

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
 Data File : BG055073.D
 Acq On : 4 Oct 2022 21:42
 Operator : CG/JU
 Sample : N4936-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SASP2-T-2-(16-22)

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-BG100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055073.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.379	10	15	33	rVB	283181	461038	28.50%	4.549%
2	4.772	247	252	260	rVB	36840	56930	3.52%	0.562%
3	5.394	350	358	369	rVB	527322	831277	51.40%	8.202%
4	5.864	431	438	447	rBV	430447	696548	43.07%	6.873%
5	6.493	539	545	551	rVB	36173	55203	3.41%	0.545%
6	7.468	703	711	720	rBV	465441	797937	49.33%	7.873%
7	8.344	853	860	872	rBV	118077	200532	12.40%	1.979%
8	9.513	1051	1059	1067	rBV	272528	477992	29.55%	4.716%
9	10.917	1290	1298	1307	rBV	16628	26255	1.62%	0.259%
10	11.176	1333	1342	1350	rBV	164529	299805	18.54%	2.958%
11	13.579	1744	1751	1758	rVB	795263	1176607	72.75%	11.610%
12	14.948	1977	1984	1991	rVB	286534	430159	26.60%	4.244%
13	16.423	2228	2235	2244	rBV	609501	896624	55.44%	8.847%
14	17.680	2443	2449	2454	rBV	326314	503921	31.16%	4.972%
15	17.721	2454	2456	2462	rVB	56767	73380	4.54%	0.724%
16	17.798	2464	2469	2470	rBV2	12014	18110	1.12%	0.179%
17	18.532	2588	2594	2601	rBV4	30687	51060	3.16%	0.504%
18	19.472	2751	2754	2759	rVB2	31486	34167	2.11%	0.337%
19	19.707	2790	2794	2799	rVB	63237	87083	5.38%	0.859%
20	20.071	2851	2856	2861	rVB	50529	76613	4.74%	0.756%
21	20.259	2882	2888	2894	rBV	1232227	1617426	100.00%	15.960%
22	21.575	3109	3112	3118	rBV3	20723	31042	1.92%	0.306%
23	21.975	3171	3180	3186	rBV	313298	594340	36.75%	5.864%
