

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
 Data File : BG060216.D
 Acq On : 3 Jan 2024 6:38
 Operator : MA/JU
 Sample : 05899-07
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-14-0-2

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-BG122923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060216.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.118	3	5	12	rVB	372082	420020	3.01%	0.531%
2	5.509	405	412	430	rBV	3481421	5711556	40.87%	7.218%
3	6.620	595	601	607	rBV3	145615	235471	1.68%	0.298%
4	7.101	674	683	699	rBV	3426003	6088058	43.57%	7.693%
5	7.378	724	730	739	rVB	343285	598631	4.28%	0.756%
6	7.936	819	825	837	rBV	757175	1319742	9.44%	1.668%
7	9.099	1015	1023	1038	rBV	2017385	3682366	26.35%	4.653%
8	10.738	1292	1302	1310	rBV	1127689	2053536	14.69%	2.595%
9	13.200	1713	1721	1731	rBV	6522353	10293078	73.66%	13.007%
10	13.312	1735	1740	1749	rVB3	121921	221713	1.59%	0.280%
11	13.447	1758	1763	1769	rVB3	158636	255571	1.83%	0.323%
12	14.575	1947	1955	1962	rBV	2249505	3453662	24.71%	4.364%
13	14.640	1962	1966	1972	rVB2	110884	156893	1.12%	0.198%
