

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
 Data File : BM046358.D
 Acq On : 28 Jun 2024 18:43
 Operator : MA/JU
 Sample : P3076-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 7-E-1

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_M\Methods\8270-BM062724.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM046358.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.287	65	68	84	rBV	218711	393413	8.41%	1.033%
2	4.593	280	290	301	rBV	167307	318053	6.80%	0.835%
3	5.051	361	368	390	rBV	2609834	4029480	86.12%	10.582%
4	6.628	627	636	664	rBV	2245164	4176255	89.26%	10.968%
5	7.369	756	762	778	rBV	656053	1100761	23.53%	2.891%
6	8.534	953	960	985	rBV	1283352	2669904	57.06%	7.012%
7	10.133	1223	1232	1251	rBV	687585	1448336	30.95%	3.804%
8	10.939	1362	1369	1379	rBV2	40567	114984	2.46%	0.302%
9	12.639	1650	1658	1686	rBV	2689208	4678900	100.00%	12.288%
10	14.021	1883	1893	1900	rBV	977790	1545468	33.03%	4.059%
11	14.086	1901	1904	1917	rVB	44774	91155	1.95%	0.239%
12	14.257	1927	1933	1935	rBV	849577	1235804	26.41%	3.245%
13	14.280	1935	1937	1961	rVB	1075196	1392952	29.77%	3.658%
14	15.527	2142	2149	2172	rBV	2206349	3462247	74.00%	9.093%
15	16.774	2355	2361	2366	rBV	966012	1451778	31.03%	3.813%
16	16.815	2366	2368	2380	rVV	288245	443828	9.49%	1.166%
17	16.915	2381	2385	2391	rVB	46361	74535	1.59%	0.196%
18	17.221	2428	2437	2445	rBV6	17862	52313	1.12%	0.137%
19	17.704	2515	2519	2530	rBV	270051	493415	10.55%	1.296%
20	17.845	2539	2543	2547	rBV2	37903	59836	1.28%	0.157%
21	18.574	2662	2667	2671	rBV6	22162	48791	1.04%	0.128%
22	18.645	2676	2679	2683	rVB4	42942	51221	1.09%	0.135%
23	18.845	2707	2713	2718	rBV	469576	655373	14.01%	1.721%
24	18.992	2734	2738	2747	rBV2	117642	242245	5.18%	0.636%
25	19.127	2758	2761	2765	rVB3	48928	56174	1.20%	0.148%
26	19.209	2767	2775	2779	rBV	386982	596188	12.74%	1.566%
27	19.421	2806	2811	2824	rVB	3296528	4157731	88.86%	10.919%
28	20.709	3026	3030	3037	rBV2	182125	309323	6.61%	0.812%
29	20.992	3072	3078	3083	rBV2	927834	1505876	32.18%	3.955%
30	23.668	3526	3533	3541	rVB	588540	1221415	26.10%	3.208%