24	24.325	3573	3580	3584	rBV3	12629	32825	2.03%	0.324%
25	25.107	3711	3713	3725	rVB4	9018	20777	1.28%	0.205%
26	25.259	3735	3739	3747	rVB	11986	25125	1.55%	0.248%
27	25.442	3758	3770	3788	rBV	186420	561764	34.73%	5.543%

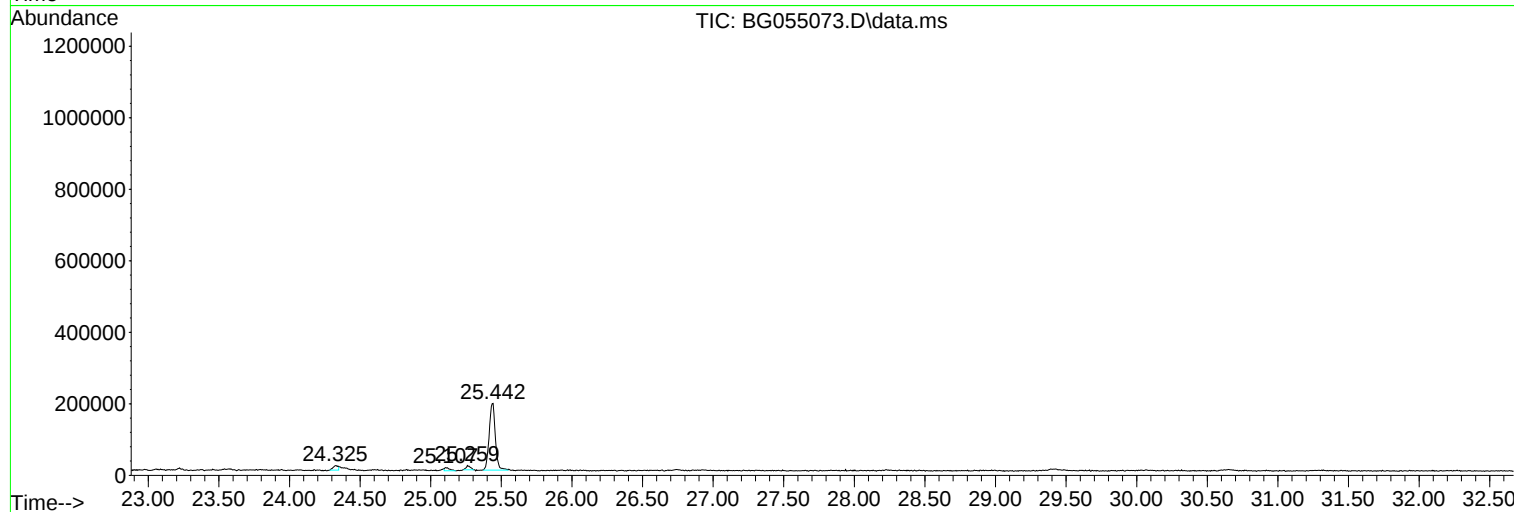
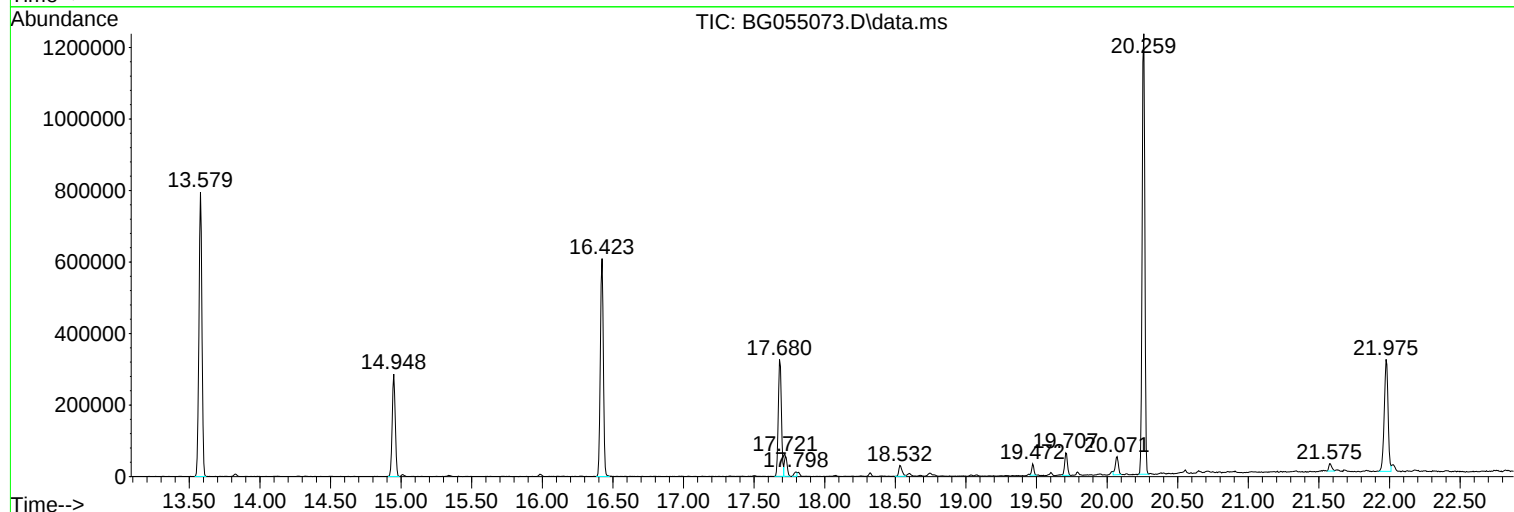
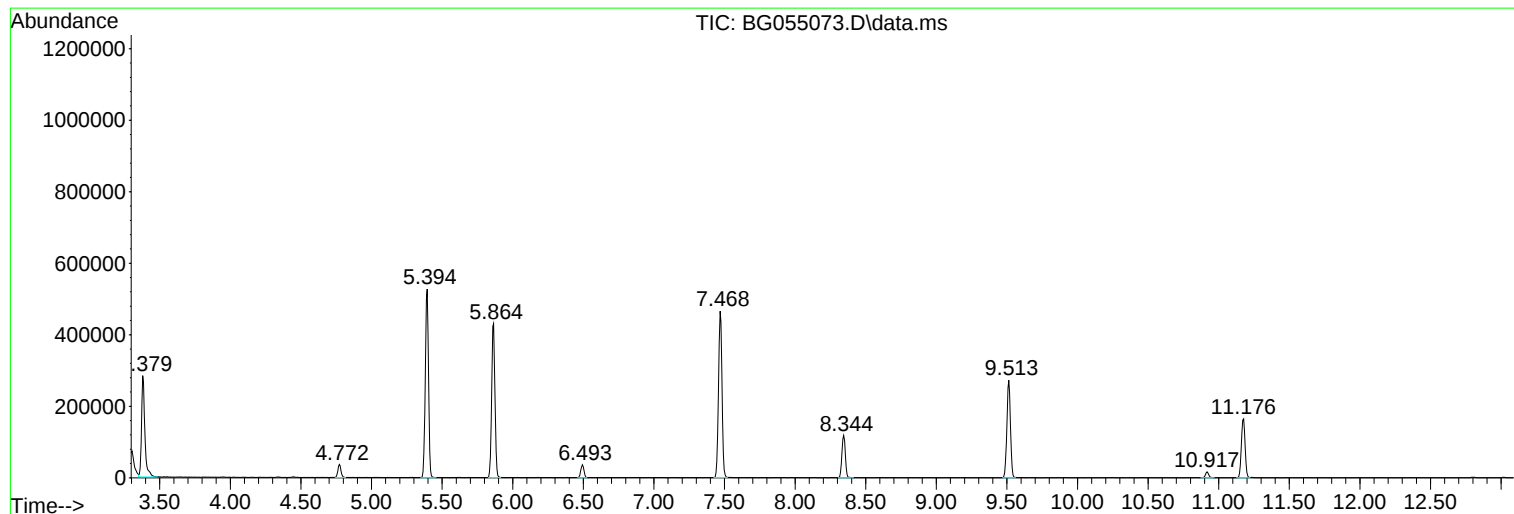
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Instrument :
BNA_G
ClientSampleId :
SASP2-T-2-(16-22)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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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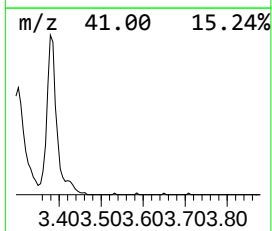
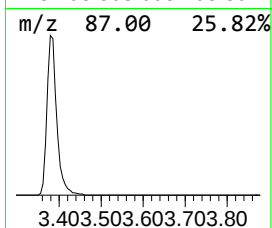
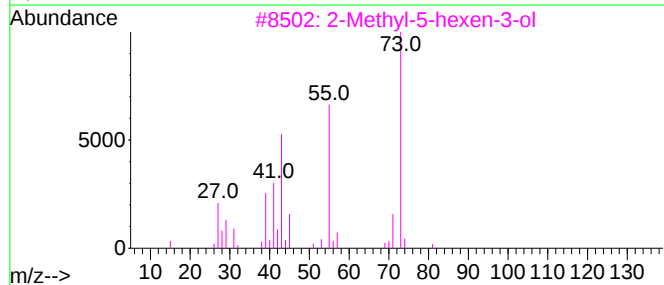
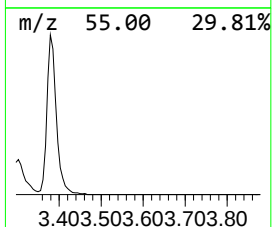
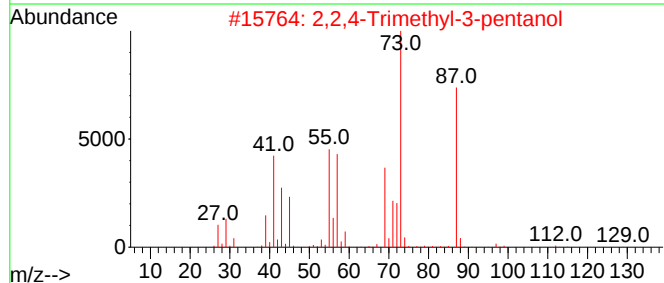
