

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
 Data File : BG055166.D
 Acq On : 13 Oct 2022 16:32
 Operator : CG/JU
 Sample : N5105-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-4

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-BG101322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055166.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.329	3	7	22	rVB	222376	352318	26.52%	3.941%
2	3.881	97	101	108	rBV	12323	19157	1.44%	0.214%
3	5.344	344	350	358	rVB	115199	170105	12.80%	1.903%
4	5.820	424	431	444	rVB	418685	669067	50.36%	7.485%
5	7.436	698	706	717	rBV	419000	744091	56.01%	8.324%
6	8.300	846	853	860	rBV	147481	250912	18.89%	2.807%
7	9.469	1044	1052	1060	rBV	260331	462331	34.80%	5.172%
8	10.873	1286	1291	1300	rVB	9698	15961	1.20%	0.179%
9	11.132	1327	1335	1344	rBV	211942	376025	28.30%	4.206%
10	13.541	1738	1745	1751	rBV	708858	1068761	80.45%	11.956%
11	14.345	1877	1882	1890	rVB	15332	24779	1.87%	0.277%
12	14.910	1971	1978	1987	rVB	322911	502041	37.79%	5.616%
13	16.384	2222	2229	2239	rBV	532167	800426	60.25%	8.954%
14	17.642	2436	2443	2453	rVB	360391	556425	41.88%	6.224%
15	18.494	2584	2588	2596	rBV	37333	67183	5.06%	0.752%
16	19.669	2784	2788	2792	rBV	10021	16309	1.23%	0.182%
17	19.751	2799	2802	2805	rBV5	13963	17321	1.30%	0.194%
18	20.027	2847	2849	2857	rVB	22652	29442	2.22%	0.329%
19	20.215	2876	2881	2886	rVB	1062942	1328497	100.00%	14.861%
