

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
 Data File : BG055631.D
 Acq On : 15 Nov 2022 21:09
 Operator : CG/JU
 Sample : N5431-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DISSOLVED-20221177-COMP-12-MODIFIED-ELUTRIATE

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: BG055631.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.695	232	239	244	rBV	22134	33752	1.00%	0.258%
2	5.306	338	343	354	rBV	57670	88005	2.62%	0.674%
3	5.782	417	424	433	rVB	371676	593952	17.66%	4.548%
4	7.392	690	698	710	rBV	277796	484619	14.41%	3.711%
5	8.256	835	845	852	rBV	154199	253909	7.55%	1.944%
6	9.425	1036	1044	1054	rVB	425859	755844	22.47%	5.787%
7	11.082	1318	1326	1335	rBV	203830	361435	10.75%	2.767%
8	13.503	1731	1738	1746	rBV	1115129	1704357	50.67%	13.050%
9	14.313	1870	1876	1882	rBV	31093	45940	1.37%	0.352%
10	14.878	1965	1972	1979	rVB	360624	550070	16.35%	4.212%
11	16.358	2217	2224	2235	rBV	1079731	1672393	49.72%	12.805%
12	17.615	2431	2438	2449	rBV	496697	768240	22.84%	5.882%
13	18.262	2542	2548	2554	rBV2	30989	44784	1.33%	0.343%
14	18.479	2579	2585	2595	rBV	122241	214523	6.38%	1.643%
15	19.737	2795	2799	2809	rBV	77127	135405	4.03%	1.037%
16	20.207	2872	2879	2886	rBV	2498528	3363726	100.00%	25.755%
17	21.552	3100	3108	3119	rBV6	40427	173708	5.16%	1.330%
18	21.916	3163	3170	3177	rBV	519169	853628	25.38%	6.536%
19	23.679	3466	3470	3477	rVB2	27910	55600	1.65%	0.426%
20	25.330	3740	3751	3764	rVB	298077	906480	26.95%	6.941%

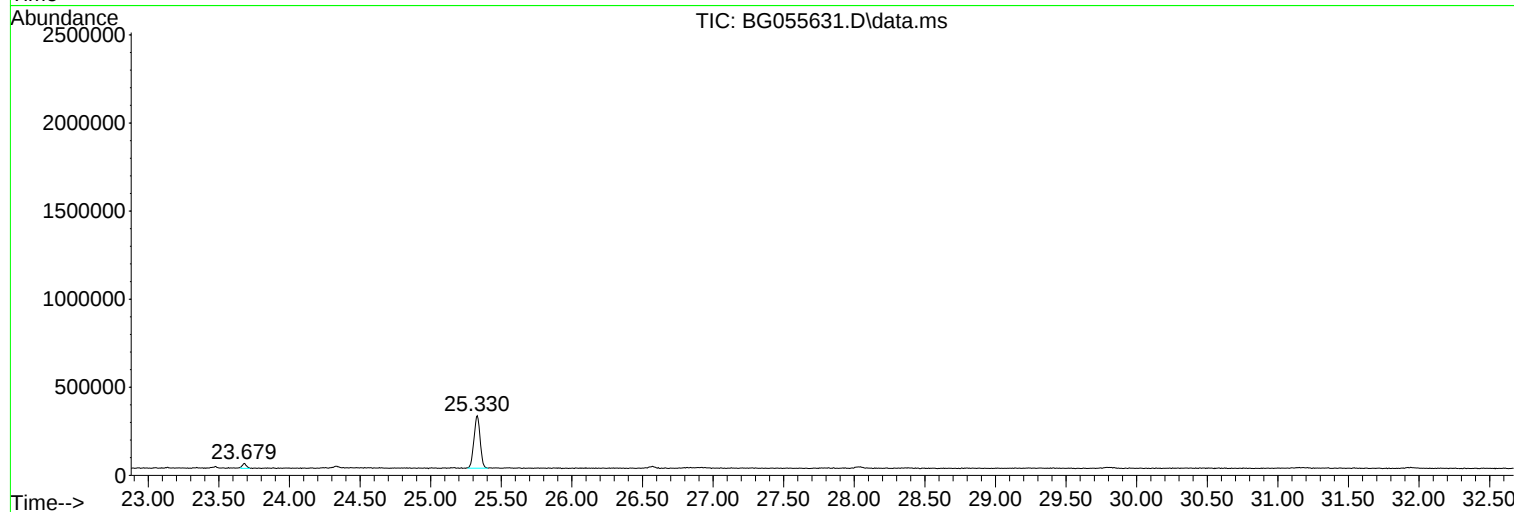