14	14.851	1994	2002	2006	rBV3	119832	187029	1.34%	0.236%
15	16.061	2199	2208	2225	rBV	4449421	6875804	49.20%	8.689%
16	16.355	2253	2258	2262	rBV2	127958	197378	1.41%	0.249%
17	17.325	2416	2423	2434	rBV	2834921	4541161	32.50%	5.739%
18	18.212	2569	2574	2584	rBV	968342	1528442	10.94%	1.931%
19	19.369	2767	2771	2780	rBV2	666820	1472455	10.54%	1.861%
20	19.493	2788	2792	2807	rBV	2150955	3227891	23.10%	4.079%
21	19.945	2863	2869	2883	rVB	10065191	13974612	100.00%	17.660%
22	21.232	3083	3088	3095	rBV	795926	1237778	8.86%	1.564%
23	21.479	3126	3130	3135	rVB4	126220	179087	1.28%	0.226%
24	21.590	3142	3149	3156	rBV	2603254	4395177	31.45%	5.554%
25	22.383	3279	3284	3285	rBV2	135021	196894	1.41%	0.249%
26	23.083	3398	3403	3410	rVB3	166967	325795	2.33%	0.412%
27	23.858	3530	3535	3540	rVV3	105612	202803	1.45%	0.256%
28	23.911	3540	3544	3556	rVB6	106765	255512	1.83%	0.323%
29	24.469	3633	3639	3647	rVB6	92633	216094	1.55%	0.273%
30	24.763	3678	3689	3705	rBV	1606325	4606496	32.96%	5.821%
31	25.298	3776	3780	3792	rVB	87784	242746	1.74%	0.307%
32	25.903	3876	3883	3892	rVB5	148920	395653	2.83%	0.500%
33	26.026	3898	3904	3914	rBV4	127984	383824	2.75%	0.485%