20	21.531	3101	3105	3114	rBV2	49935	87939	6.62%	0.984%
21	21.925	3166	3172	3179	rVB	319248	546727	41.15%	6.116%
22	23.458	3429	3433	3445	rVB4	116993	243380	18.32%	2.723%
23	25.350	3748	3755	3767	rVB3	187433	590105	44.42%	6.601%

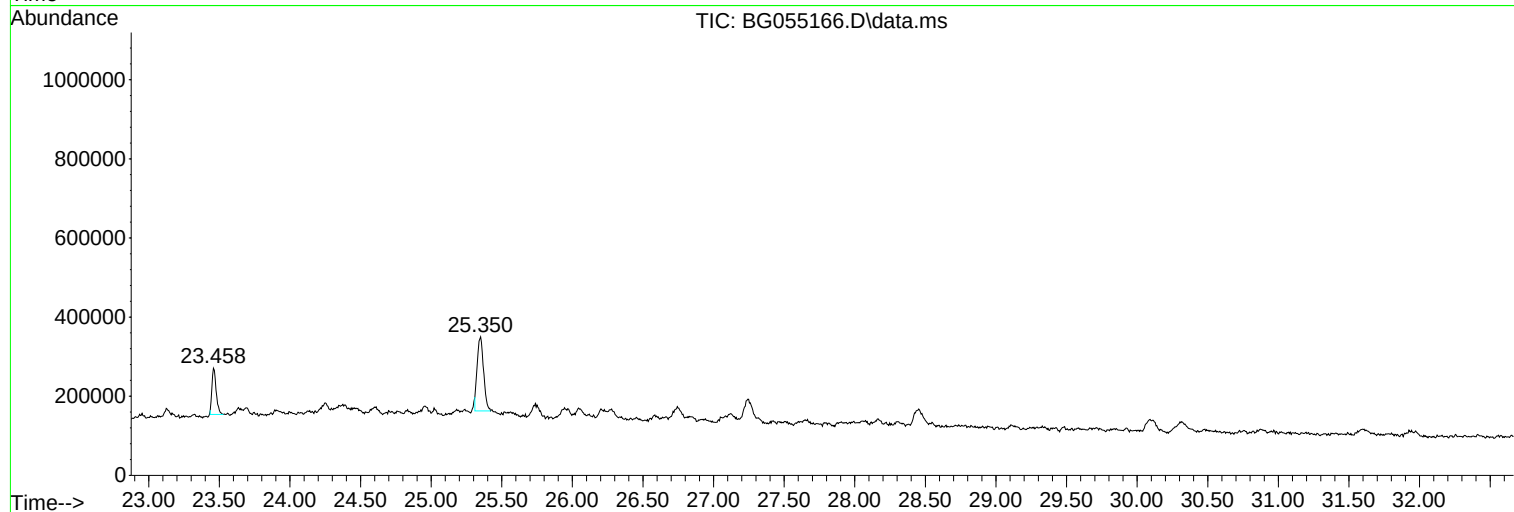
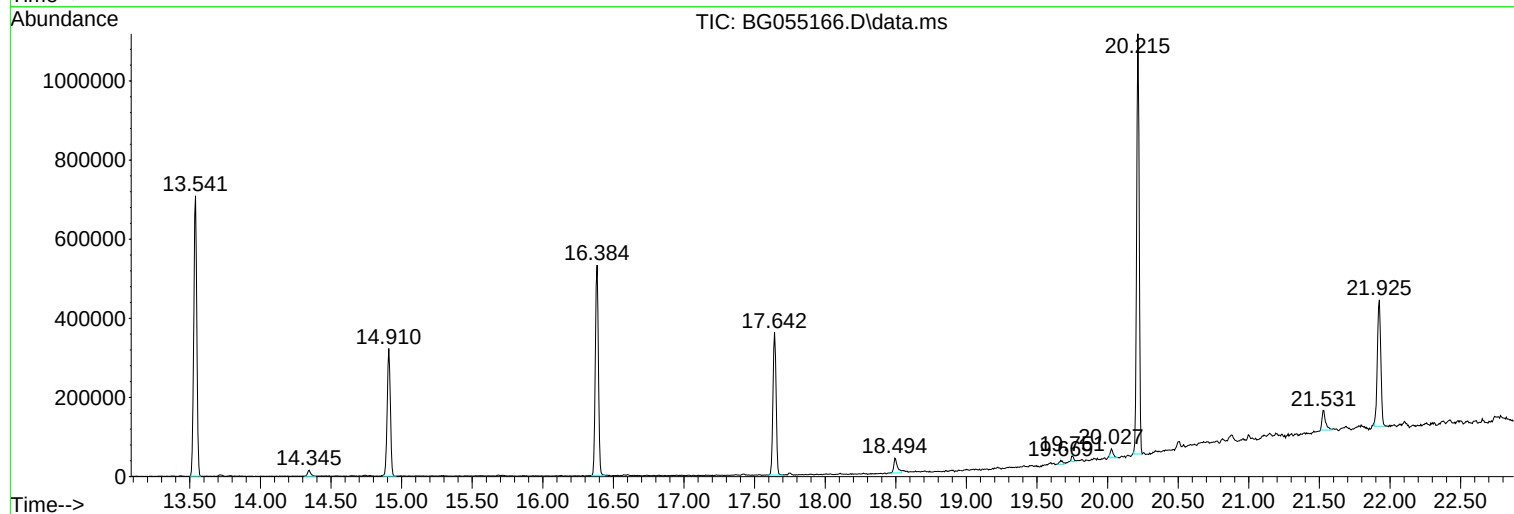
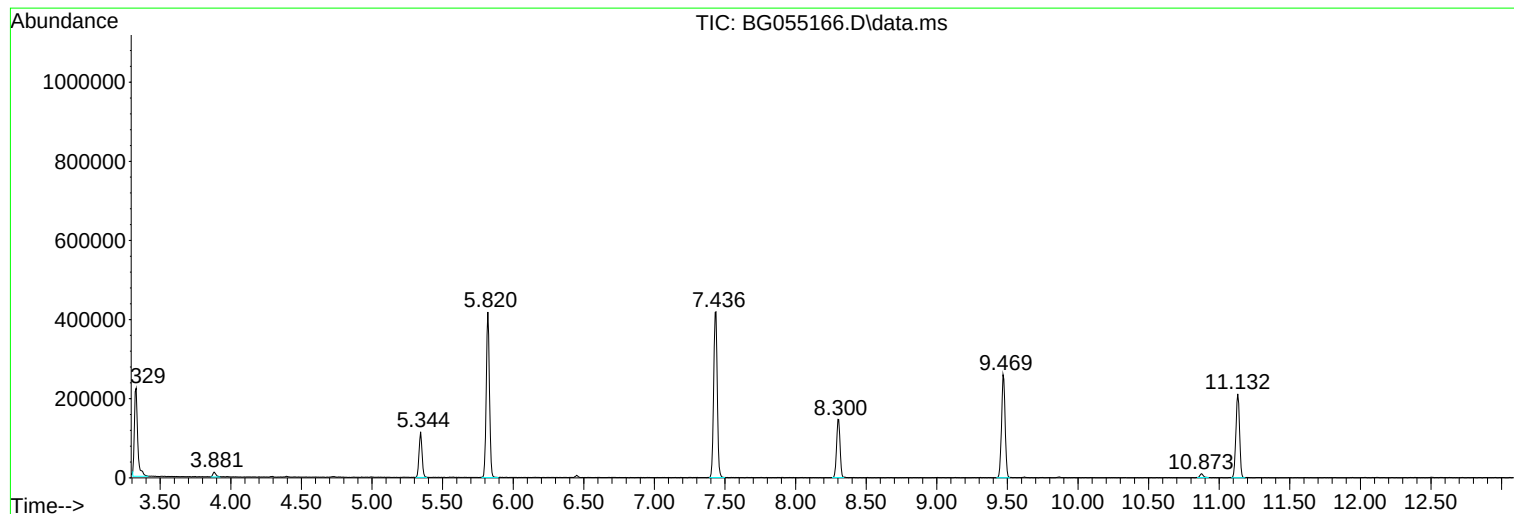
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Instrument :
BNA_G
ClientSampleId :
WC-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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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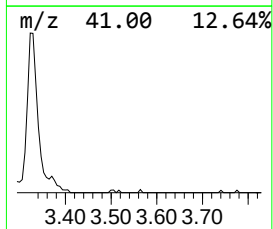
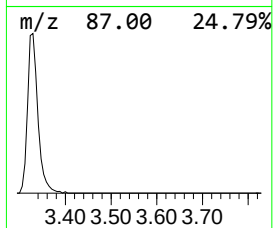
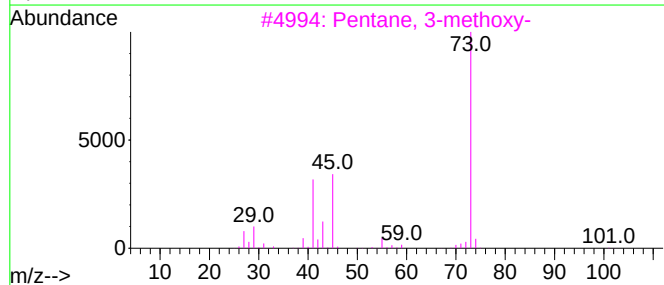
