

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102922\
 Data File : BG055371.D
 Acq On : 29 Oct 2022 18:50
 Operator : CG/JU
 Sample : N5313-15
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMPOSITE-SE-QUARTER

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-BG102422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055371.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.323	4	6	15	rVB2	15438	21982	1.31%	0.231%
2	5.303	337	343	351	rVB	67486	101342	6.04%	1.065%
3	5.785	418	425	438	rBV	444236	733906	43.75%	7.713%
4	6.924	612	619	625	rVB	36351	57310	3.42%	0.602%
5	7.406	693	701	722	rBV	443099	781801	46.60%	8.216%
6	8.258	838	846	854	rBV	107564	183427	10.93%	1.928%
7	9.433	1038	1046	1055	rBV	265296	470379	28.04%	4.943%
8	10.832	1277	1284	1296	rBV	25824	56816	3.39%	0.597%
9	11.090	1321	1328	1335	rBV	155404	275876	16.44%	2.899%
10	13.499	1731	1738	1746	rBV	757624	1162759	69.31%	12.220%
11	14.874	1965	1972	1979	rBV	267745	406823	24.25%	4.275%
12	16.355	2217	2224	2241	rBV	573392	920764	54.89%	9.676%
13	17.606	2430	2437	2442	rBV	344672	509390	30.36%	5.353%
14	17.647	2442	2444	2449	rVB	30482	38028	2.27%	0.400%
15	18.464	2578	2583	2590	rBV3	46569	99129	5.91%	1.042%
16	18.523	2591	2593	2600	rVB4	13334	21588	1.29%	0.227%
17	18.669	2612	2618	2623	rBV2	9527	21758	1.30%	0.229%
18	19.639	2777	2783	2790	rVB	82229	121212	7.23%	1.274%
19	19.715	2792	2796	2805	rBV6	24900	51351	3.06%	0.540%
20	19.962	2834	2838	2840	rBV2	14170	21127	1.26%	0.222%
21	19.997	2840	2844	2850	rVB	77541	112543	6.71%	1.183%
