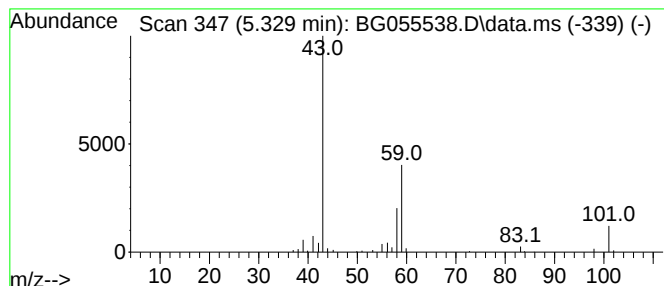
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.329	8.54 ng	138848	1,4-Dichlorobenzene-d4	8.272

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	8



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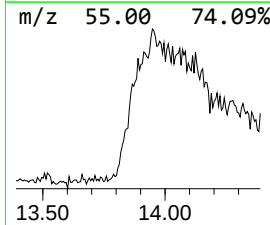
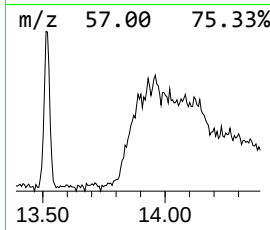
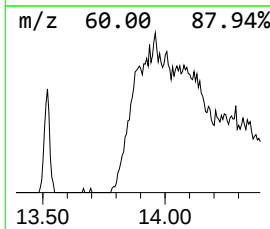
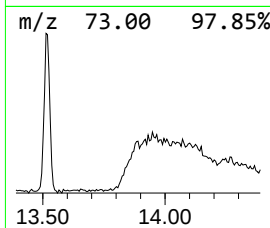
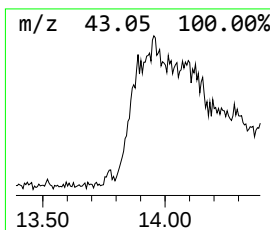
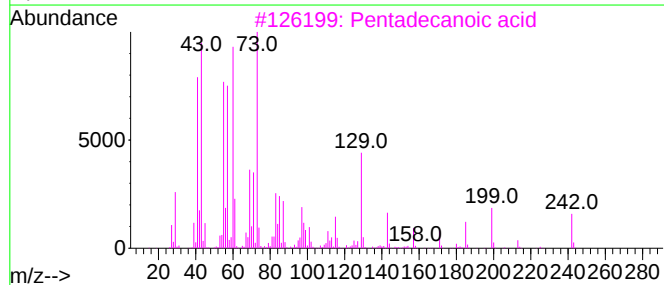
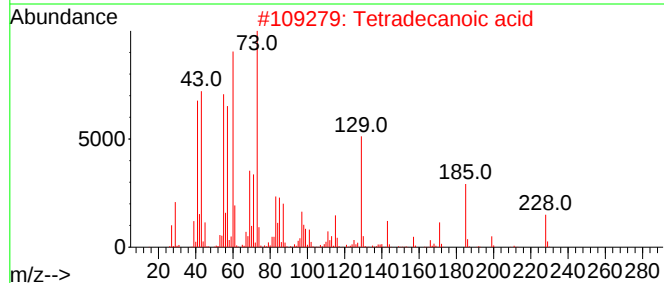
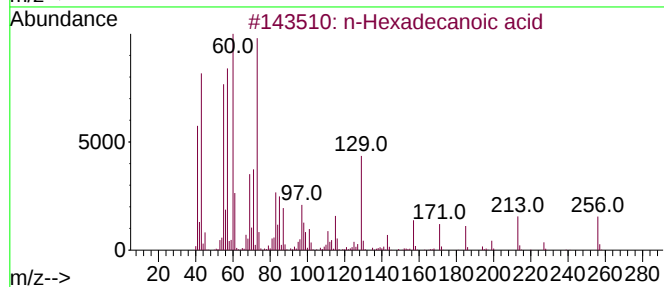
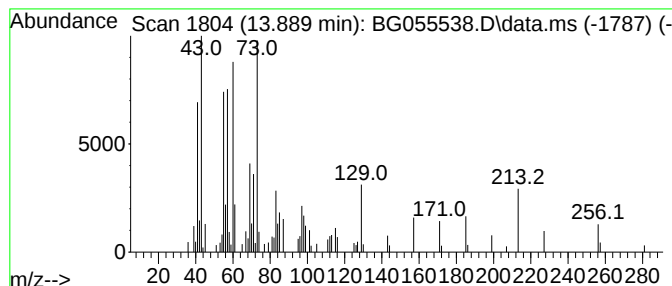
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.889	6.47 ng	193477	Acenaphthene-d10	14.888