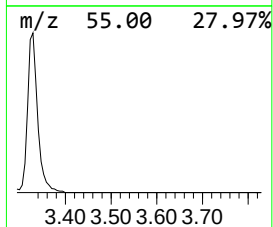
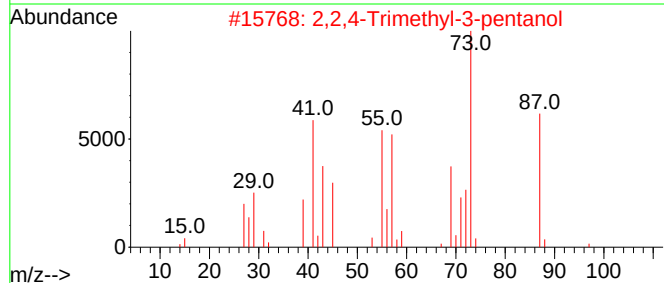
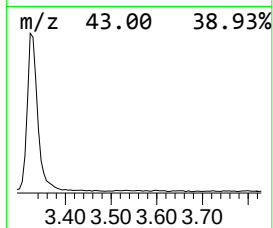
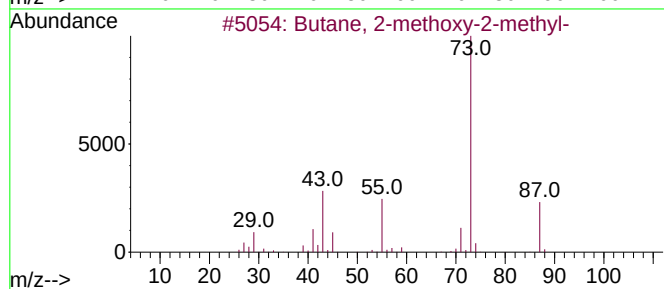
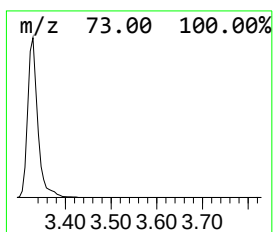
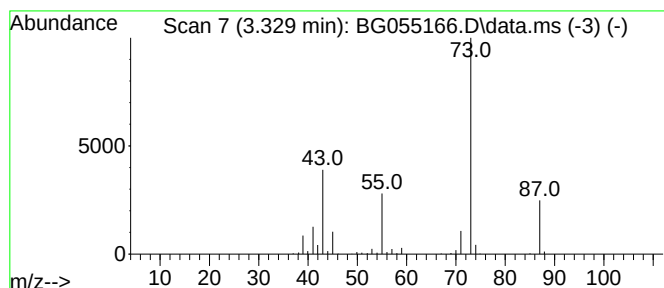
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.329	28.08 ng	352318	1,4-Dichlorobenzene-d4	8.306

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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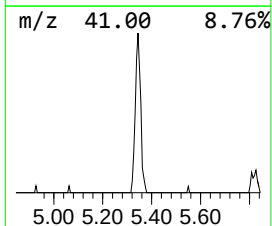
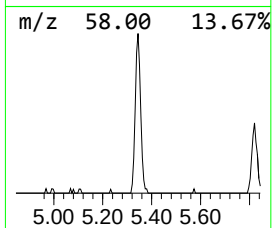
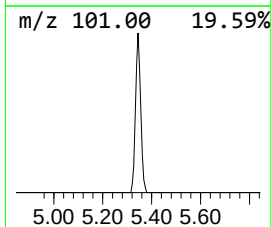
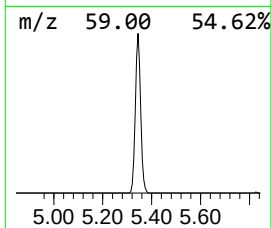
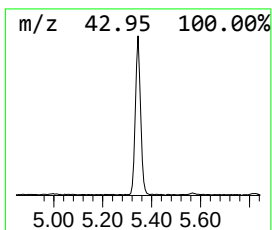
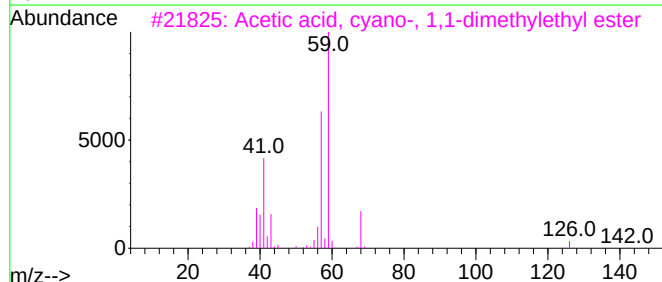