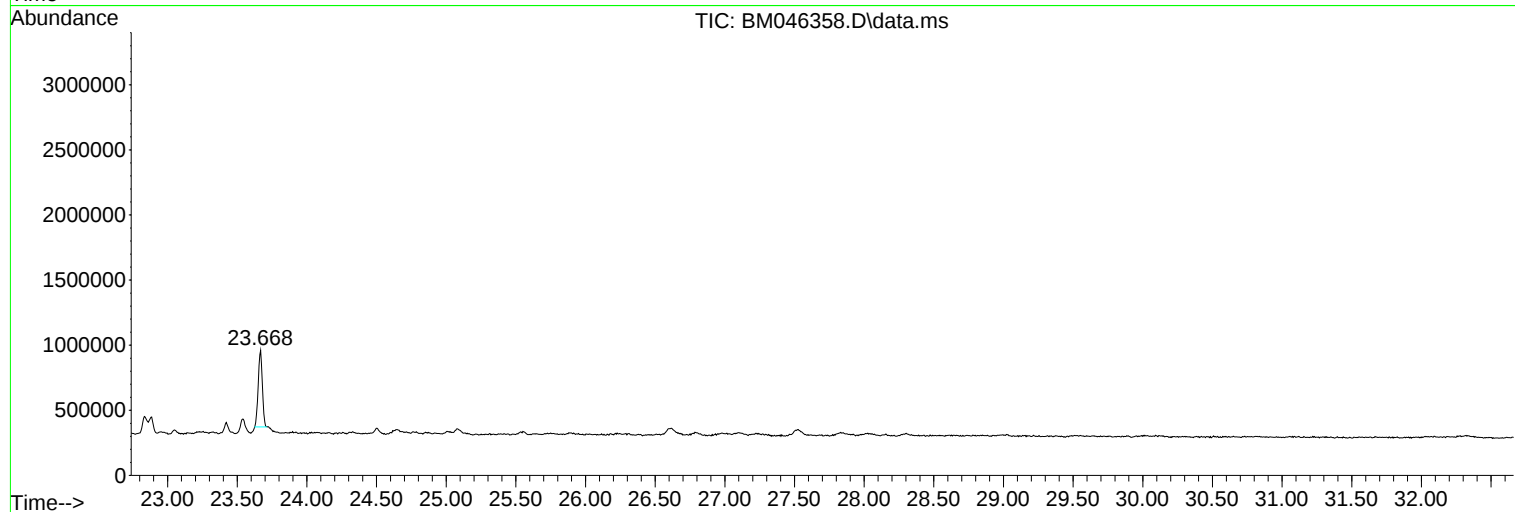
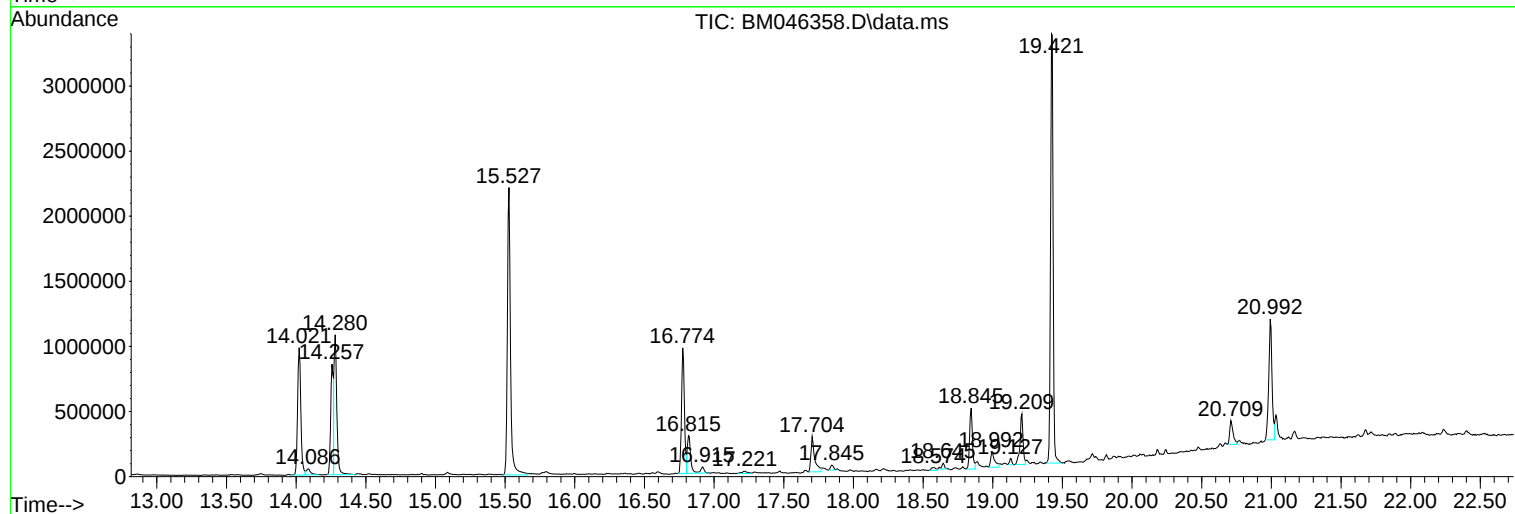
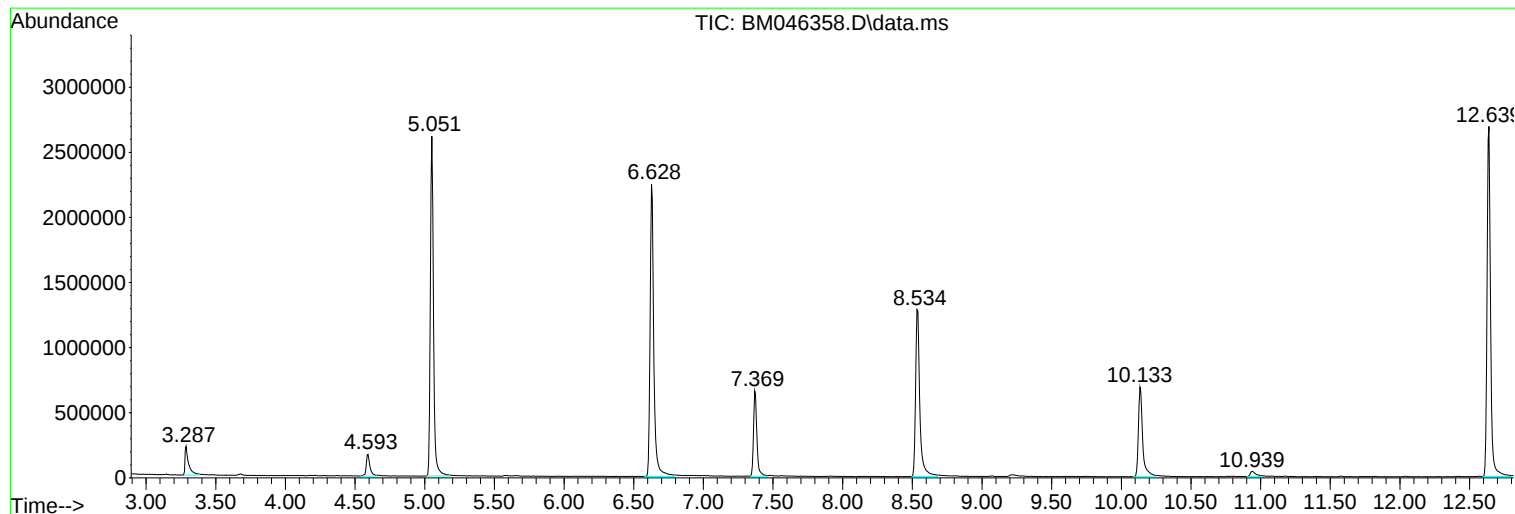
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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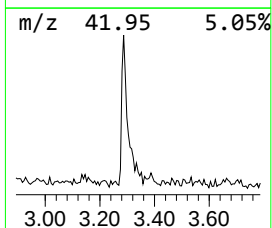
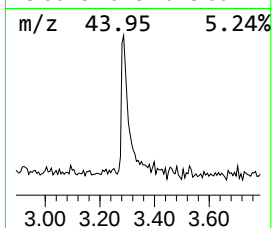
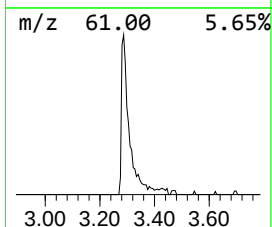
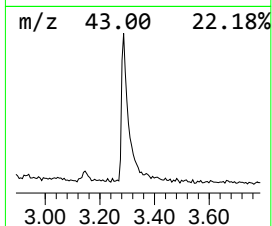
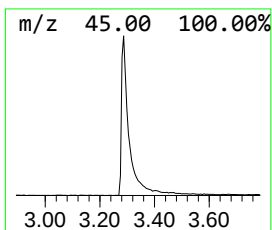
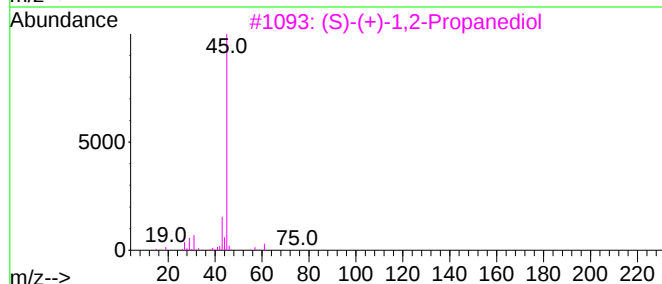
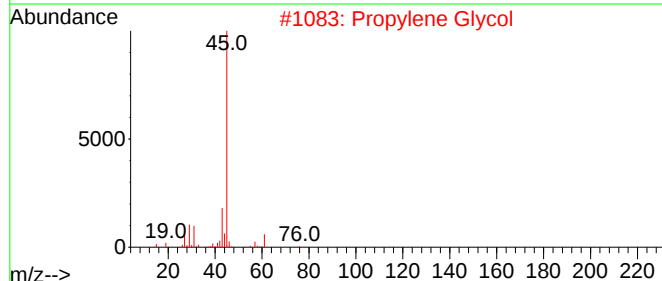
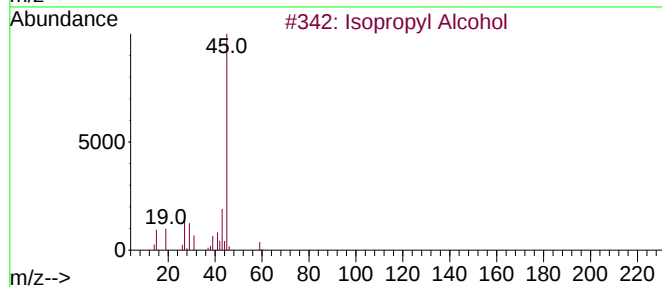
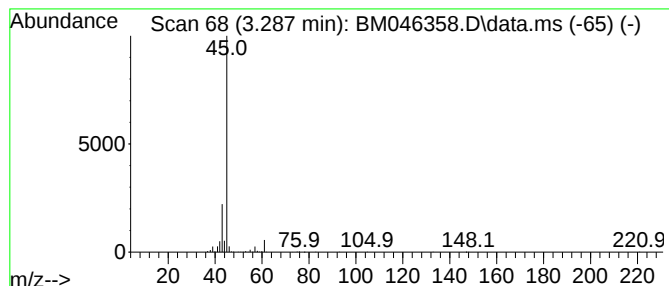
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.287	7.15 ng	393413	1,4-Dichlorobenzene-d4	7.369

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2		Propylene Glycol	76	C3H8O2	000057-55-6	37
3		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5		Acetic acid, cyano-, 2-methoxyet...	143	C6H9NO3	010258-54-5	9



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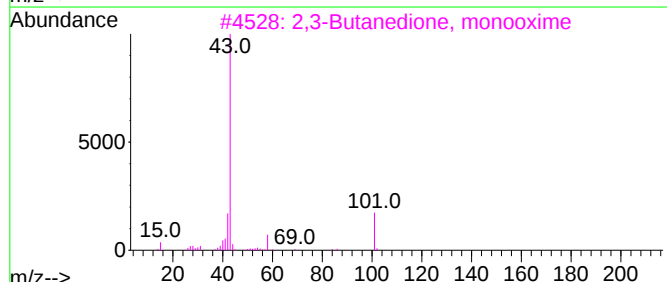
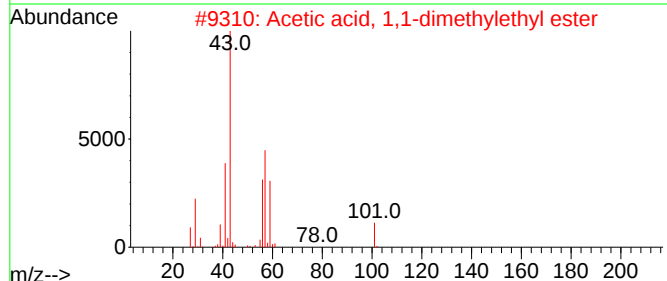