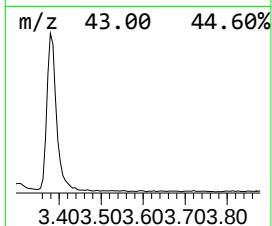
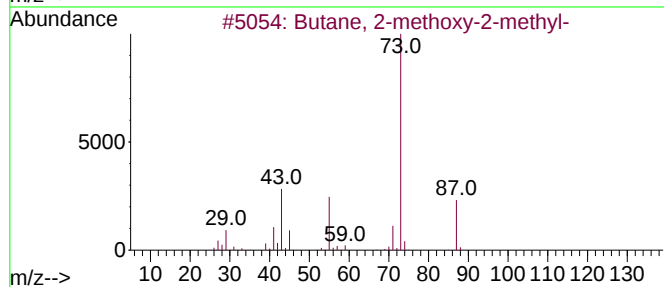
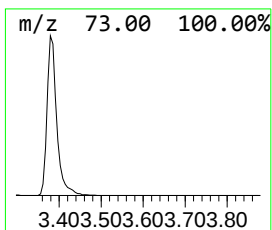
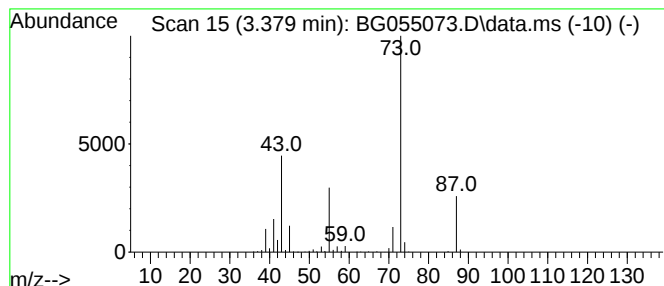
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.379	45.98 ng	461038	1,4-Dichlorobenzene-d4	8.344

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			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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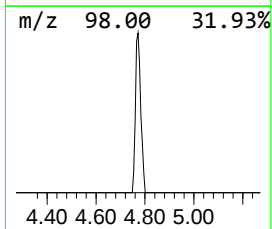
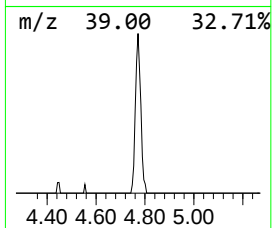
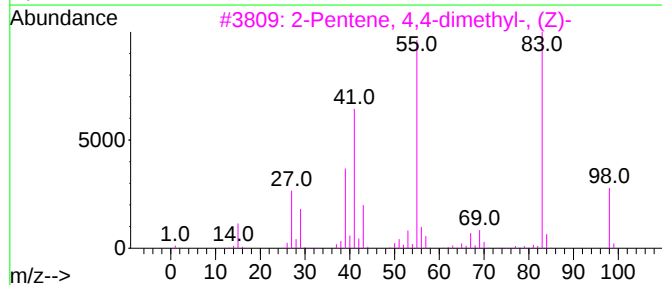
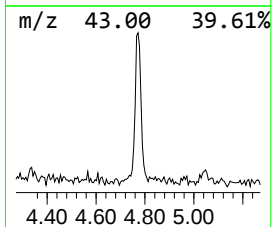
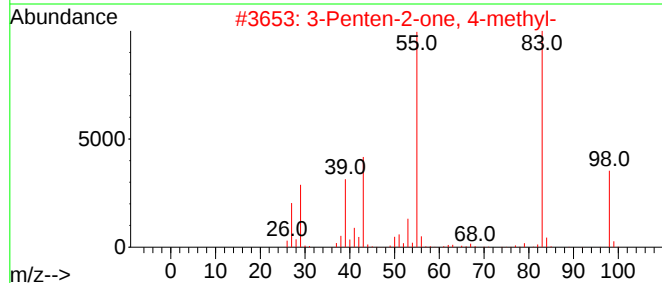
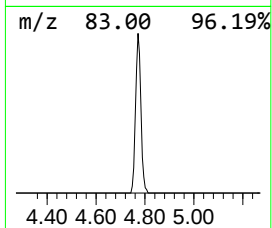
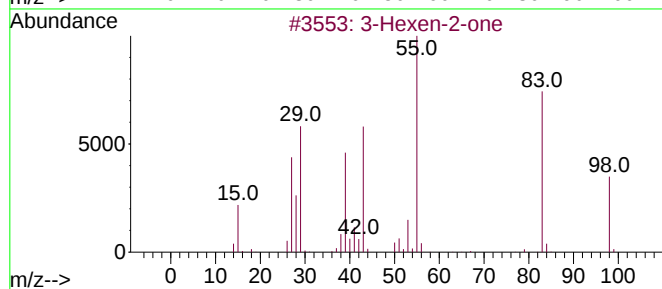
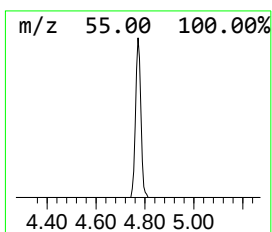
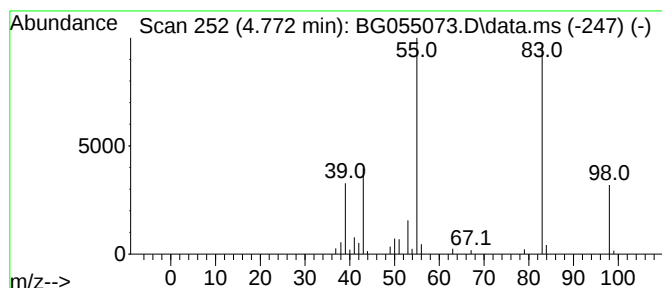