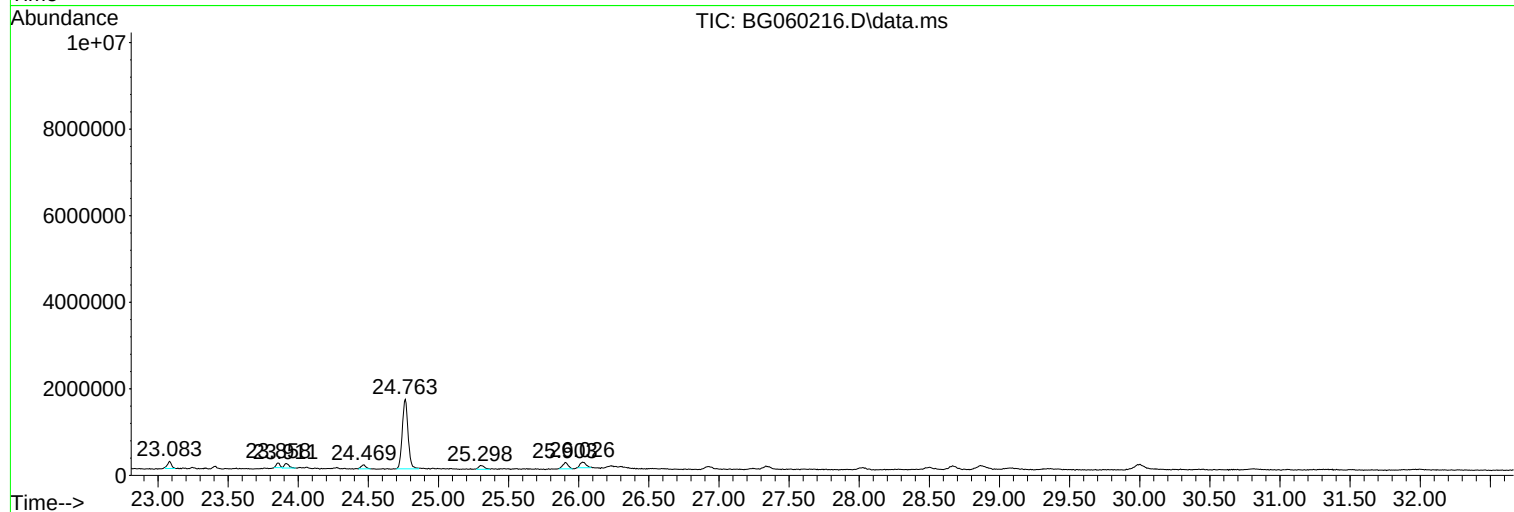
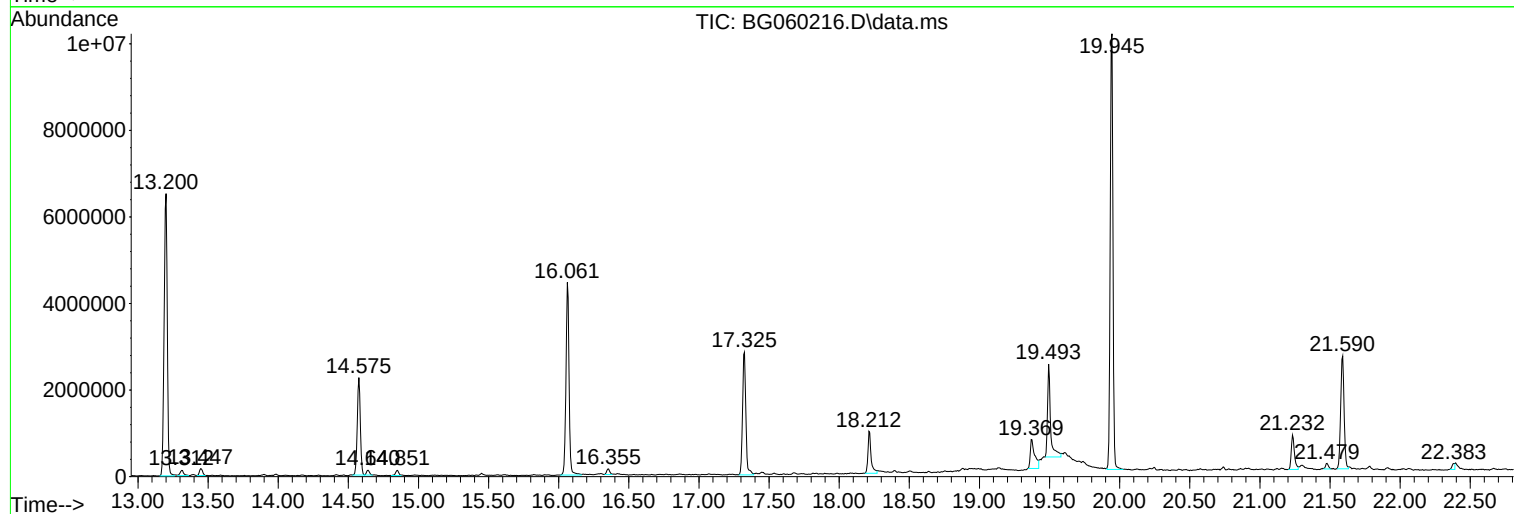
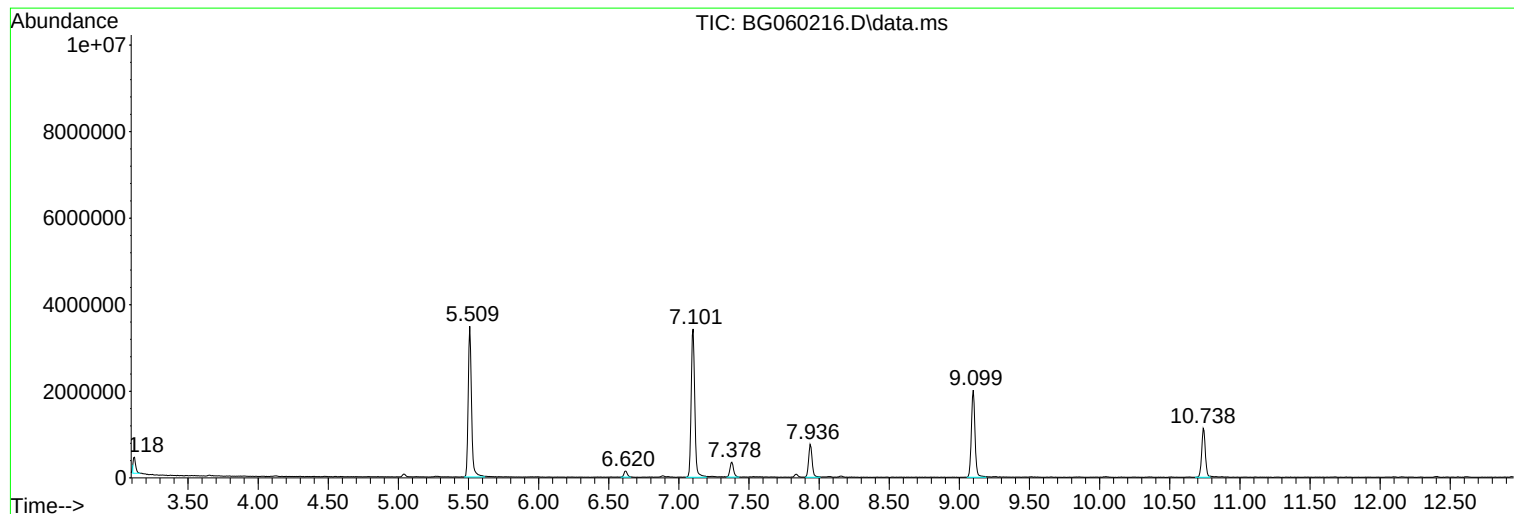
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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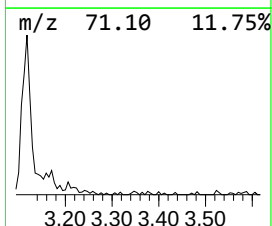
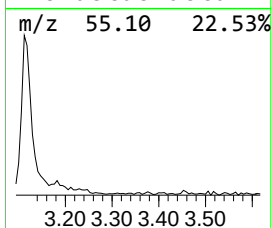
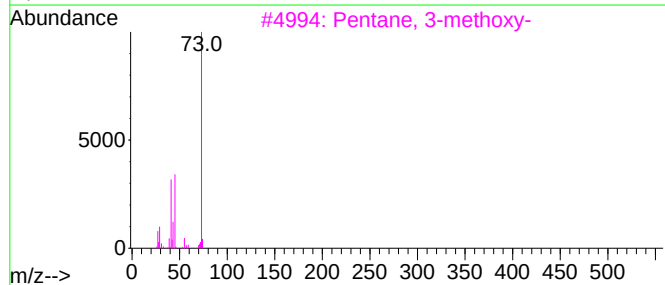
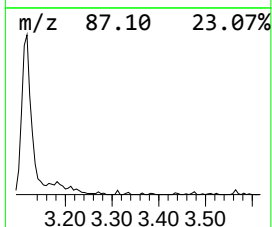
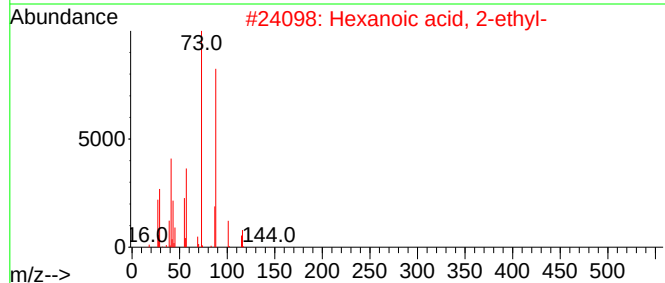
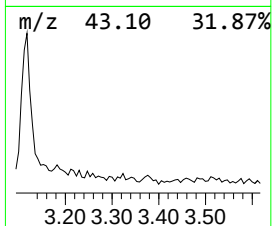
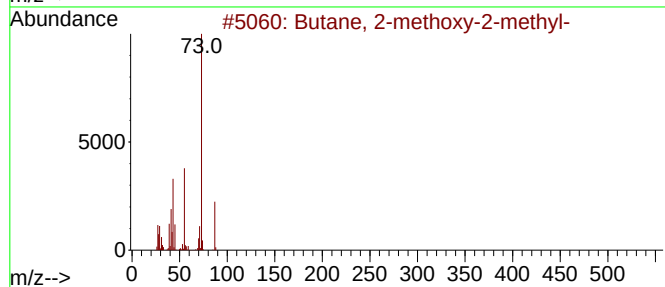
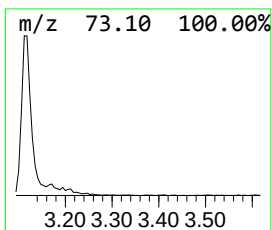
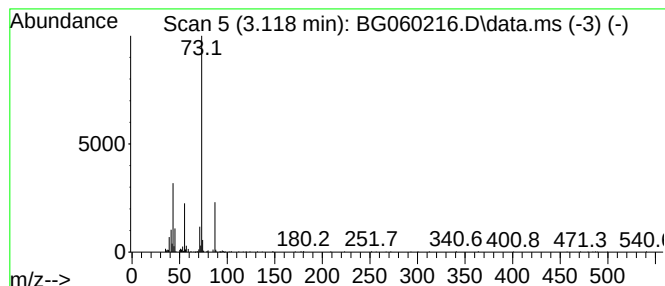
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.118	6.37 ng	420020	1,4-Dichlorobenzene-d4	7.936

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	53
2			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	33
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
5			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	12



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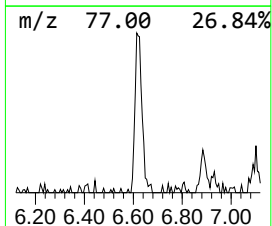
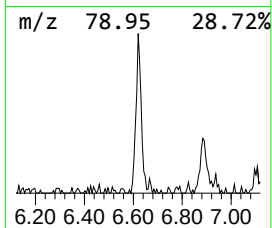
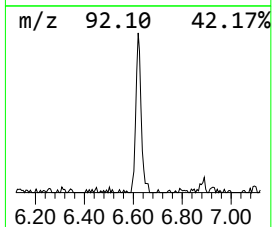