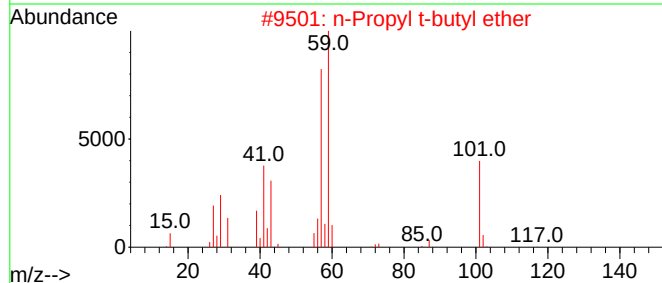
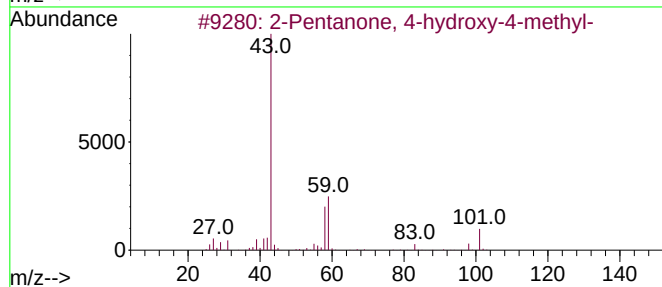
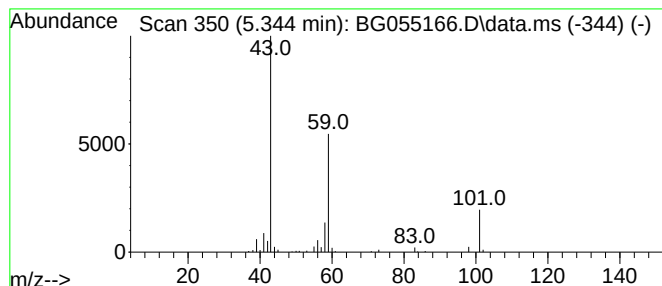
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.344	13.56 ng	170105	1,4-Dichlorobenzene-d4	8.306

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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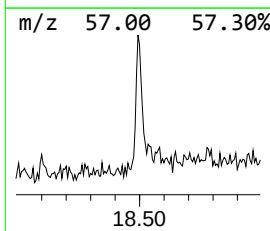
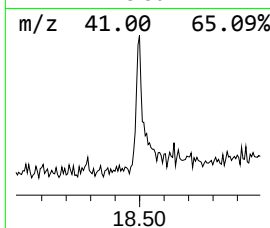
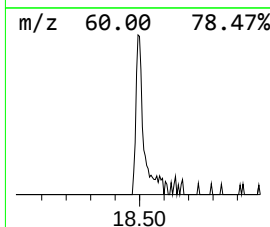
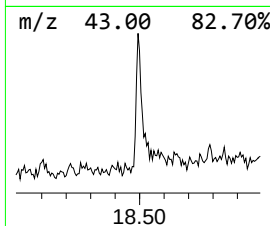
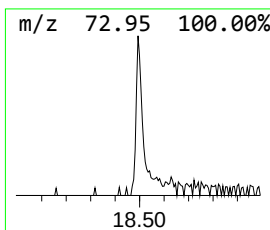
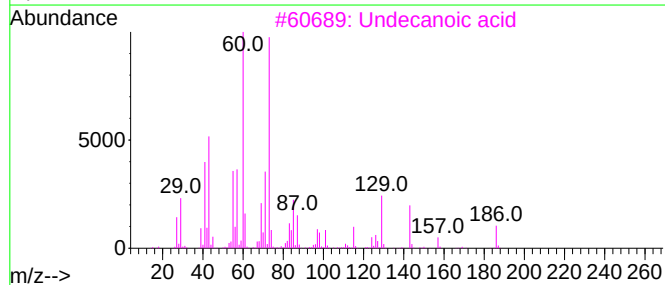
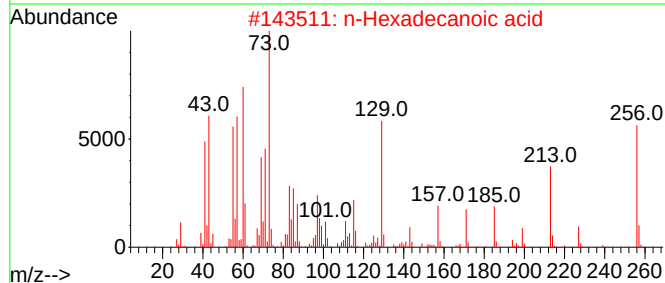
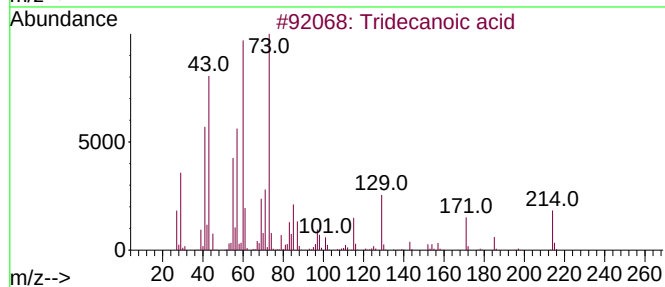
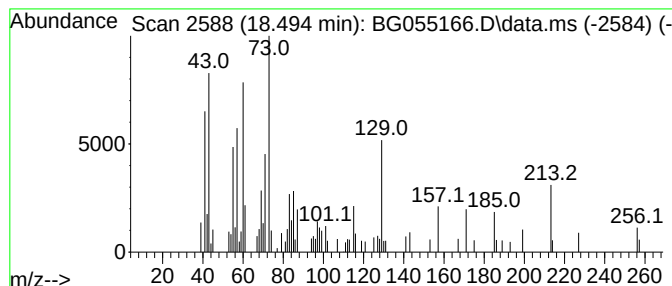