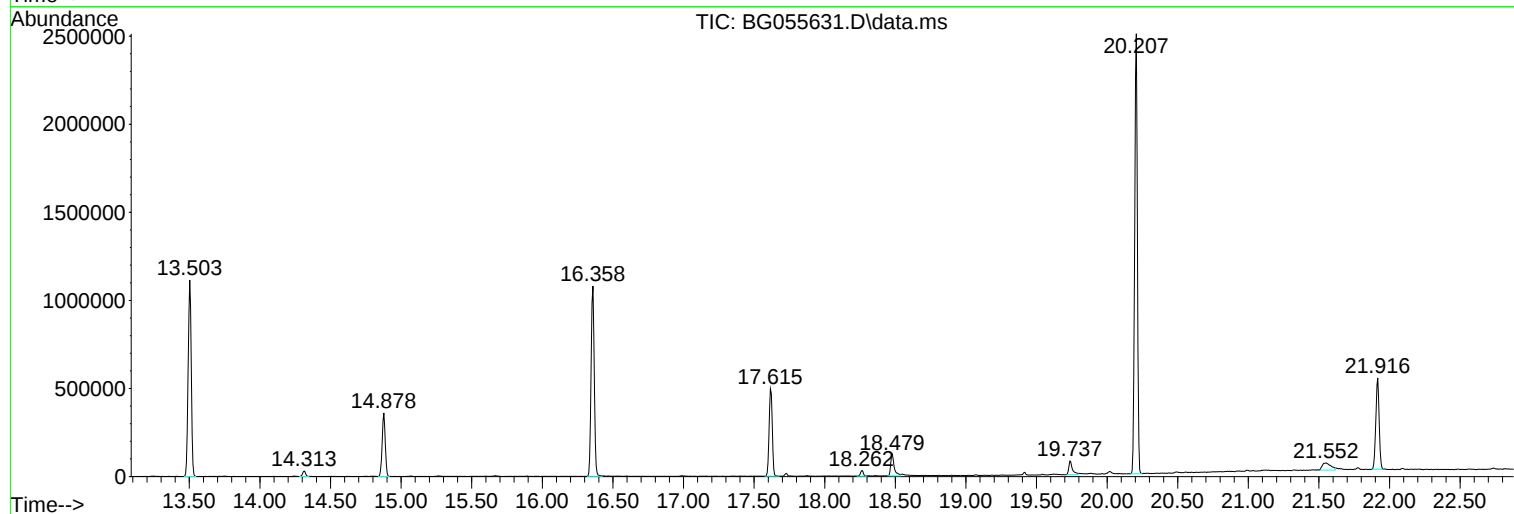
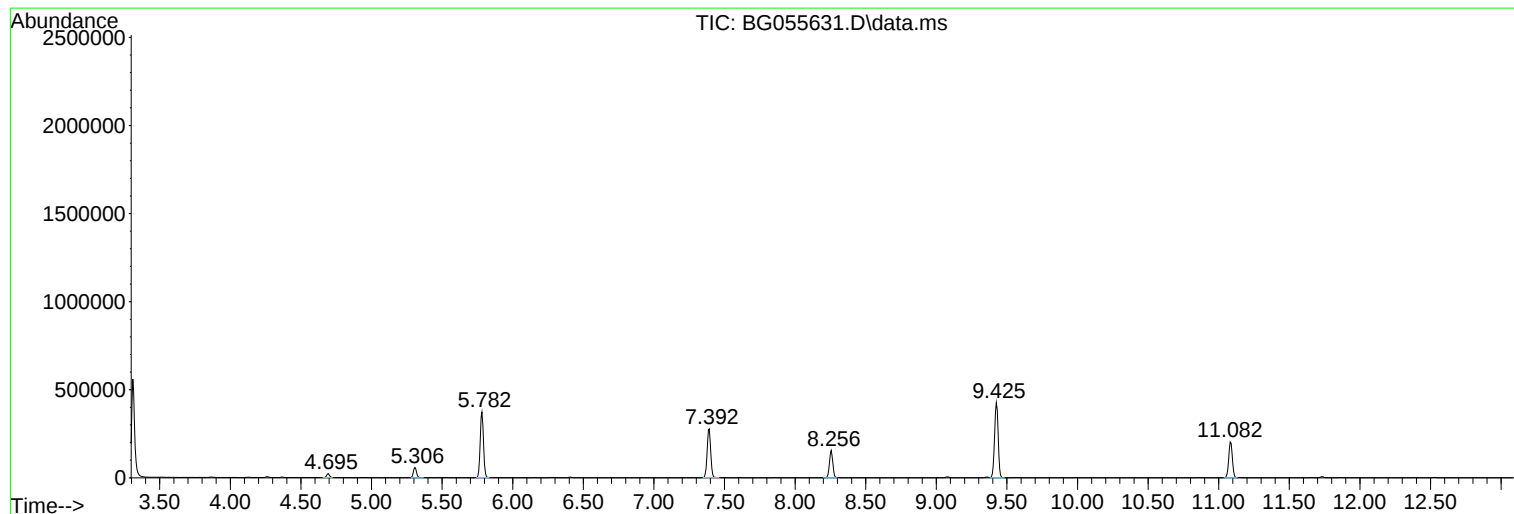
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG055631.D
Acq On : 15 Nov 2022 21:09
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Instrument :
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ClientSampleId :
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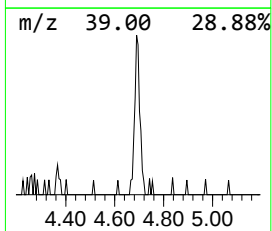
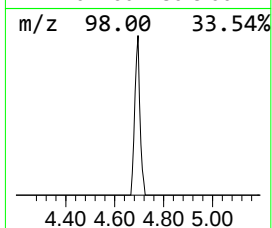
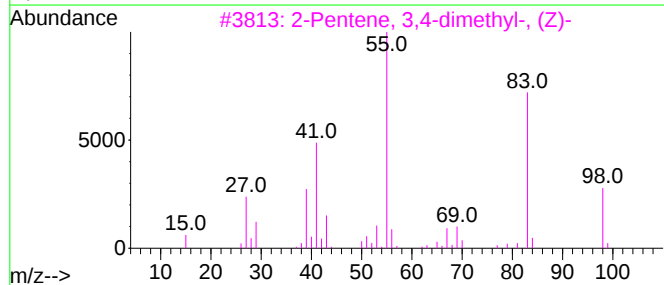
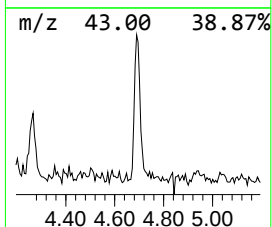
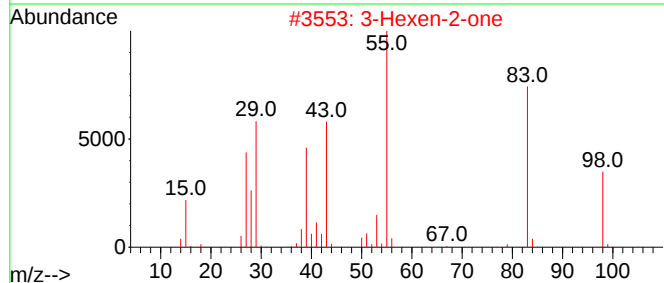
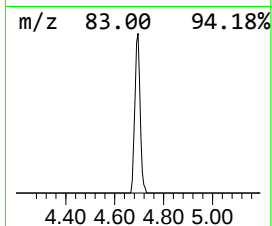
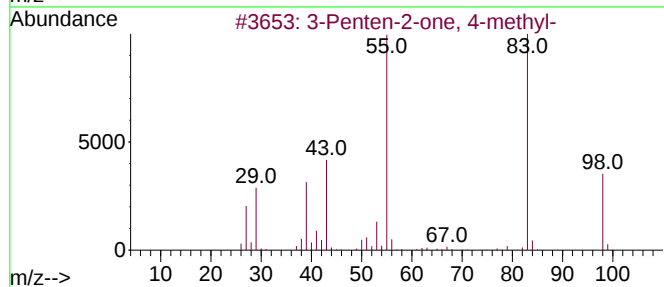
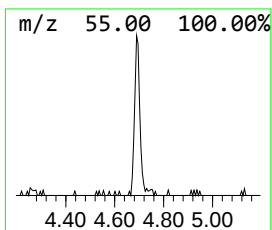
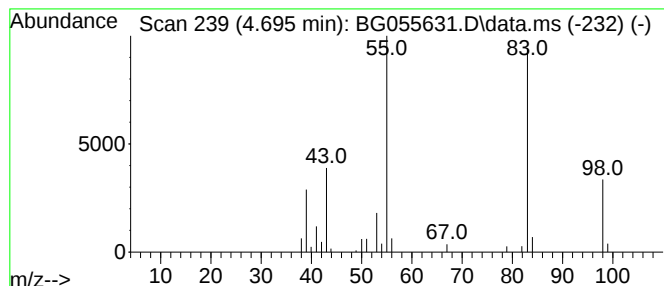