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.772	5.68 ng	56930	1,4-Dichlorobenzene-d4	8.344

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72
4			2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	72
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72



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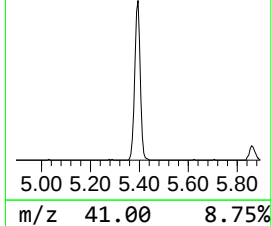
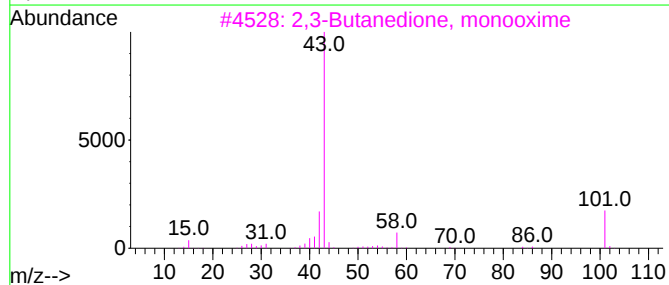
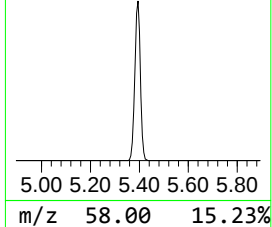
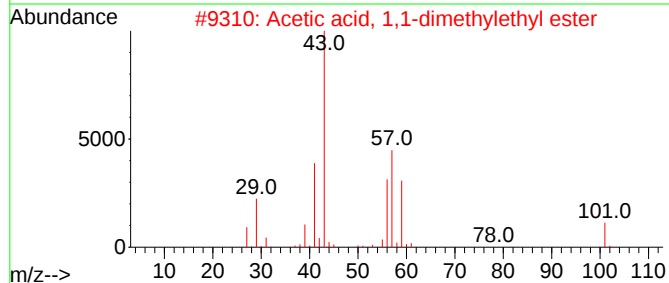
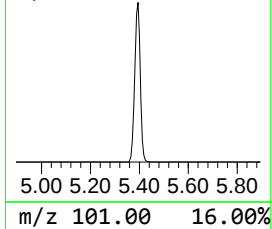
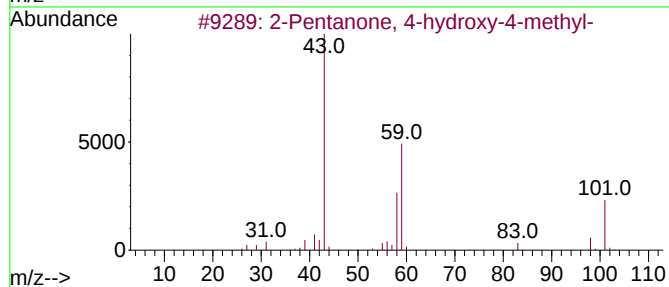
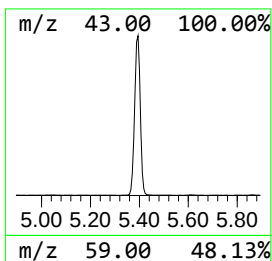
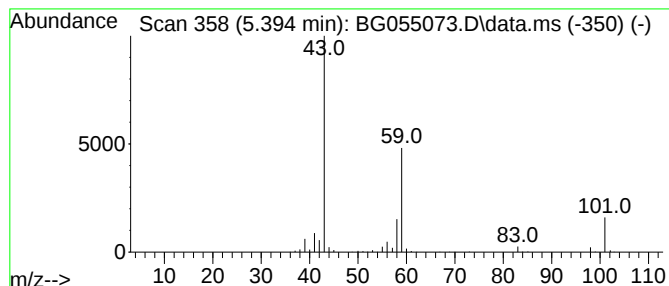
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.394	82.91 ng	831277	1,4-Dichlorobenzene-d4	8.344