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.494	2.41 ng	67183	Phenanthrene-d10	17.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Undecanoic acid	186	C11H22O2	000112-37-8	70
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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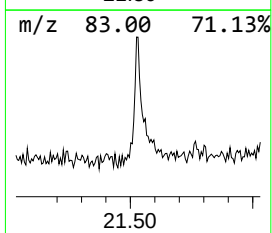
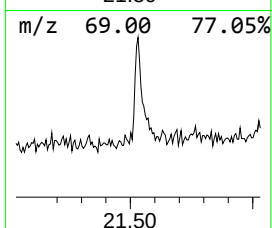
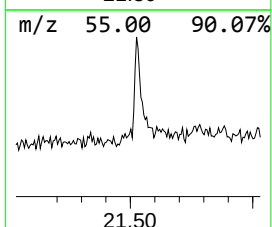
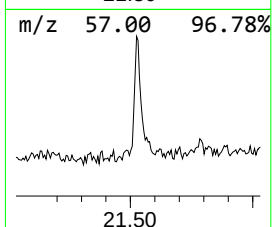
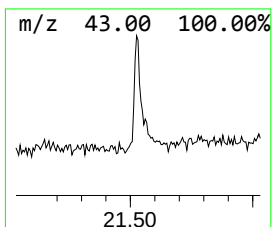
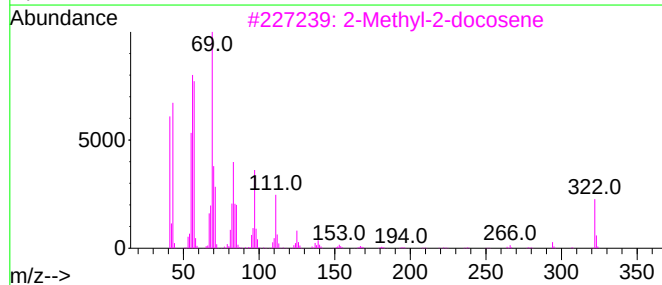
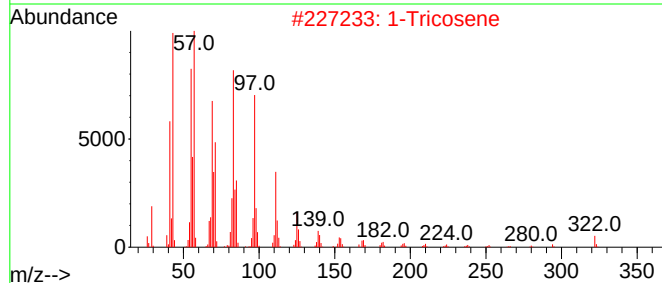
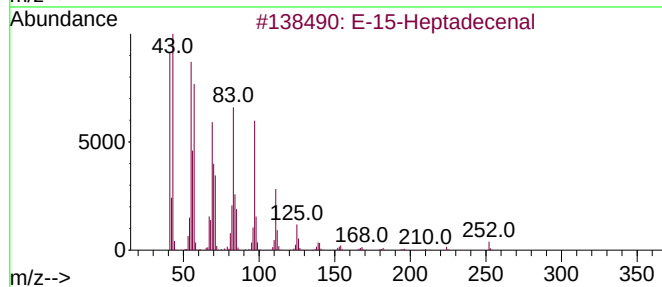
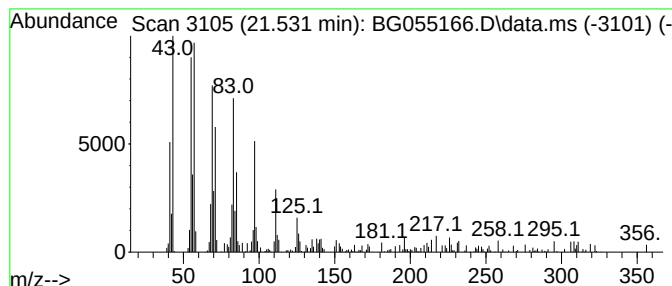