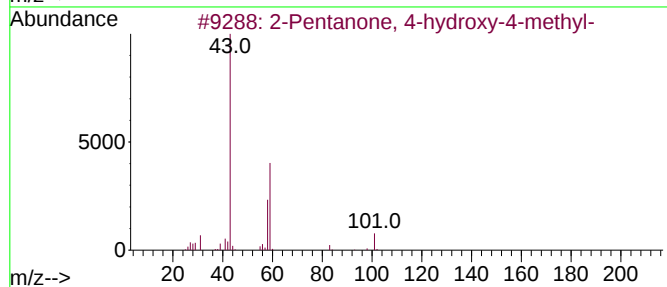
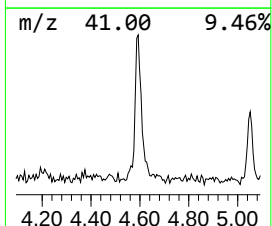
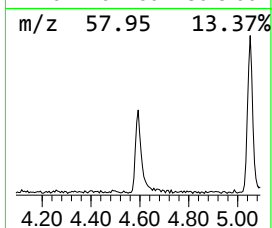
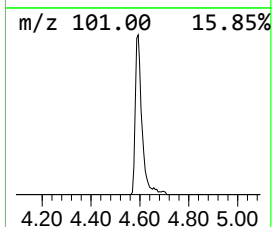
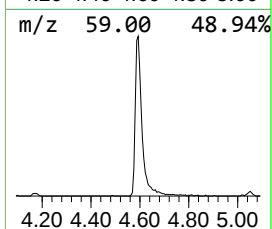
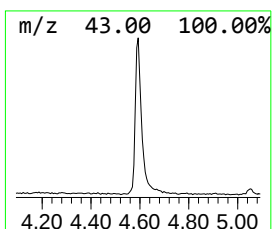
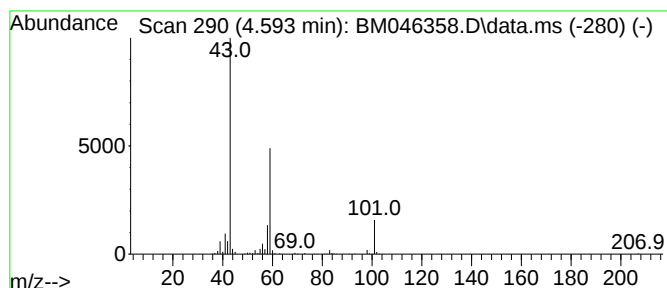
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.593	5.78 ng	318053	1,4-Dichlorobenzene-d4	7.369	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9



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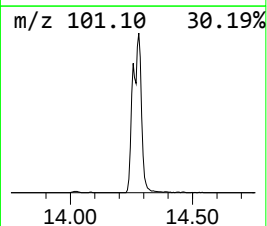
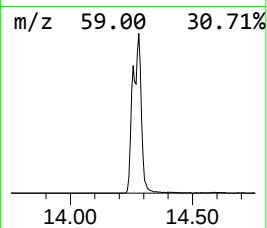
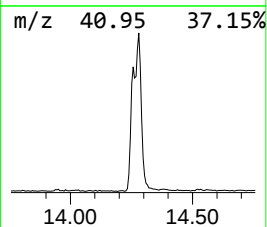
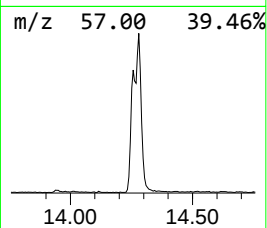
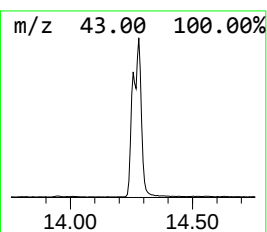
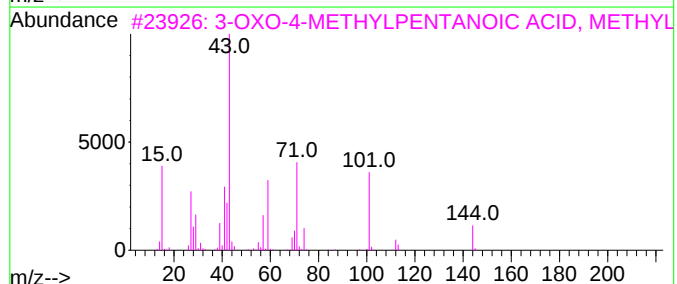
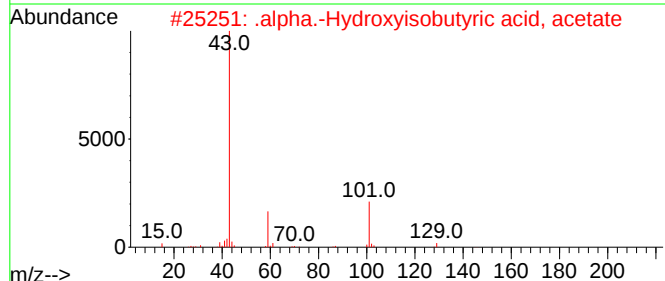
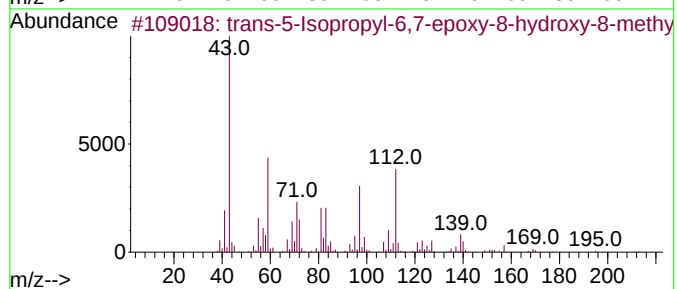
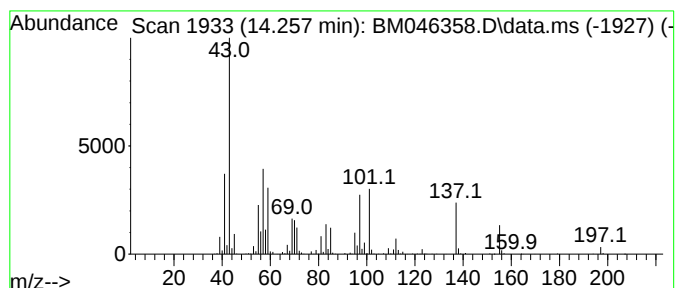
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown14.257 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	15.99 ng	1235800	Acenaphthene-d10	14.021