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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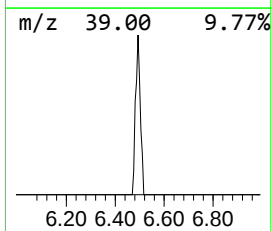
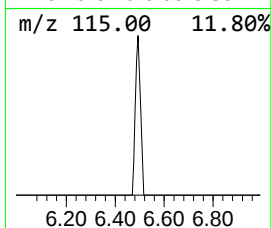
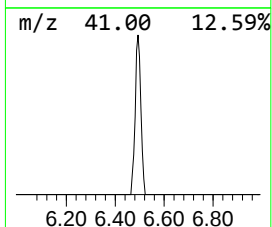
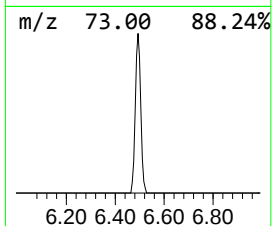
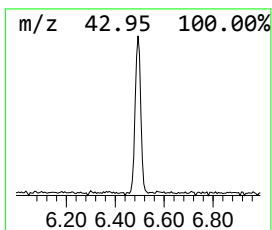
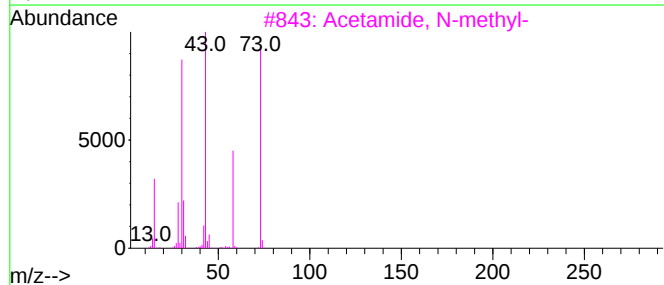
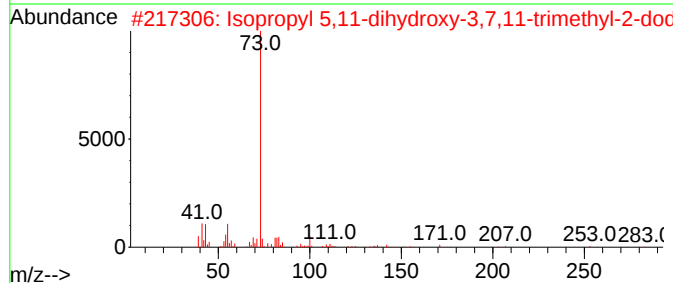
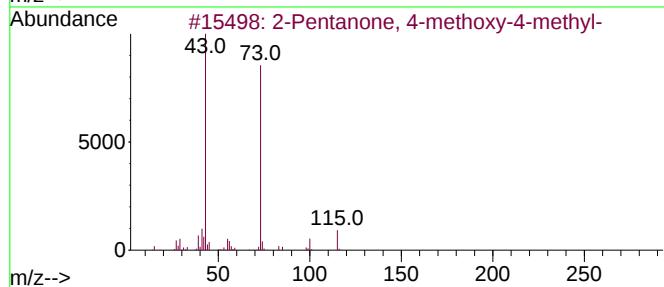
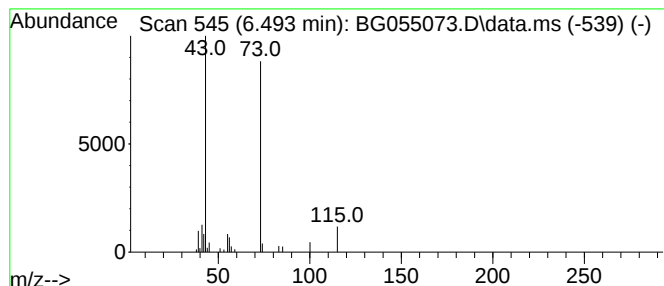
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.493	5.51 ng	55203	1,4-Dichlorobenzene-d4	8.344

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Isopropyl 5,11-dihydroxy-3,7,11-...	314	C18H34O4	1000223-34-1	12
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Diacetyl(methoxyimino)methane	143	C6H9NO3	069740-33-6	9



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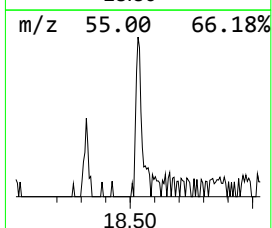