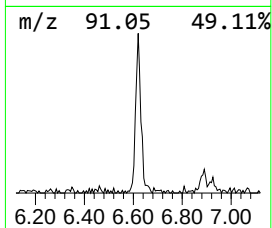
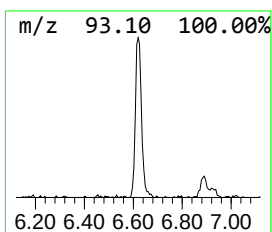
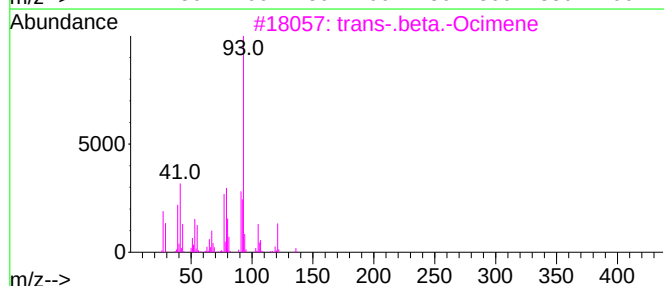
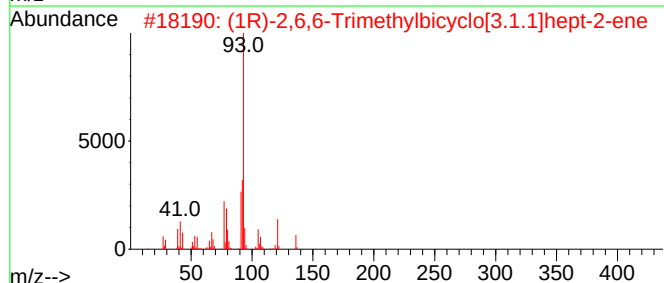
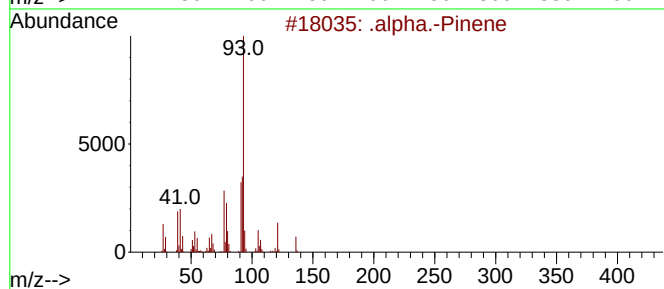
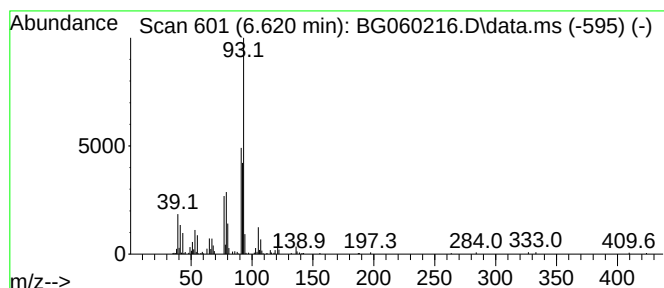
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 .alpha.-Pinene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.620	3.57 ng	235471	1,4-Dichlorobenzene-d4	7.936

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.alpha.-Pinene	136	C10H16	000080-56-8	91
2		(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	91
3		trans-.beta.-Ocimene	136	C10H16	003779-61-1	80
4		4-Carene, (1S,3S,6R)-(-)-	136	C10H16	005208-50-4	80
5		Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	72



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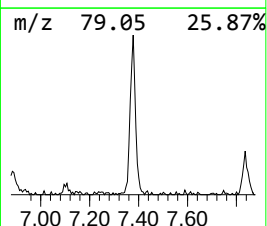
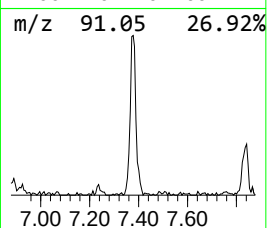
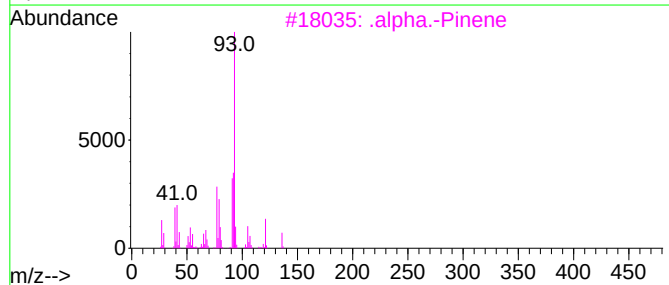
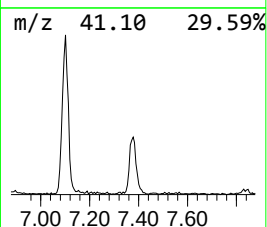
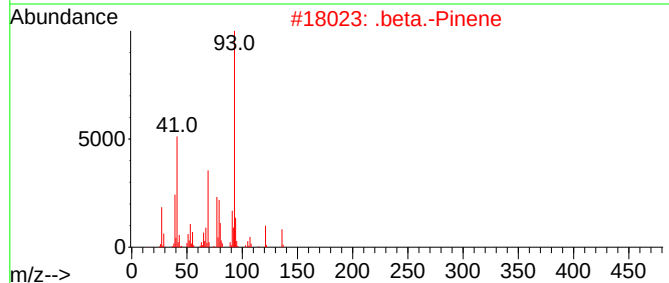
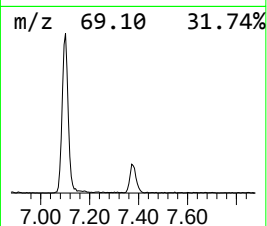
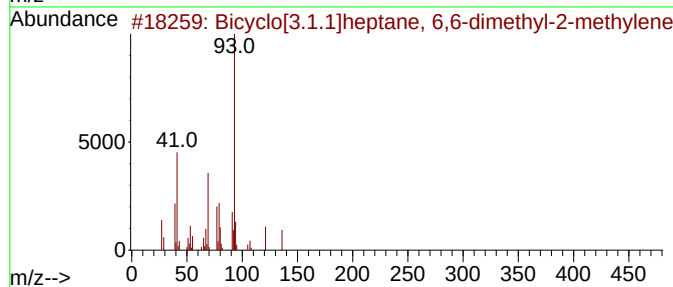
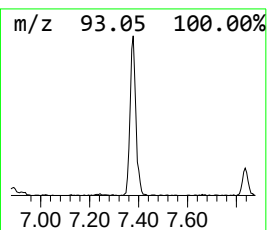