22	20.179	2869	2875	2881	rBV	1326306	1677612	100.00%	17.630%
23	20.320	2893	2899	2904	rVB5	11224	20693	1.23%	0.217%
24	20.779	2973	2977	2981	rBV4	13744	21719	1.29%	0.228%
25	21.490	3094	3098	3105	rBV5	28699	66638	3.97%	0.700%
26	21.877	3156	3164	3170	rBV2	328982	641627	38.25%	6.743%
27	21.924	3170	3172	3179	rVB	34641	52988	3.16%	0.557%
28	23.587	3453	3455	3464	rVB5	19368	37337	2.23%	0.392%
29	24.187	3551	3557	3559	rBV	28250	56816	3.39%	0.597%
30	25.109	3709	3714	3722	rVB	27309	66645	3.97%	0.700%
31	25.273	3729	3742	3751	rBV2	191130	601939	35.88%	6.326%
32	26.419	3929	3937	3947	rBV2	33212	102213	6.09%	1.074%

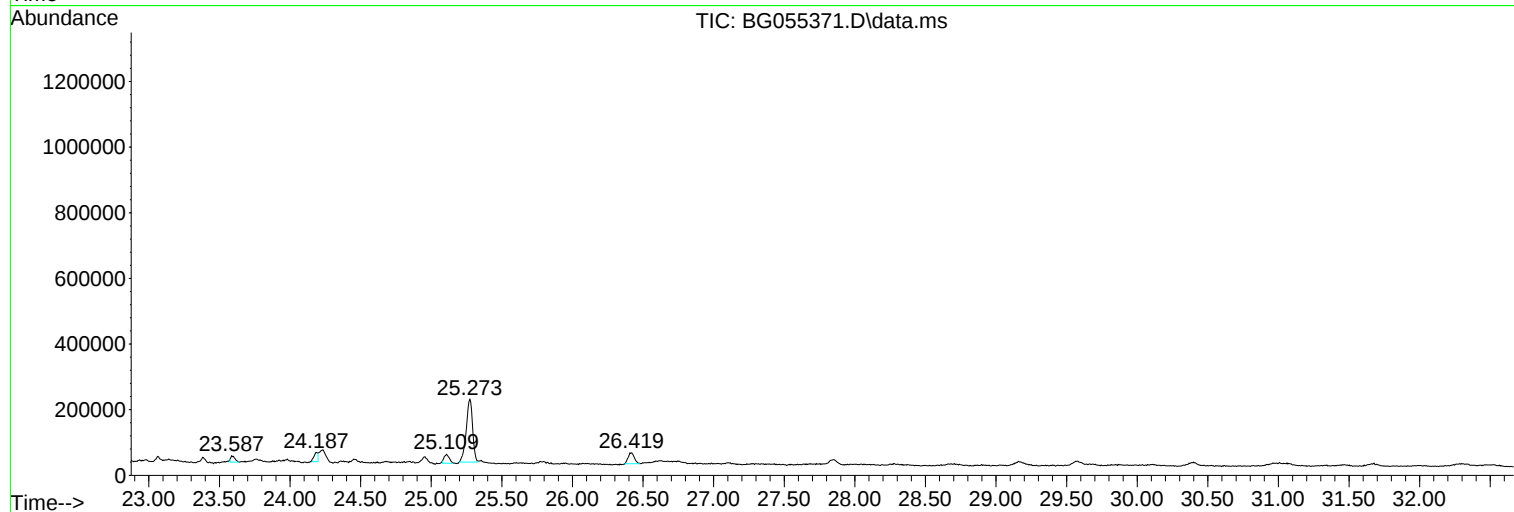
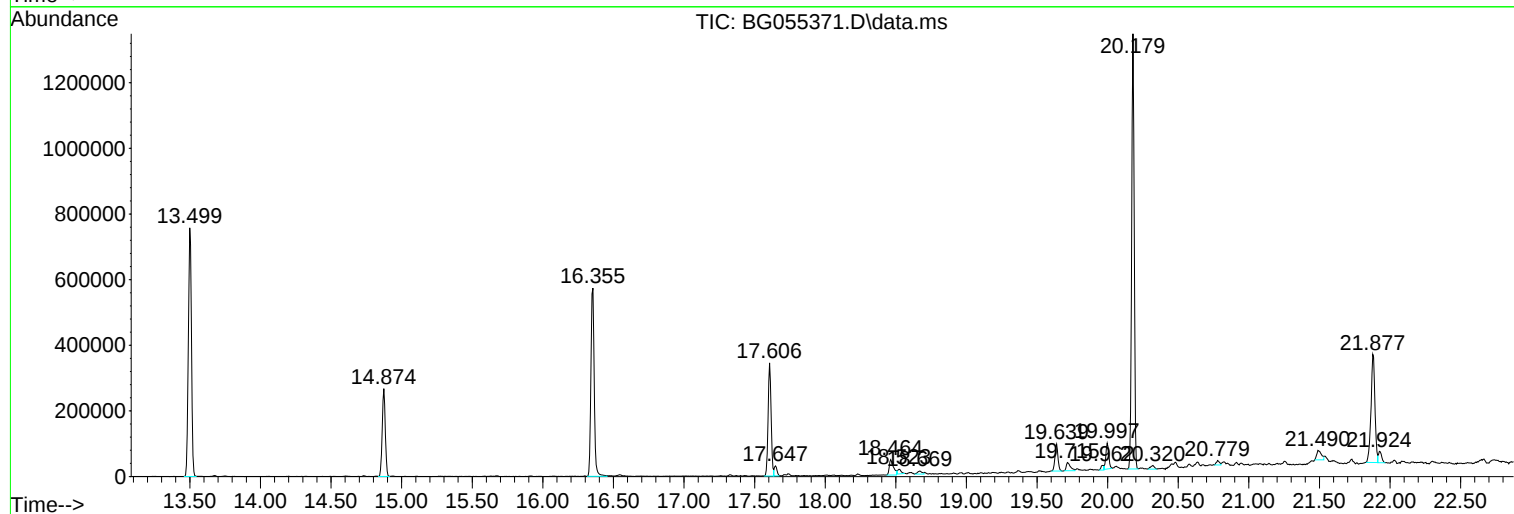
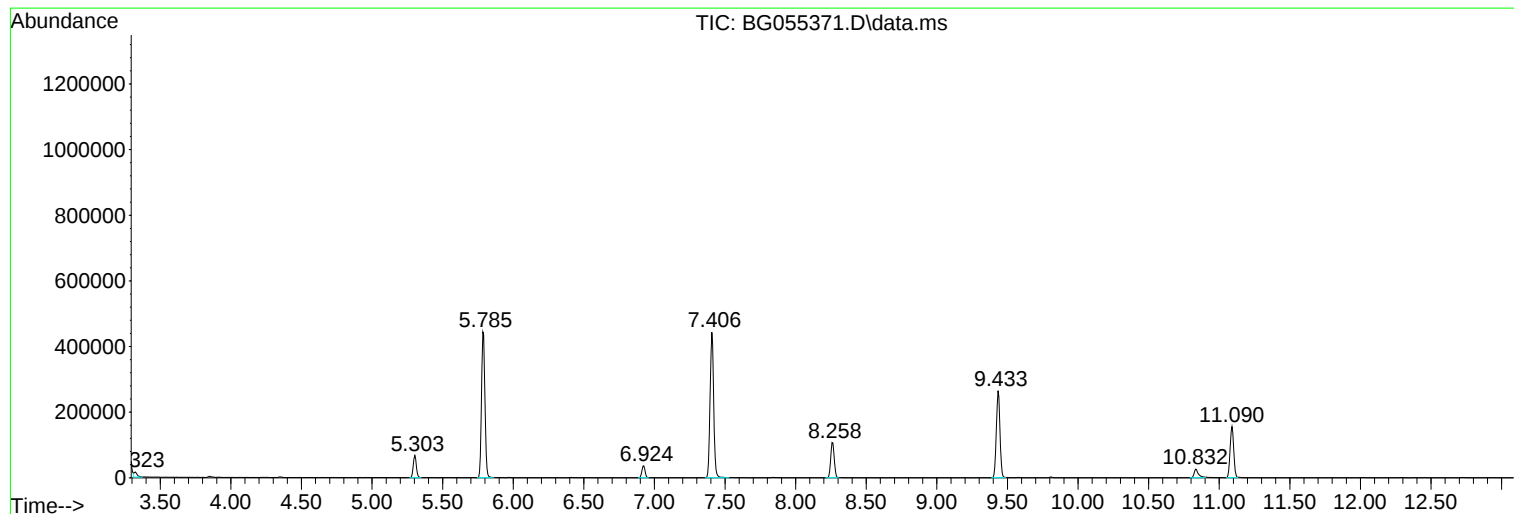