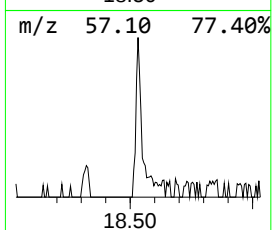
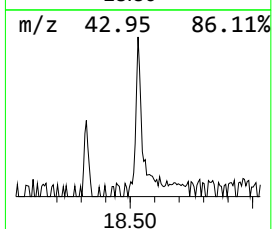
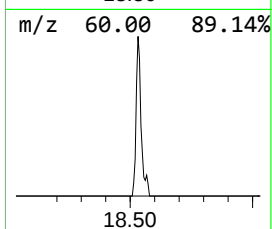
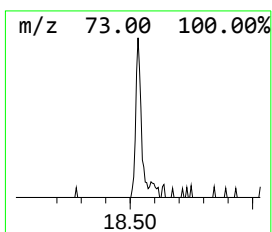
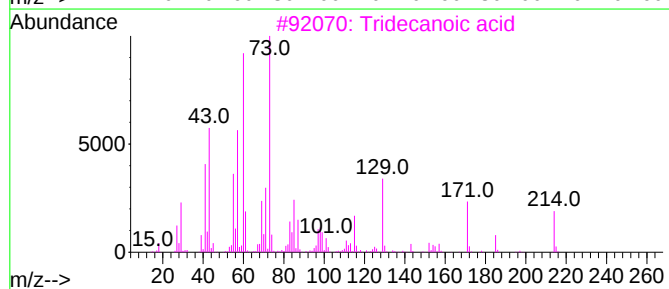
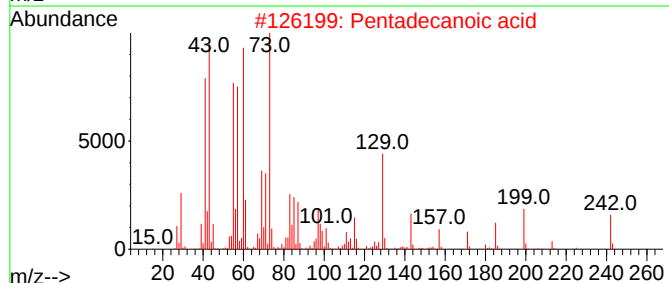
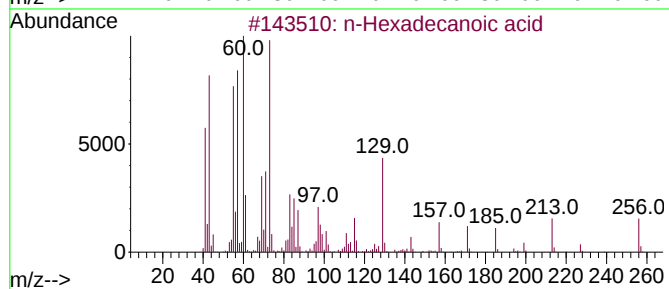
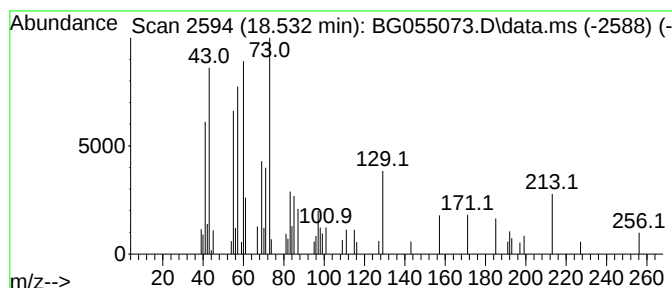
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.532	2.03 ng	51060	Phenanthrene-d10	17.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	22



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.379	46.0	ng	461038	1	8.344	200532	20.0
3-Hexen-2-one	4.772	5.7	ng	56930	1	8.344	200532	20.0
2-Pentanone, 4-...	5.394	82.9	ng	831277	1	8.344	200532	20.0
2-Pentanone, 4-...	6.493	5.5	ng	55203	1	8.344	200532	20.0
n-Hexadecanoic ...	18.532	2.0	ng	51060	4	17.680	503921	20.0