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		trans-5-Isopropyl-6,7-epoxy-8-hy...	228 C13H24O3	058002-07-6 25
2		.alpha.-Hydroxyisobutyric acid, ...	146 C6H10O4	1000374-31-3 14
3		3-OXO-4-METHYLPENTANOIC ACID, ME...	144 C7H12O3	042558-54-3 12
4		2-Pentanol, 2-methyl-, acetate	144 C8H16O2	034859-98-8 10
5		Acetic acid, 1,1-dimethylethyl e...	116 C6H12O2	000540-88-5 10



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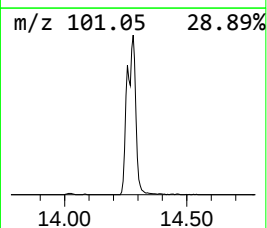
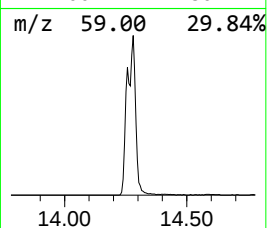
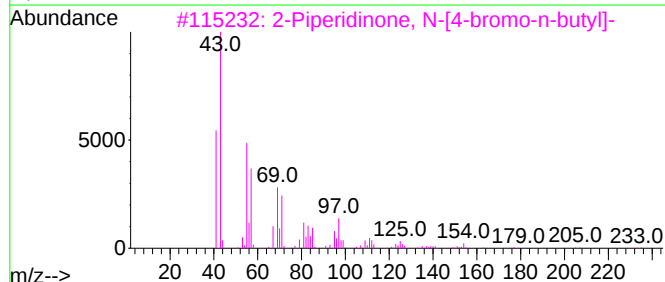
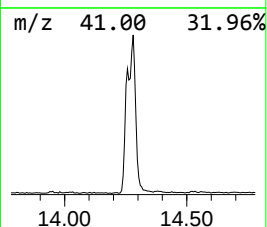
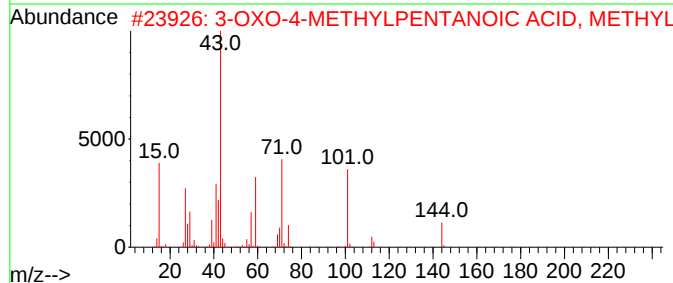
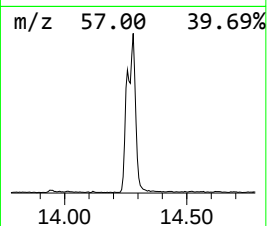
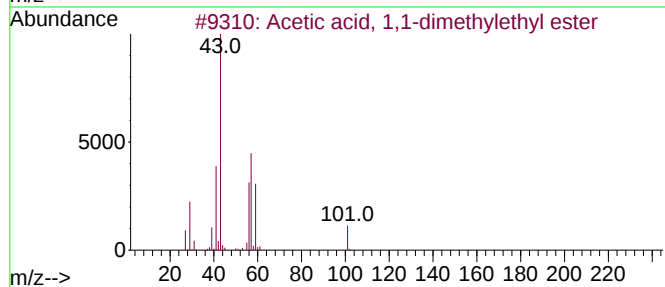
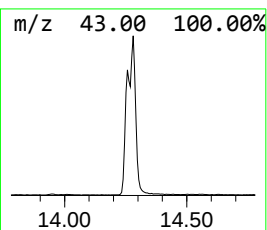
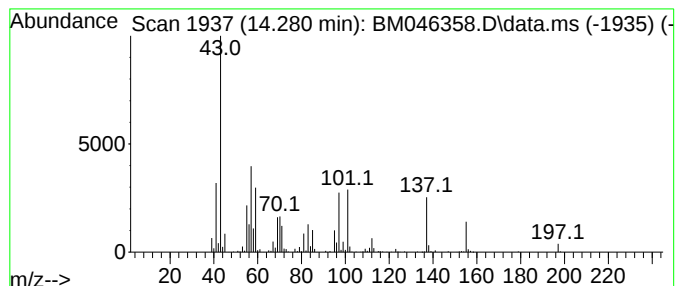
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Peak Number 4 unknown14.280 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.280	18.03 ng	1392950	Acenaphthene-d10	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