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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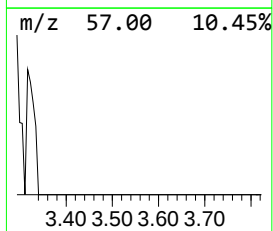
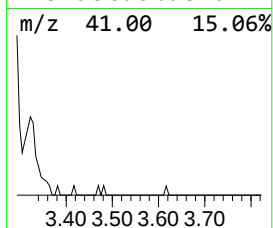
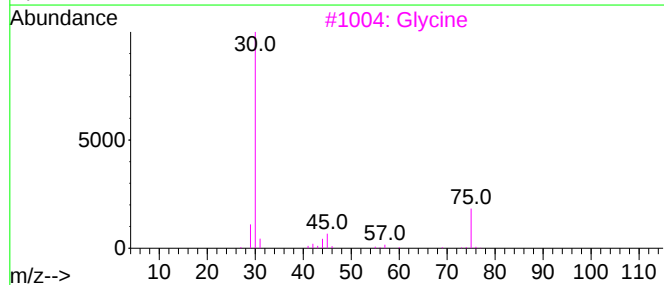
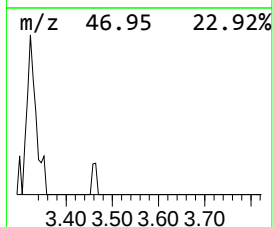
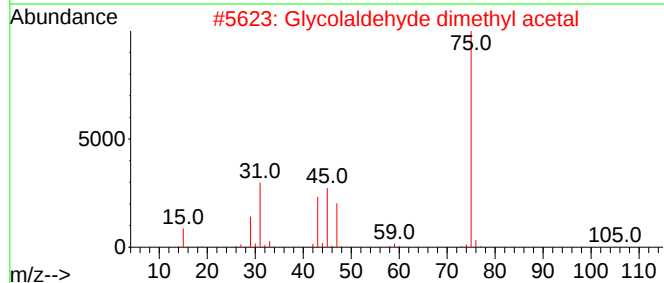
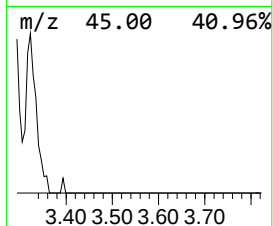
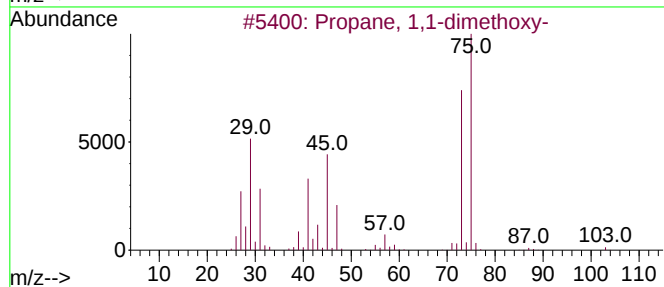
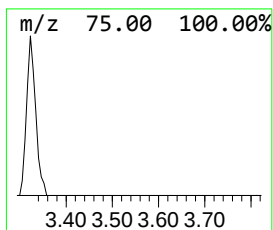
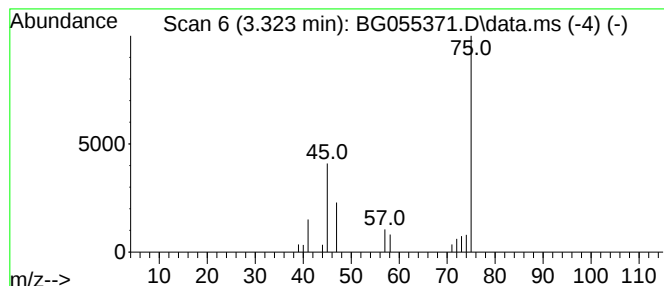
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.323	2.40 ng	21982	1,4-Dichlorobenzene-d4	8.258

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
3			Glycine	75	C2H5NO2	000056-40-6	4
4			Ethylamine	45	C2H7N	000075-04-7	3
5			Methane, nitroso-	45	CH3NO	000865-40-7	3