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.695	2.66 ng	33752	1,4-Dichlorobenzene-d4	8.256

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	93
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86



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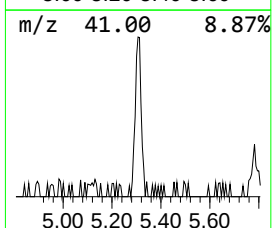
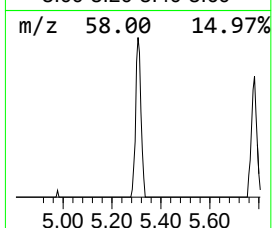
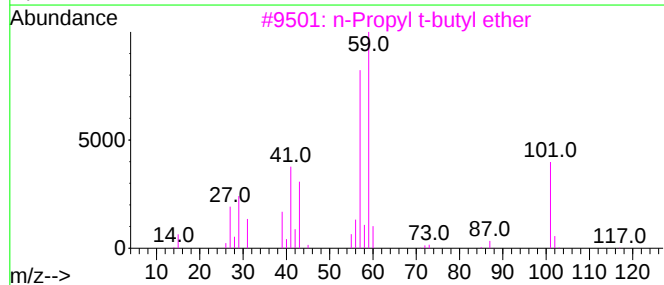
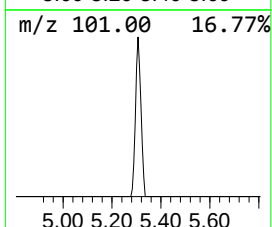
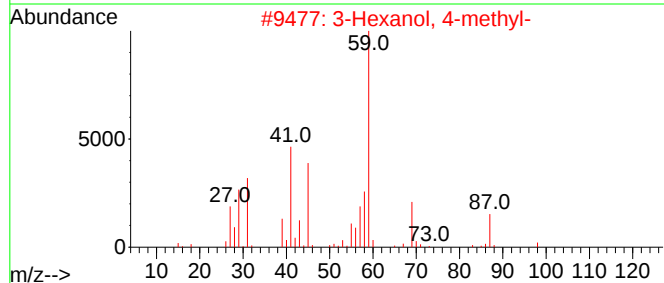
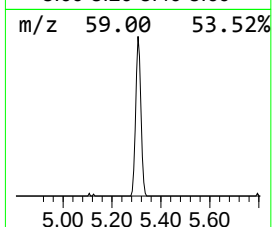
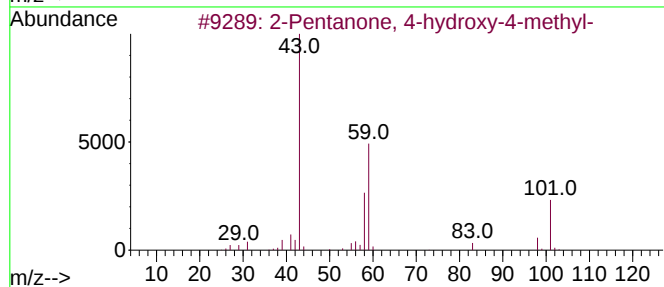
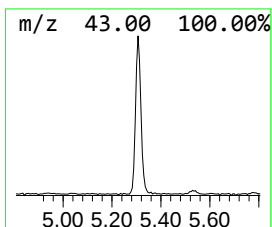
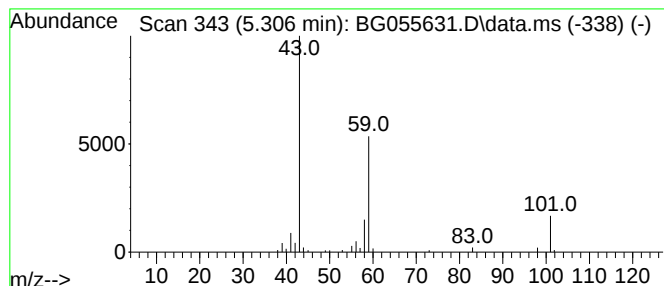
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.306	6.93 ng	88005	1,4-Dichlorobenzene-d4	8.256