2			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	10
3			2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	9
4			1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	9
5			10-Nonadecanone	282	C19H38O	000504-57-4	9



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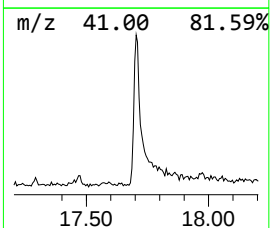
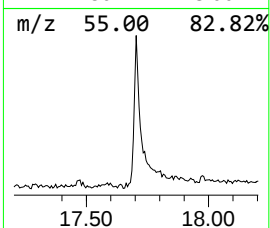
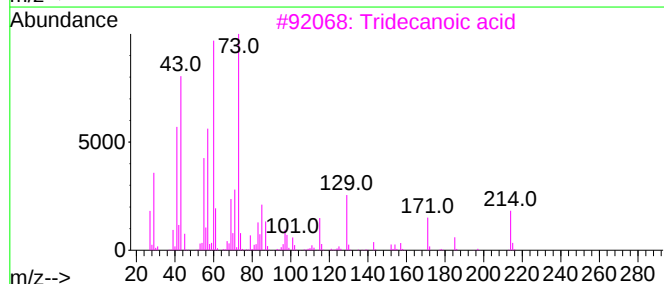
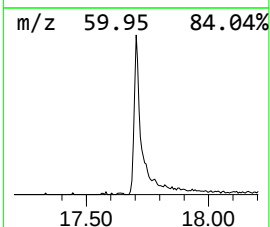
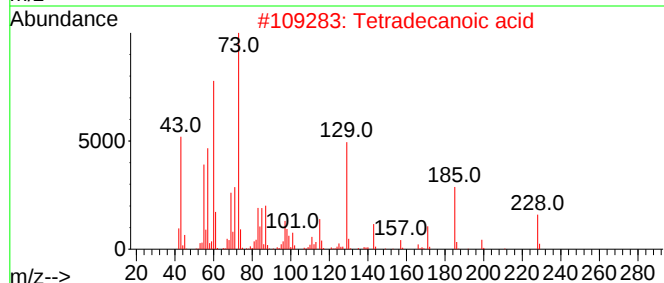
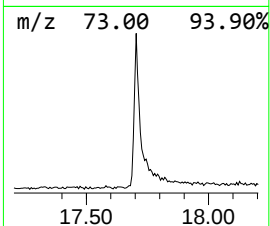
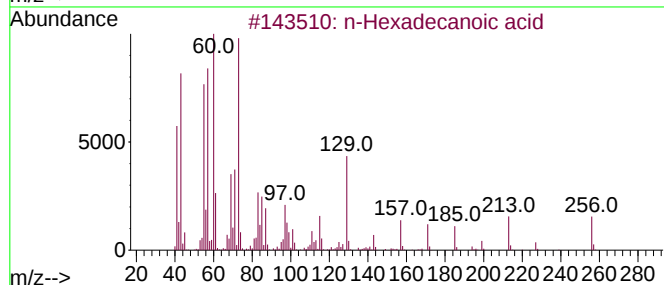
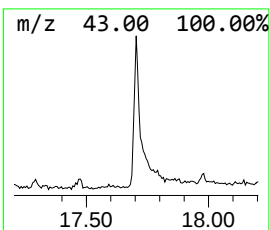
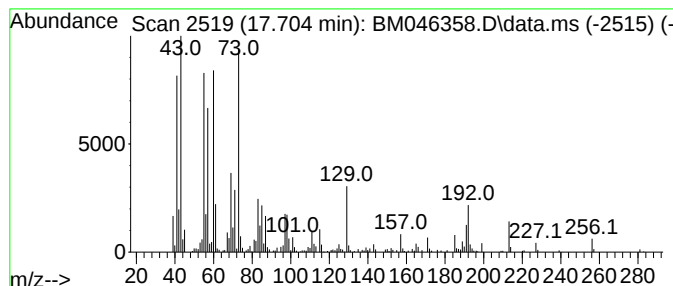
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.703	6.80 ng	493415	Phenanthrene-d10	16.774

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	89
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			d-Gluco-heptulosan	210	C7H14O7	1000126-85-2	46



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7-E-1

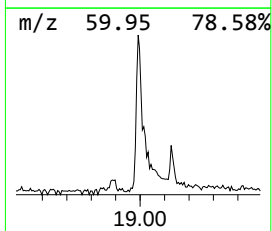
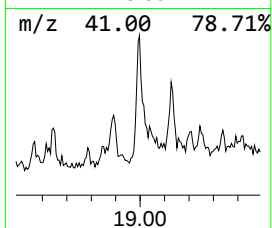