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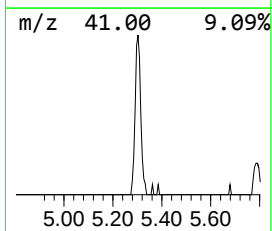
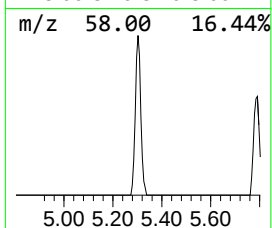
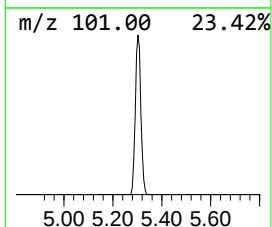
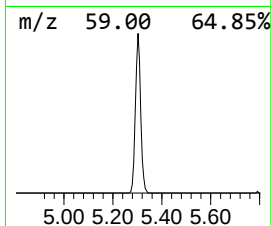
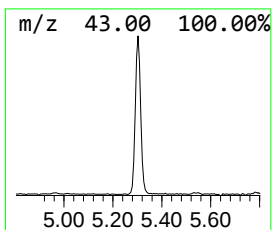
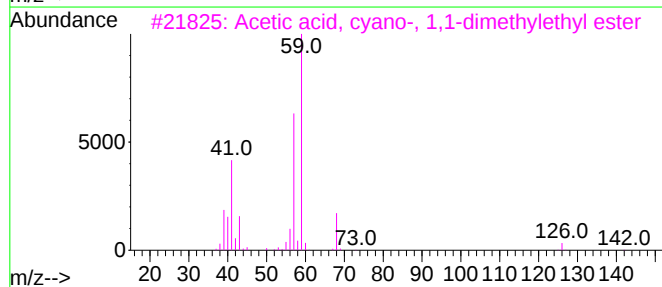
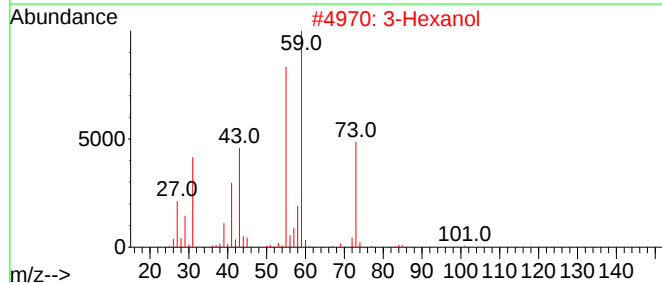
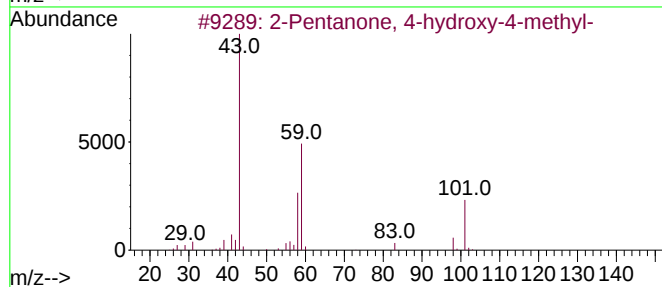
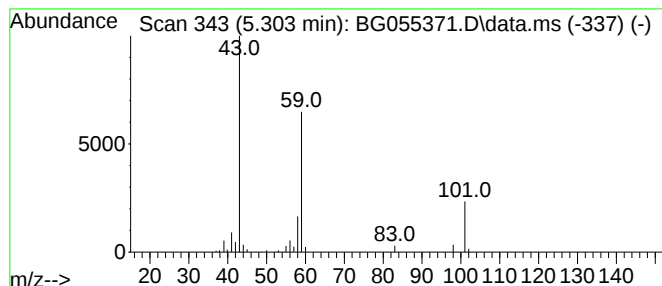
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.303	11.05 ng	101342	1,4-Dichlorobenzene-d4	8.258

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol	102	C6H14O	000623-37-0	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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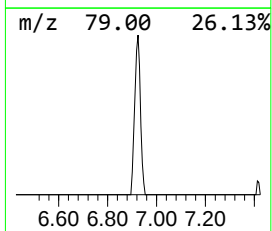