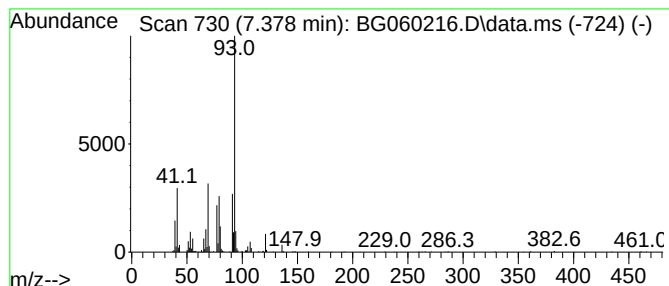
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Bicyclo[3.1.1]heptane, 6,6-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.378	9.07 ng	598631	1,4-Dichlorobenzene-d4	7.936

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	90
2			.beta.-Pinene	136	C10H16	000127-91-3	87
3			.alpha.-Pinene	136	C10H16	000080-56-8	87
4			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	86
5			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	72



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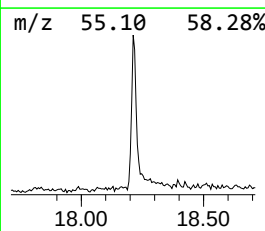
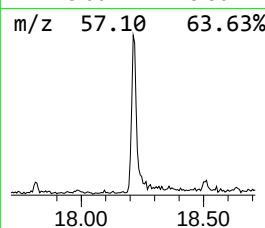
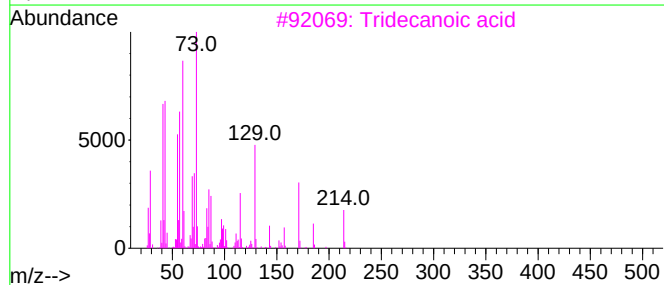
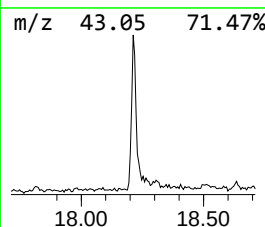
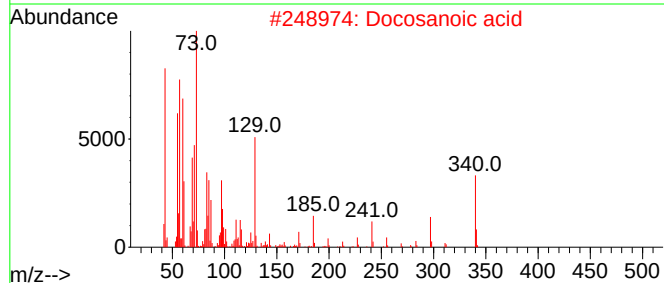
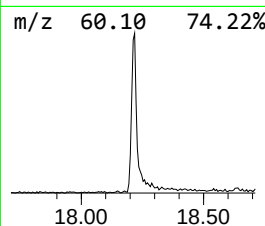
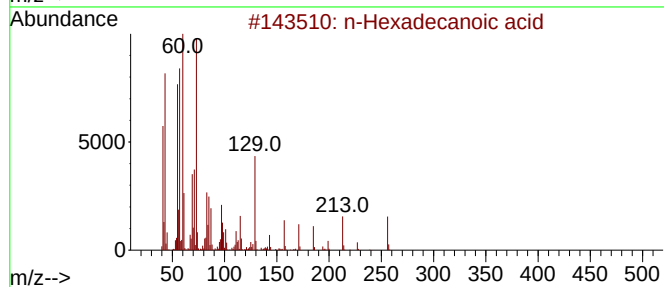
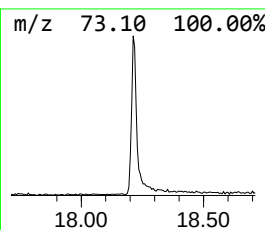
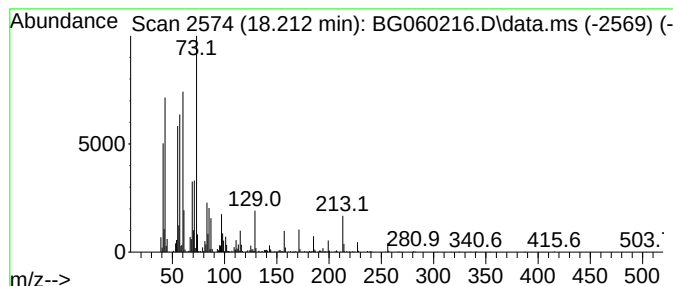
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.212	6.73 ng	1528440	Phenanthrene-d10	17.325