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	64
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4			n-Decanoic acid	172	C10H20O2	000334-48-5	60
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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ALS Vial : 6 Sample Multiplier: 1

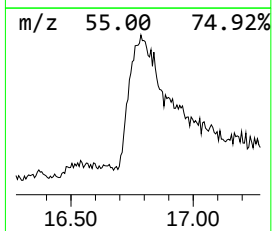
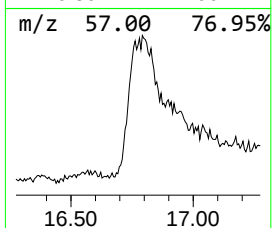
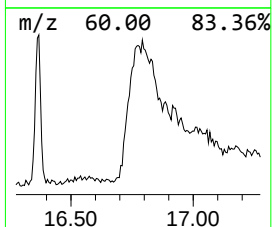
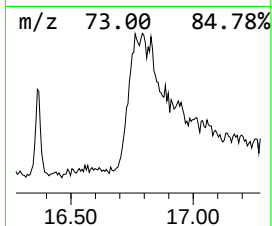
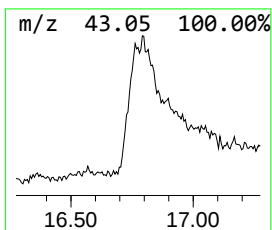
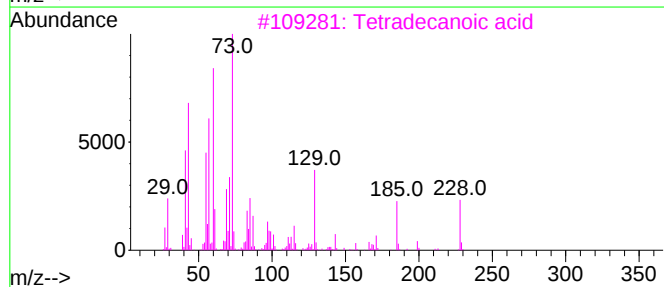
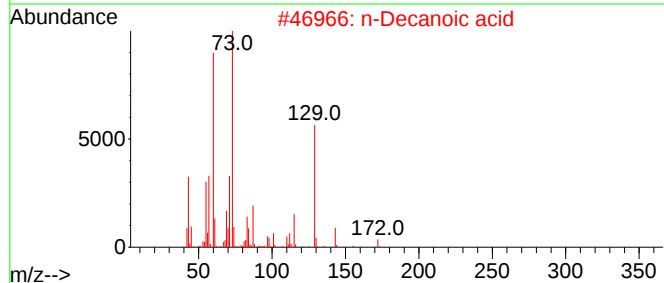
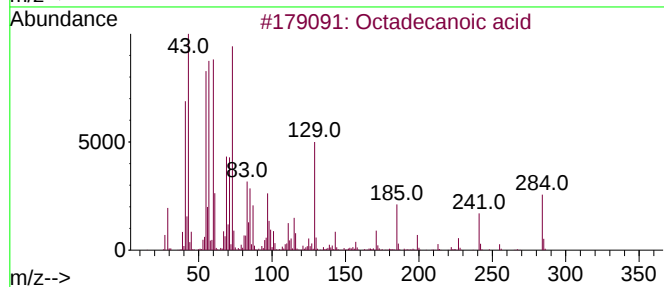
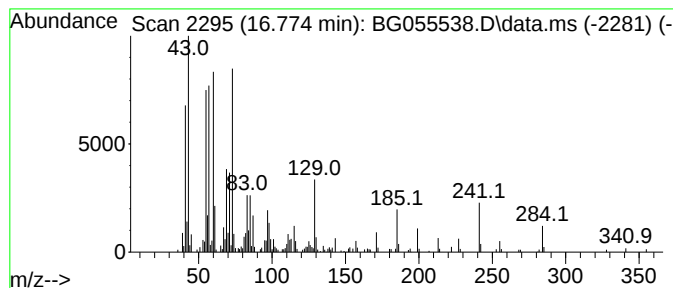
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.774	13.86 ng	509498	Phenanthrene-d10		17.626	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	n-Decanoic acid		172	C10H20O2	000334-48-5	87
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	74
4	Octadecanoic acid, 2-(2-hydroxye...		372	C22H44O4	000106-11-6	74
5	Pentadecanoic acid		242	C15H30O2	001002-84-2	72