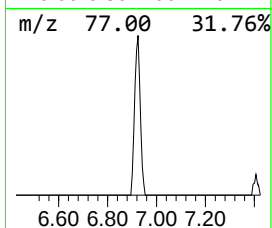
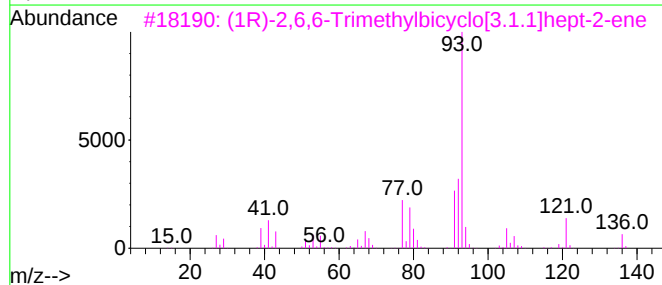
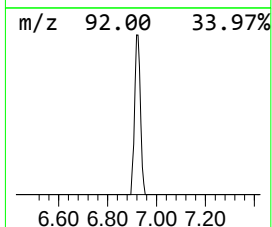
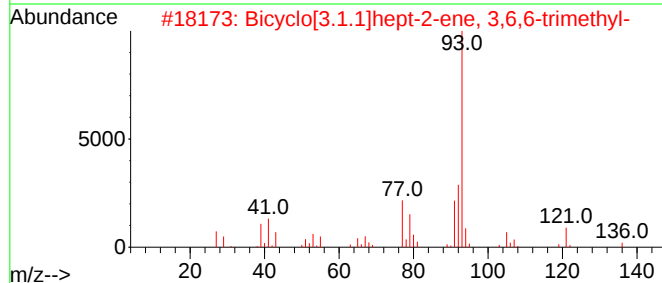
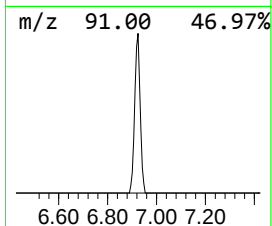
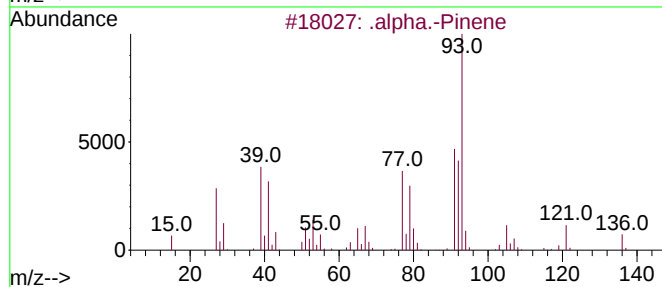
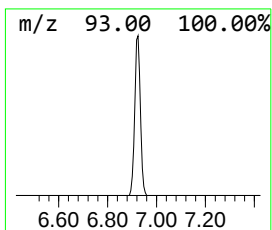
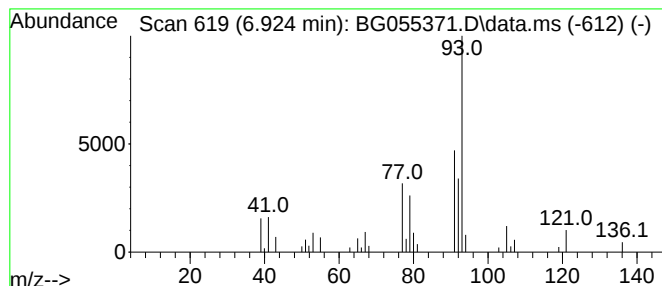
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 .alpha.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.924	6.25 ng	57310	1,4-Dichlorobenzene-d4	8.258

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.alpha.-Pinene	136	C10H16	000080-56-8	95
2		Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
3		(1R)-2,6,6-Trimethylbicyclo[3.1.1]...	136	C10H16	007785-70-8	91
4		Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	87