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.531	3.22 ng	87939	Chrysene-d12	21.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2			1-Tricosene	322	C23H46	018835-32-0	95
3			2-Methyl-2-docosene	322	C23H46	1000131-16-9	91
4			17-Pentatriacontene	491	C35H70	006971-40-0	91
5			1-Octadecene	252	C18H36	000112-88-9	90



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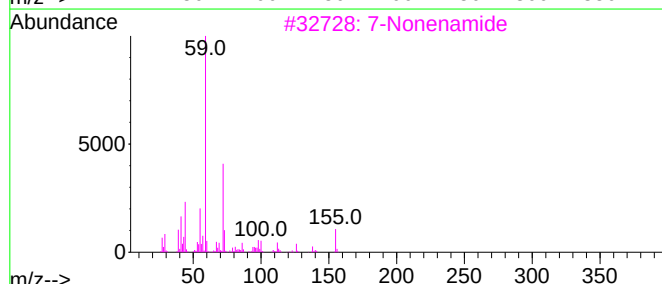
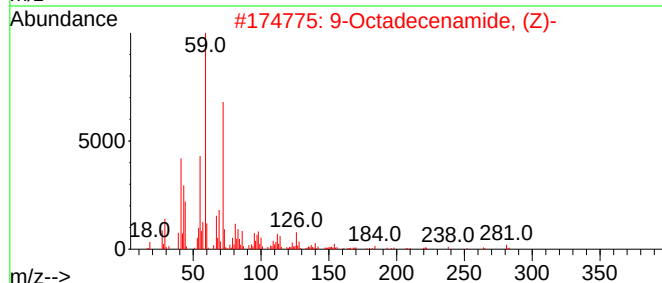
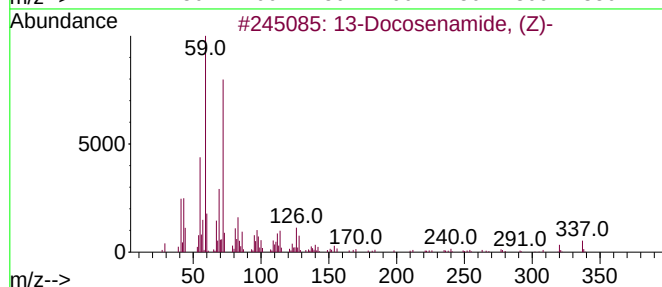
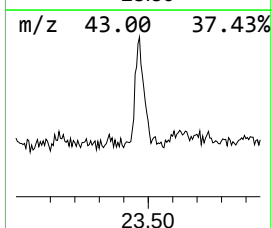
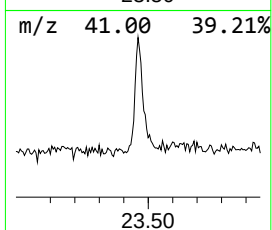
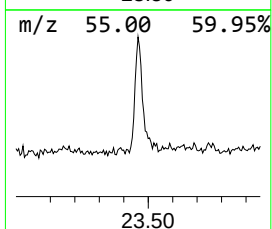
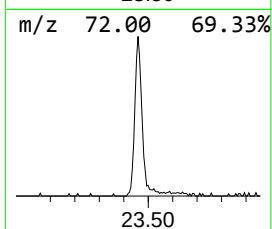
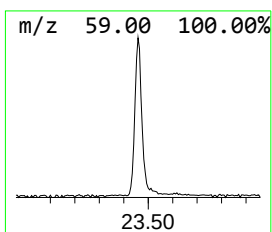
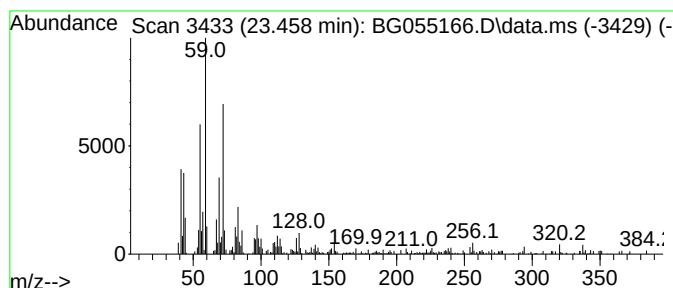
Instrument :
BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.458	8.90 ng	243380	Chrysene-d12		21.925	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-		337	C22H43NO	000112-84-5	91
2	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	68
3	7-Nonenamide		155	C9H17NO	090949-53-4	52
4	Dodecanamide		199	C12H25NO	001120-16-7	50
5	7-Octen-2-ol, 2,6-dimethyl-		156	C10H20O	018479-58-8	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.329	28.1	ng	352318	1	8.306	250912	20.0
2-Pentanone, 4-...	5.344	13.6	ng	170105	1	8.306	250912	20.0
Tridecanoic acid	18.494	2.4	ng	67183	4	17.642	556425	20.0
E-15-Heptadecenal	21.531	3.2	ng	87939	5	21.925	546727	20.0
13-Docosenamide...	23.458	8.9	ng	243380	5	21.925	546727	20.0