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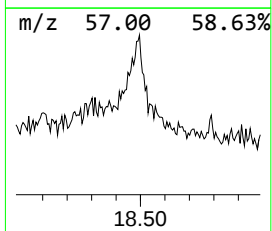
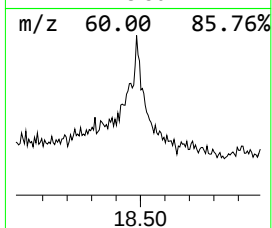
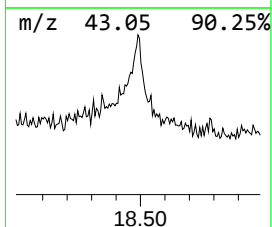
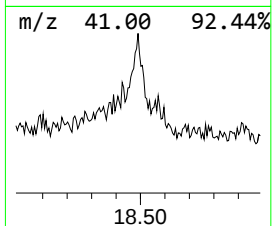
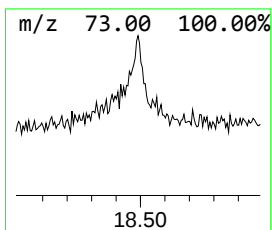
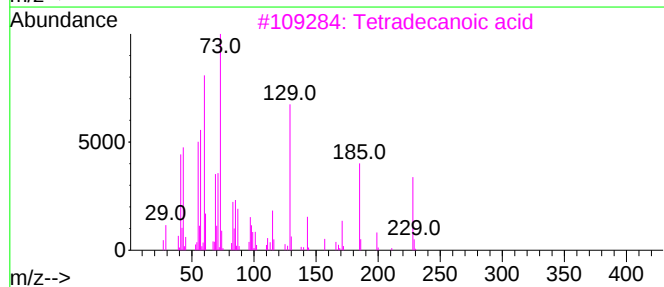
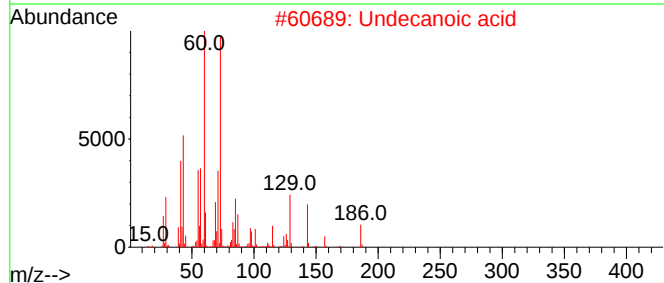
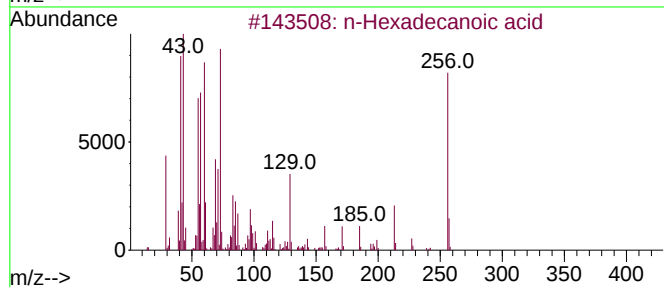
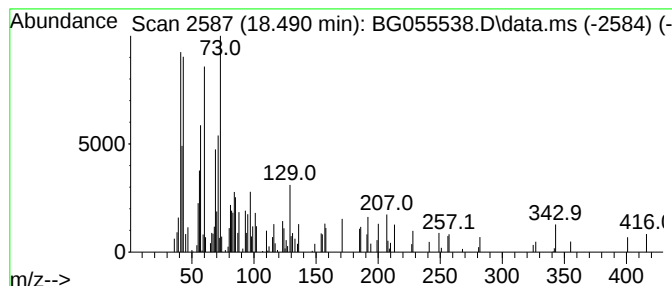
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.490	2.52 ng	92537	Phenanthrene-d10	17.626

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
2			Undecanoic acid	186	C11H22O2	000112-37-8	58
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4			Dodecanoic acid	200	C12H24O2	000143-07-7	47
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	42