5		trans-.beta.-Ocimene	136	C10H16	003779-61-1	86



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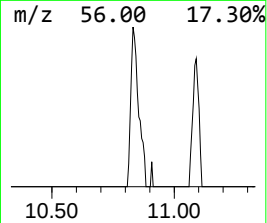
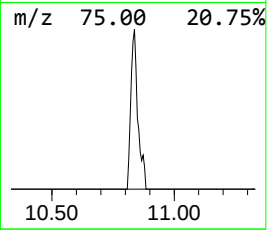
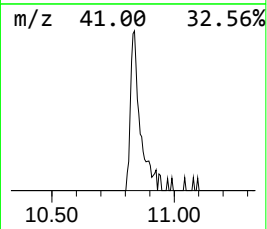
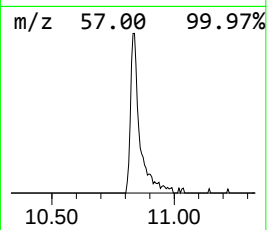
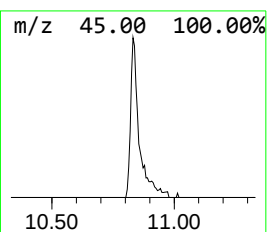
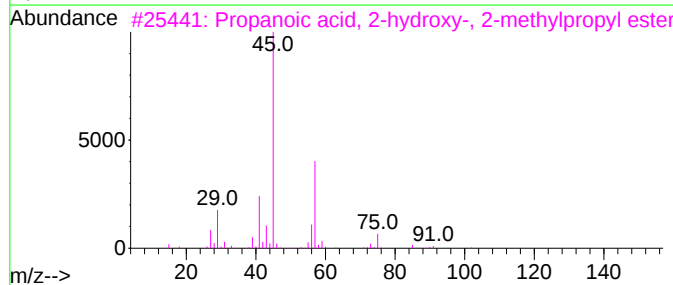
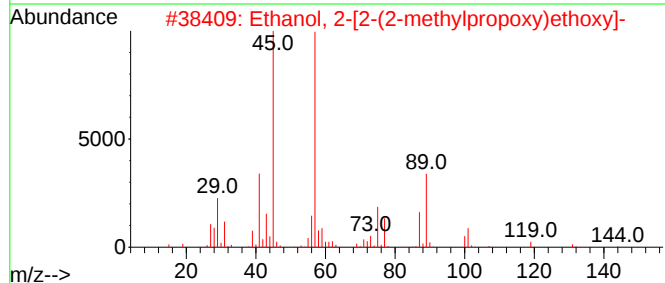
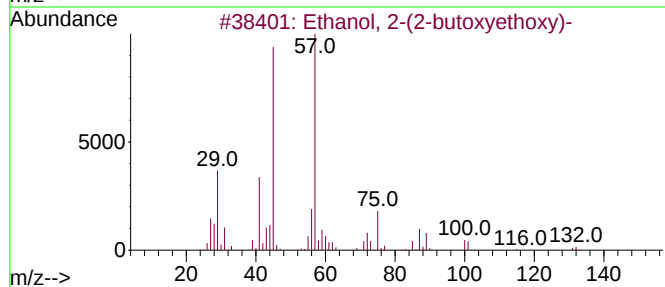
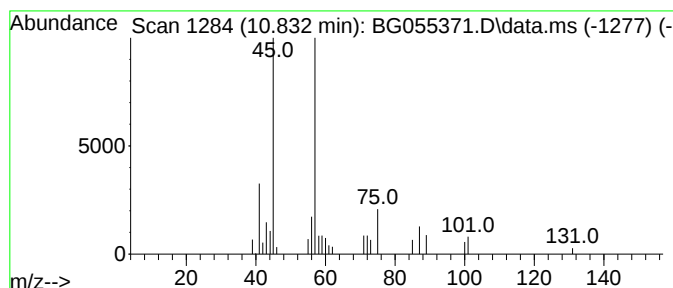
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.832	4.12 ng	56816	Naphthalene-d8	11.090	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
3	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	64
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50