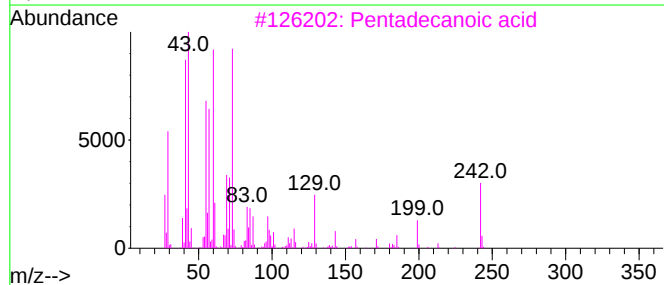
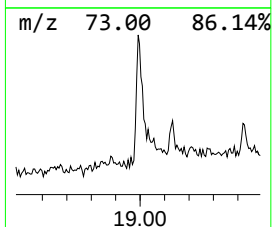
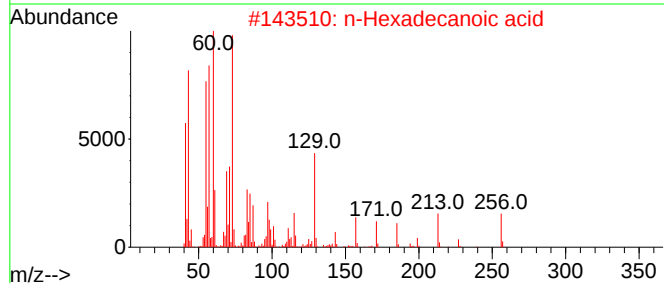
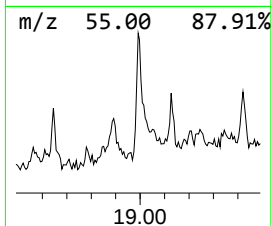
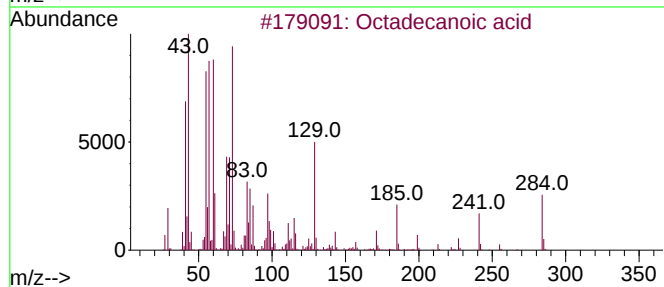
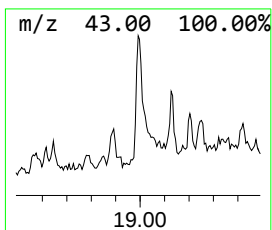
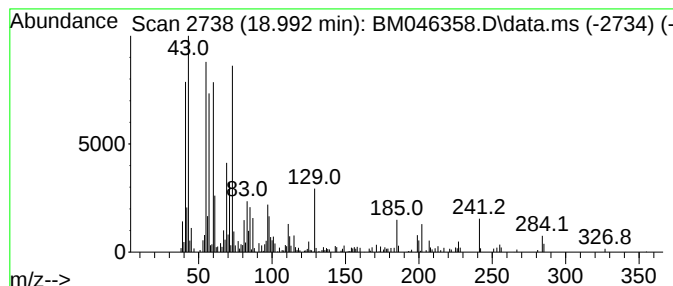
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.992	3.22 ng	242245	Chrysene-d12	20.992

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5		Tridecanoic acid	214	C13H26O2	000638-53-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046358.D
Acq On : 28 Jun 2024 18:43
Operator : MA/JU
Sample : P3076-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

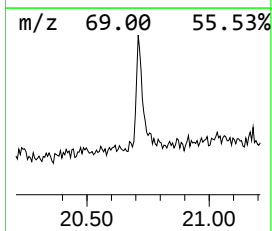
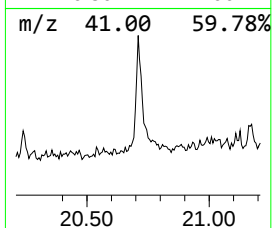
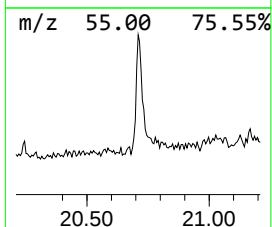
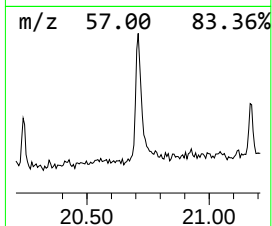
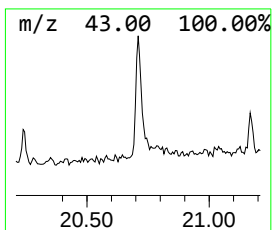
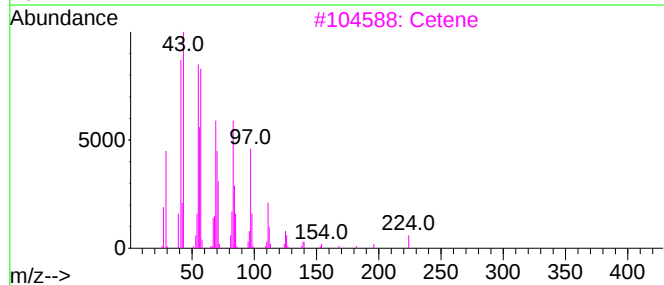
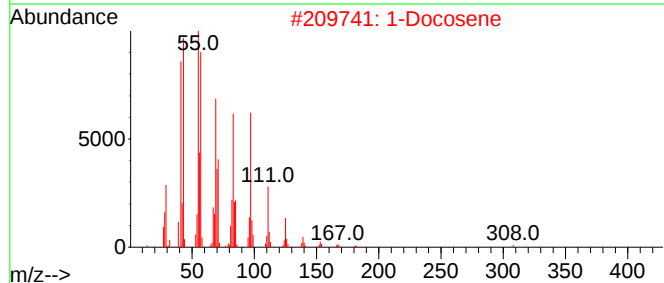
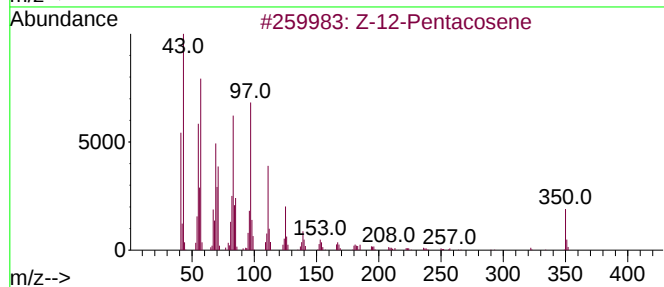
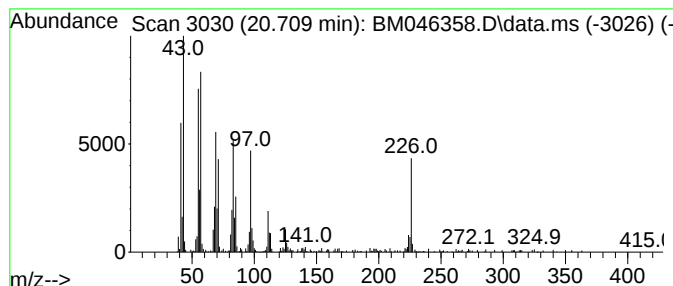
Instrument :
BNA_M
ClientSampleId :
7-E-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Z-12-Pentacosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.709	4.11 ng	309323	Chrysene-d12	20.992	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-12-Pentacosene	350	C25H50	1000131-09-4	92
2	1-Docosene	308	C22H44	001599-67-3	83
3	Cetene	224	C16H32	000629-73-2	83
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	74
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046358.D
Acq On : 28 Jun 2024 18:43
Operator : MA/JU
Sample : P3076-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
7-E-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	3.287	7.2	ng	393413	1	7.369	1100760	20.0
2-Pentanone, 4-...	4.593	5.8	ng	318053	1	7.369	1100760	20.0
unknown14.257	14.257	16.0	ng	1235800	3	14.021	1545470	20.0
unknown14.280	14.280	18.0	ng	1392950	3	14.021	1545470	20.0
n-Hexadecanoic ...	17.703	6.8	ng	493415	4	16.774	1451780	20.0
Octadecanoic acid	18.992	3.2	ng	242245	5	20.992	1505880	20.0
Z-12-Pentacosene	20.709	4.1	ng	309323	5	20.992	1505880	20.0