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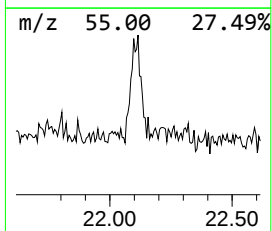
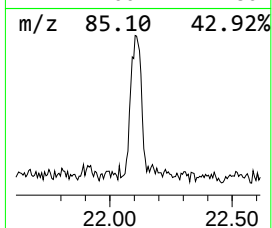
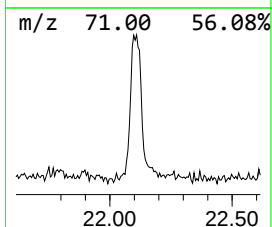
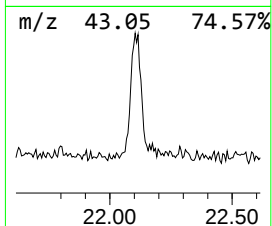
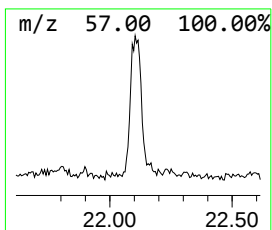
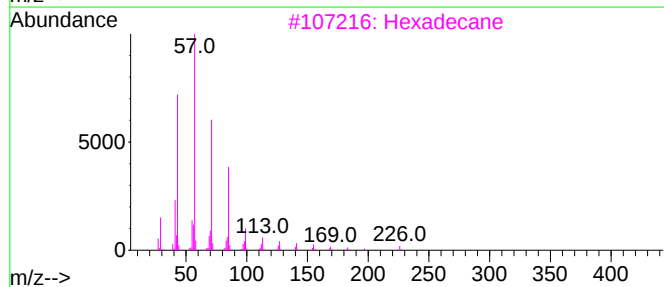
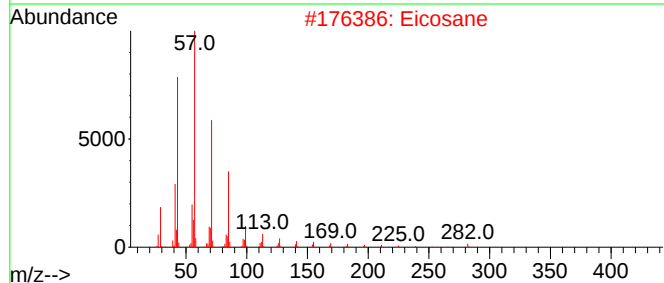
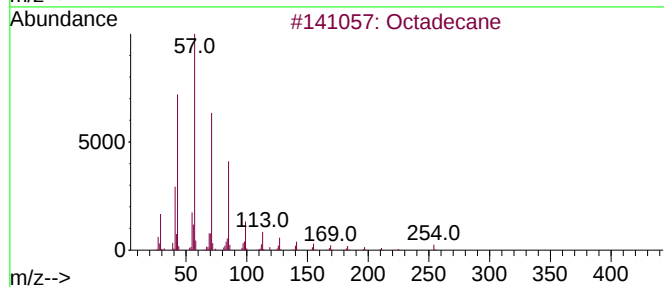
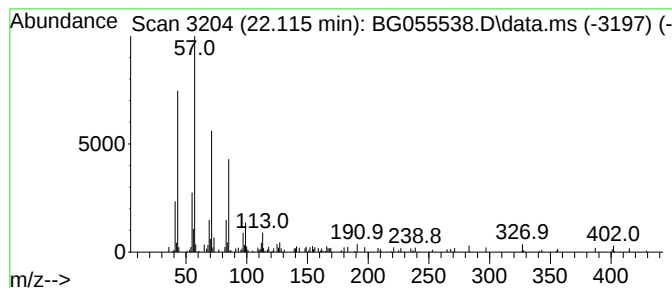
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.115	3.31 ng	148184	Chrysene-d12	21.927

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	80
2		Eicosane	282	C20H42	000112-95-8	80
3		Hexadecane	226	C16H34	000544-76-3	80
4		Nonadecane	268	C19H40	000629-92-5	72
5		Tetracosane	338	C24H50	000646-31-1	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055538.D
Acq On : 10 Nov 2022 13:48
Operator : CG/JU
Sample : N5378-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-20221028