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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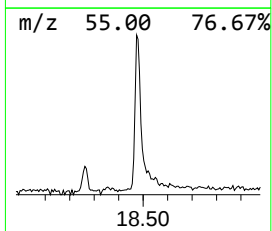
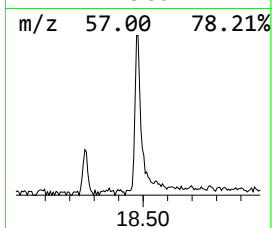
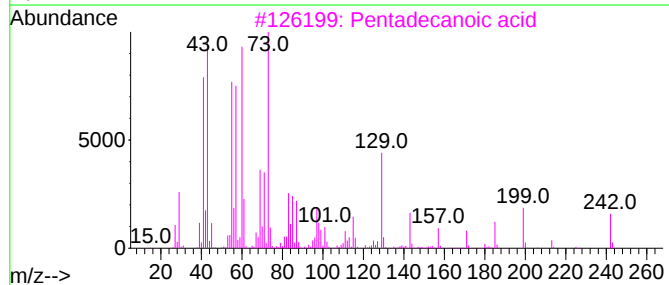
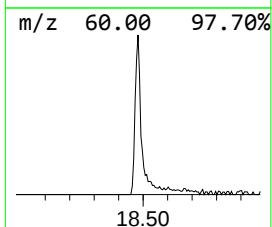
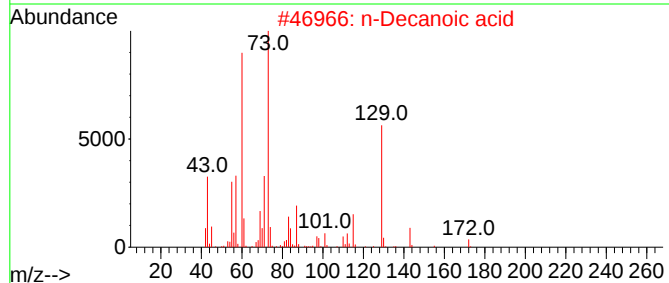
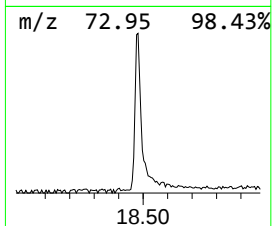
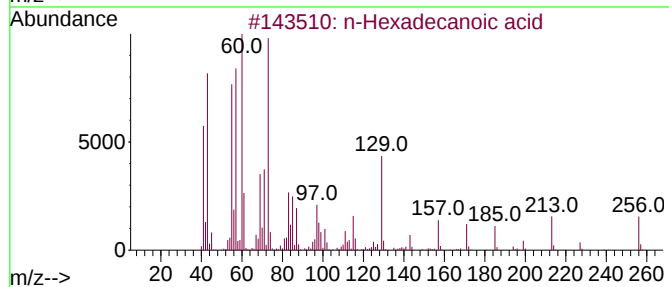
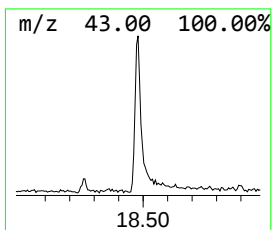
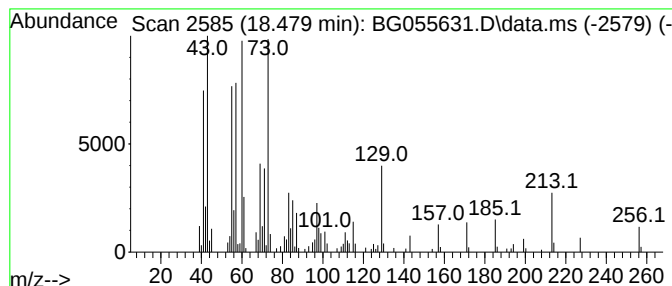
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.479	5.58 ng	214523	Phenanthrene-d10	17.616	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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Misc :
ALS Vial : 9 Sample Multiplier: 1

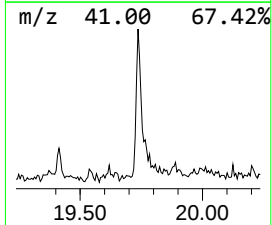
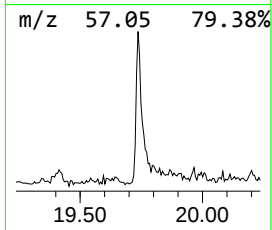