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Docosanoic acid	340	C22H44O2	000112-85-6	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Octadecanoic acid	284	C18H36O2	000057-11-4	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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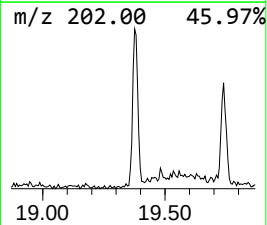
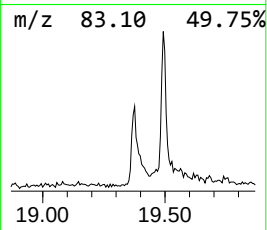
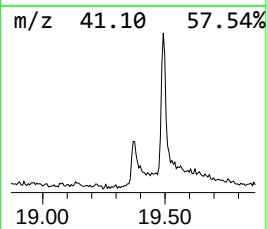
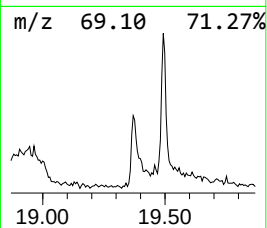
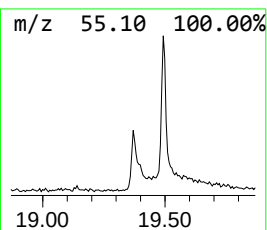
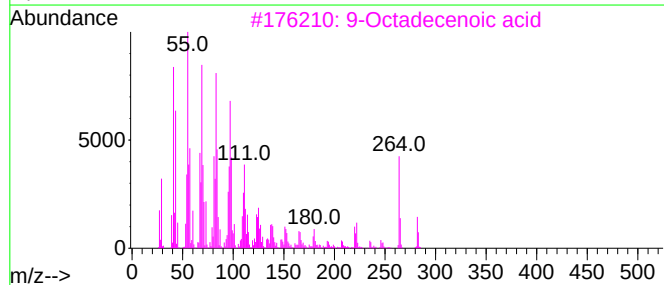
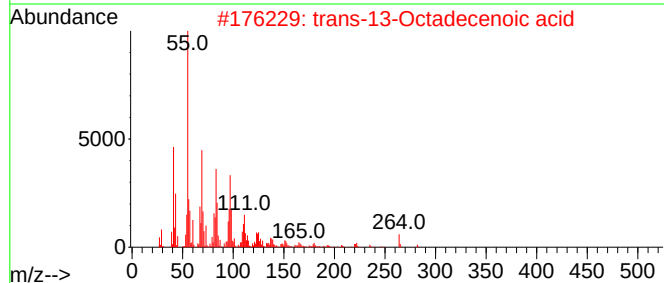
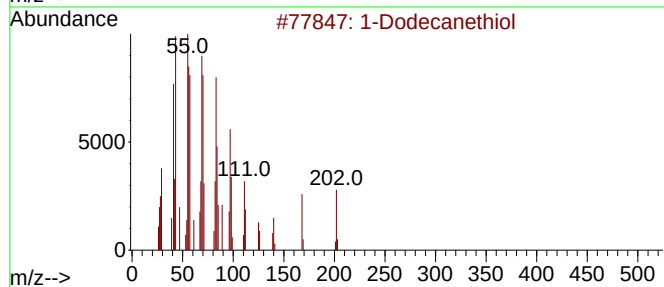
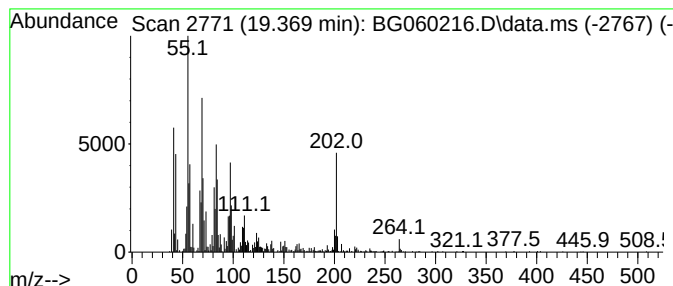
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Peak Number 5 1-Dodecanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.369	6.48 ng	1472460	Phenanthrene-d10	17.325

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dodecanethiol	202	C12H26S	000112-55-0	80
2			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	70
3			9-Octadecenoic acid	282	C18H34O2	002027-47-6	70
4			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	62
5			Erucic acid	338	C22H42O2	000112-86-7	58



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ClientSampleId :