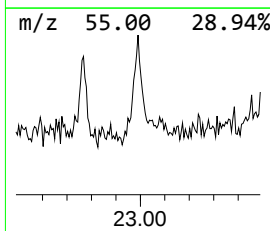
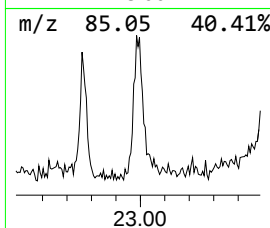
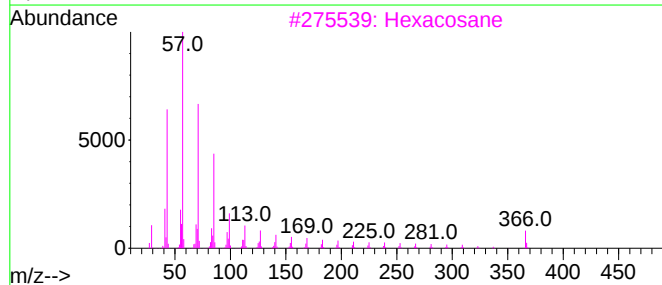
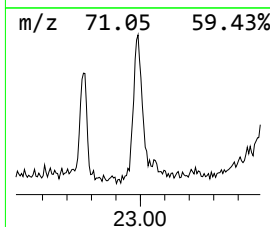
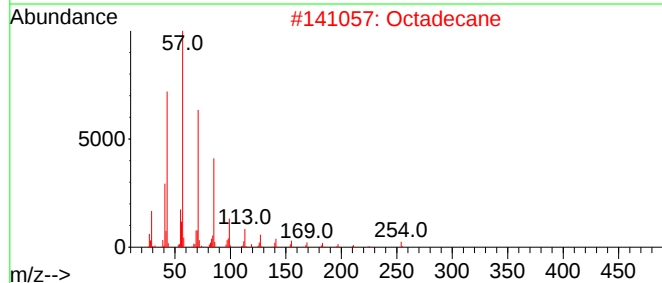
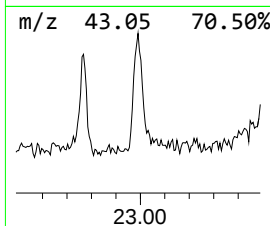
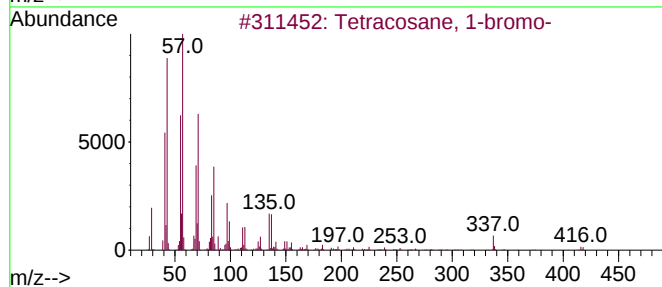
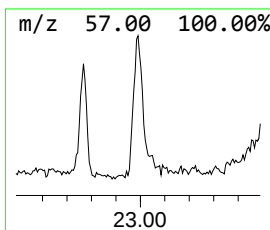
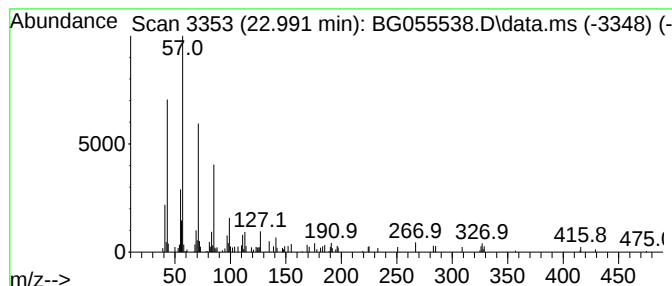
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tetracosane, 1-bromo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.991	2.01 ng	90022	Chrysene-d12	21.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane, 1-bromo-	416	C24H49Br	006946-24-3	87
2			Octadecane	254	C18H38	000593-45-3	87
3			Hexacosane	366	C26H54	000630-01-3	86
4			Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
5			Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055538.D
Acq On : 10 Nov 2022 13:48
Operator : CG/JU
Sample : N5378-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-20221028

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.331	63.8	ng	1036970	1	8.272	325081	20.0
2-Pentanone, 4-...	5.329	8.5	ng	138848	1	8.272	325081	20.0
n-Hexadecanoic ...	13.889	6.5	ng	193477	3	14.888	597847	20.0
Octadecanoic acid	16.774	13.9	ng	509498	4	17.626	735304	20.0
Undecanoic acid	18.490	2.5	ng	92537	4	17.626	735304	20.0
Octadecane	22.115	3.3	ng	148184	5	21.927	894736	20.0
Tetracosane, 1-...	22.991	2.0	ng	90022	5	21.927	894736	20.0