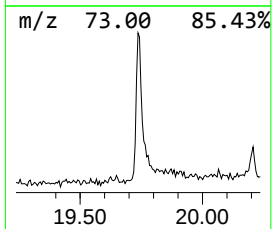
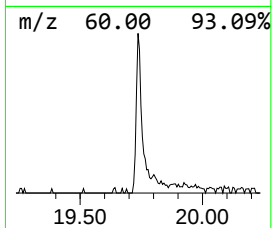
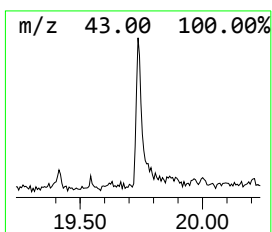
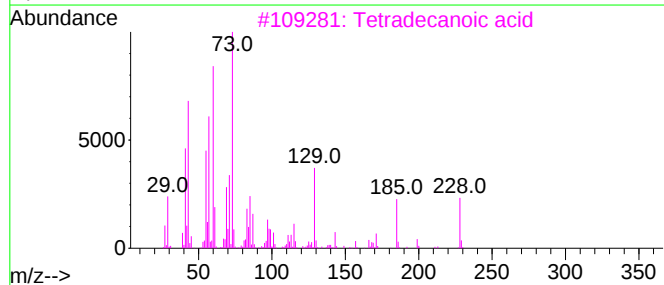
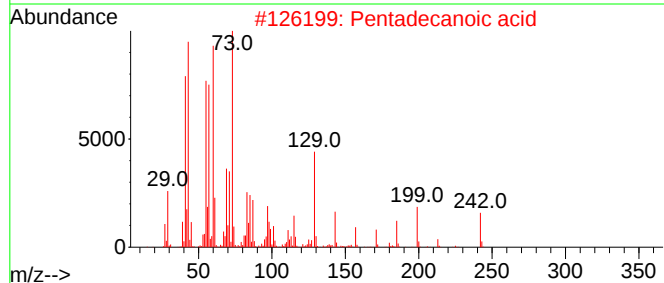
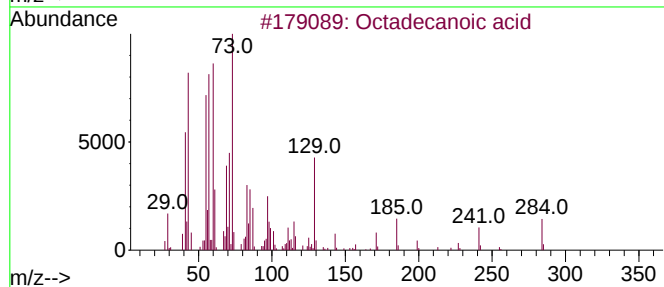
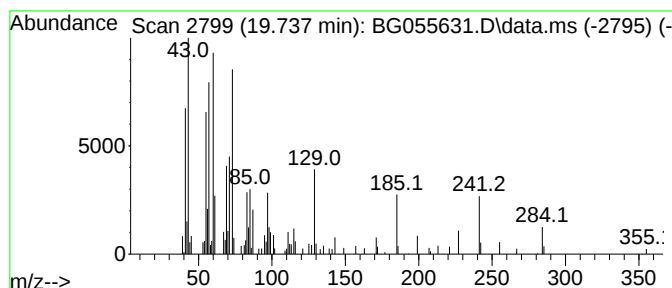
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.736	3.53 ng	135405	Phenanthrene-d10	17.616	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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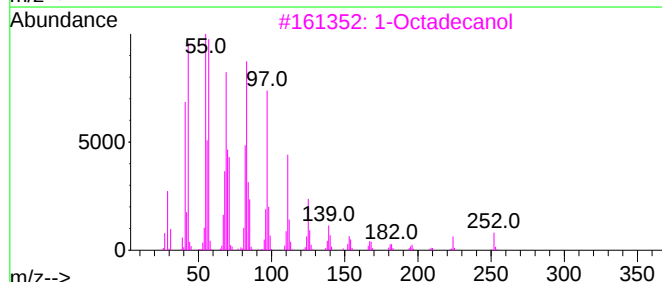
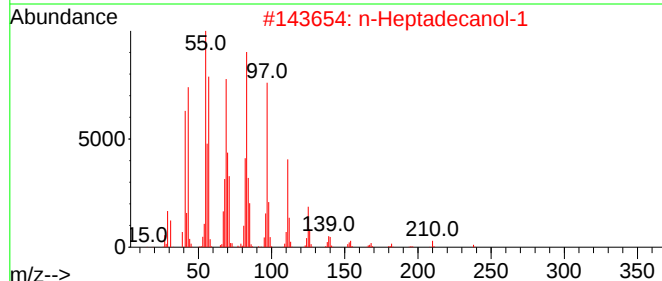
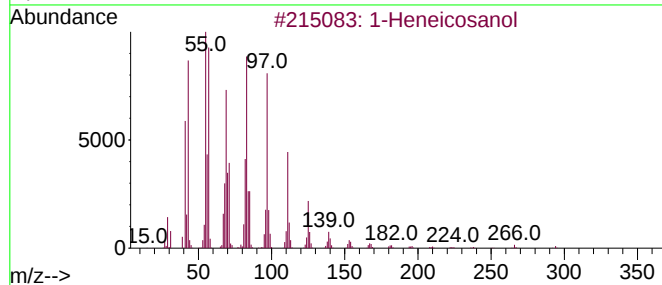
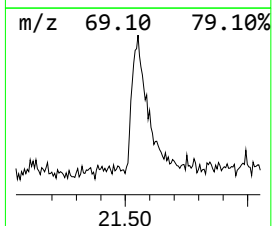
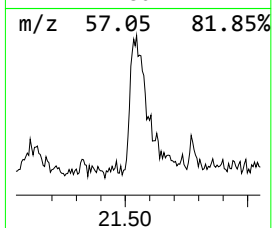
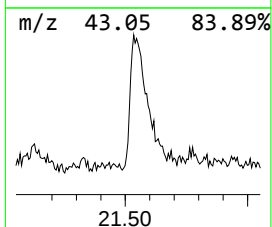
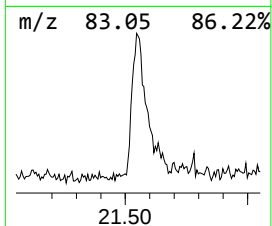