GHL-SS-14-0-2

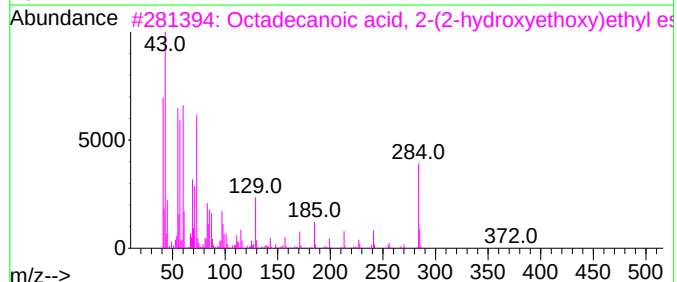
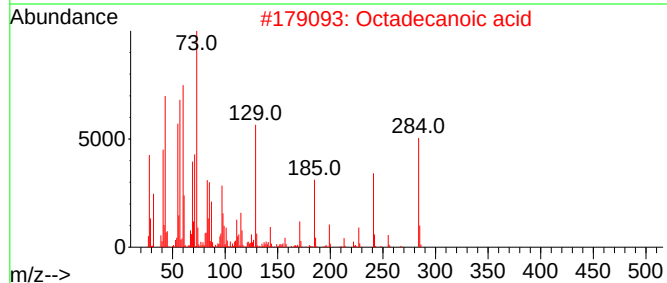
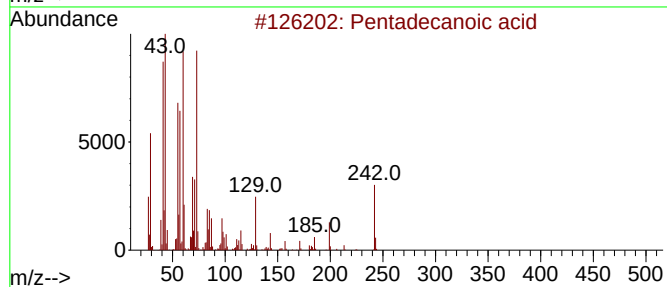
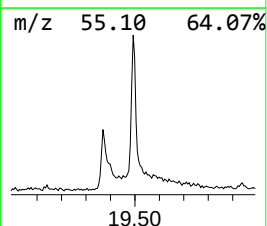
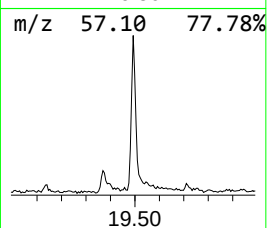
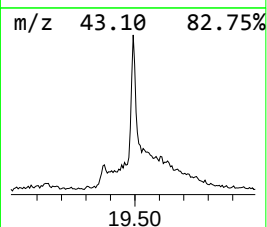
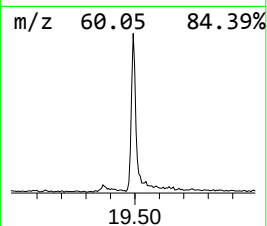
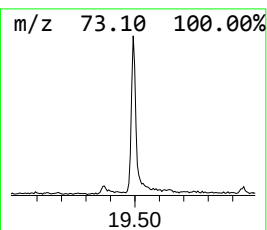
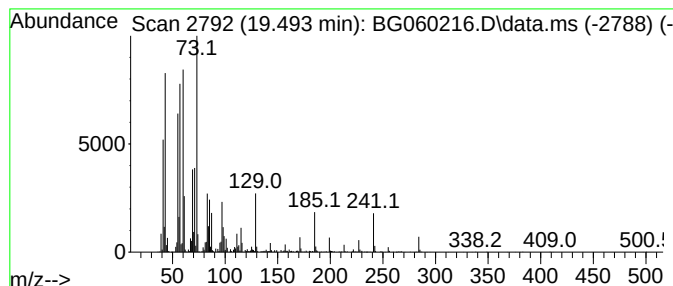
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.493	14.69 ng	3227890	Chrysene-d12	21.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2			Octadecanoic acid	284	C18H36O2	000057-11-4	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060216.D
Acq On : 3 Jan 2024 6:38
Operator : MA/JU
Sample : 05899-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-14-0-2

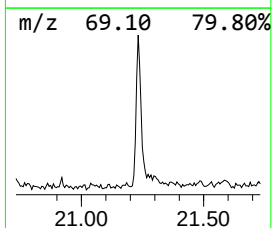
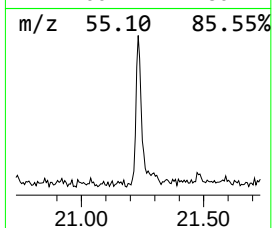
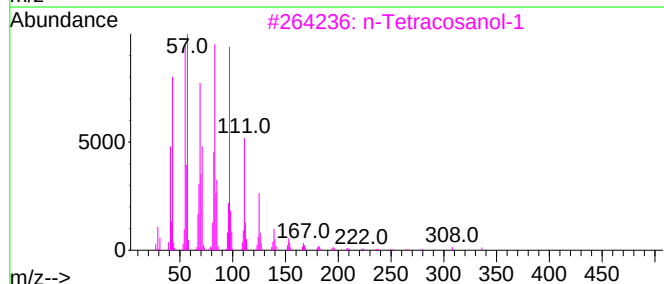
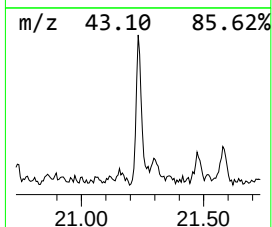
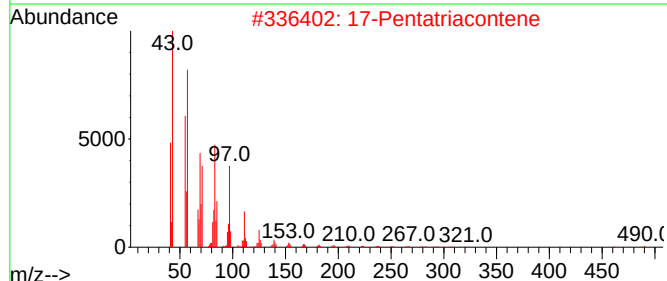
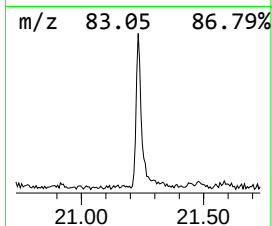
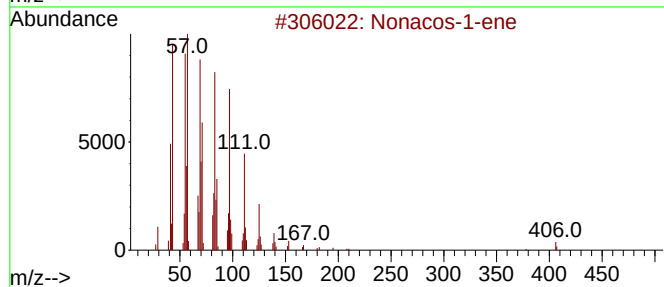
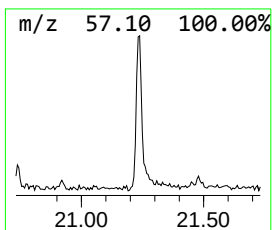
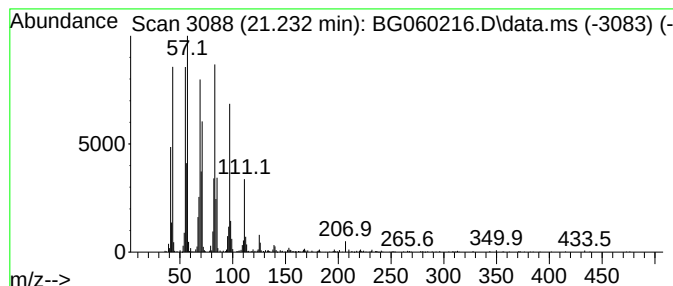
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonacos-1-ene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.232	5.63 ng	1237780	Chrysene-d12	21.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonacos-1-ene	406	C29H58	018835-35-3	91
2			17-Pentatriacontene	491	C35H70	006971-40-0	91
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4			2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
5			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060216.D
Acq On : 3 Jan 2024 6:38
Operator : MA/JU
Sample : 05899-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-14-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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...	3.118	6.4	ng	420020	1	7.936	1319740	20.0
.alpha.-Pinene	6.620	3.6	ng	235471	1	7.936	1319740	20.0
Bicyclo[3.1.1]h...	7.378	9.1	ng	598631	1	7.936	1319740	20.0
n-Hexadecanoic ...	18.212	6.7	ng	1528440	4	17.325	4541160	20.0
1-Dodecanethiol	19.369	6.5	ng	1472460	4	17.325	4541160	20.0
Pentadecanoic acid	19.493	14.7	ng	3227890	5	21.590	4395180	20.0
Nonacos-1-ene	21.232	5.6	ng	1237780	5	21.590	4395180	20.0