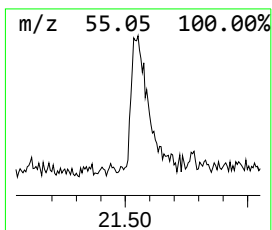
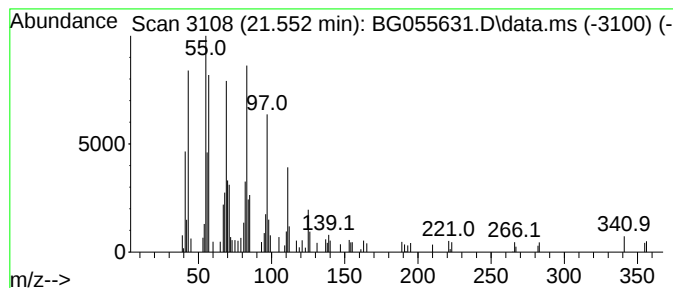
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.552	4.07 ng	173708	Chrysene-d12	21.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			n-Heptadecanol-1	256	C17H36O	001454-85-9	95
3			1-Octadecanol	270	C18H38O	000112-92-5	95
4			Cyclopentadecane	210	C15H30	000295-48-7	94
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	93



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.695	2.7	ng	33752	1	8.256	253909	20.0
2-Pentanone, 4-...	5.306	6.9	ng	88005	1	8.256	253909	20.0
n-Hexadecanoic ...	18.479	5.6	ng	214523	4	17.616	768240	20.0
Octadecanoic acid	19.736	3.5	ng	135405	4	17.616	768240	20.0
1-Heneicosanol	21.552	4.1	ng	173708	5	21.916	853628	20.0