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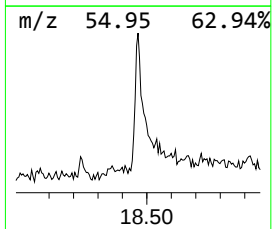
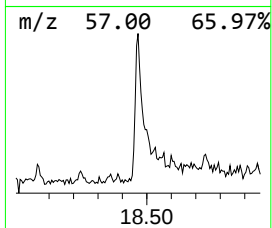
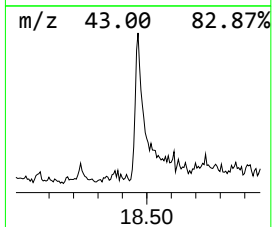
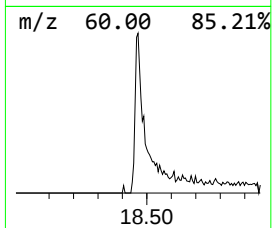
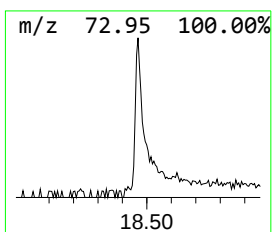
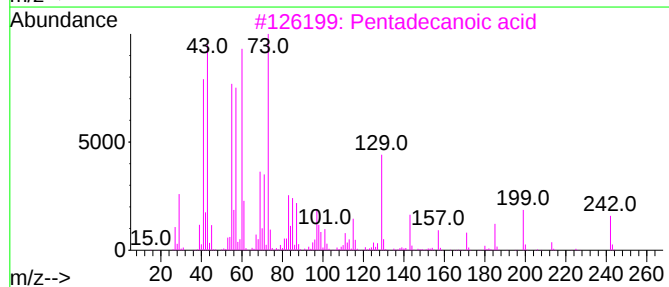
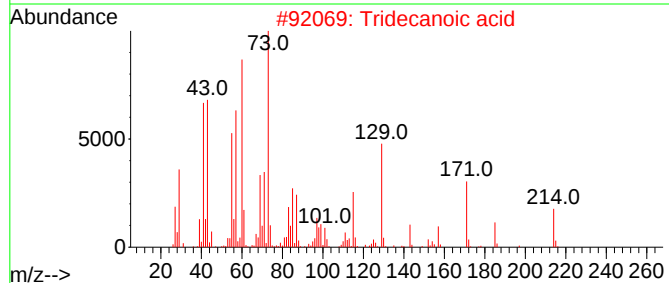
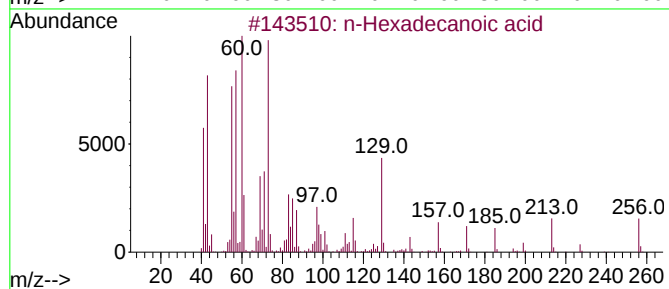
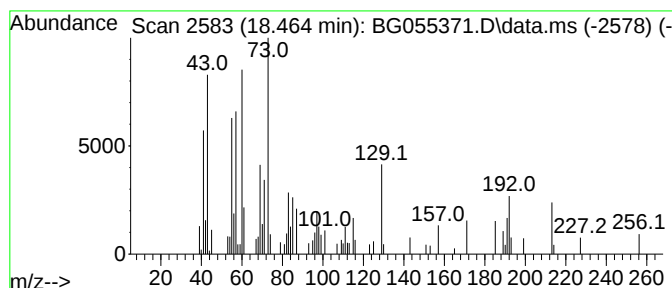
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.464	3.89 ng	99129	Phenanthrene-d10	17.606

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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ClientSampleId :
COMPOSITE-SE-QUARTER

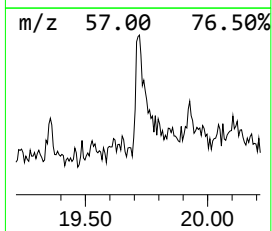
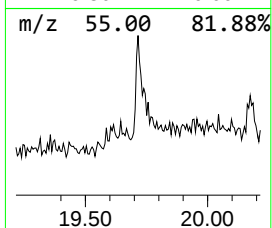
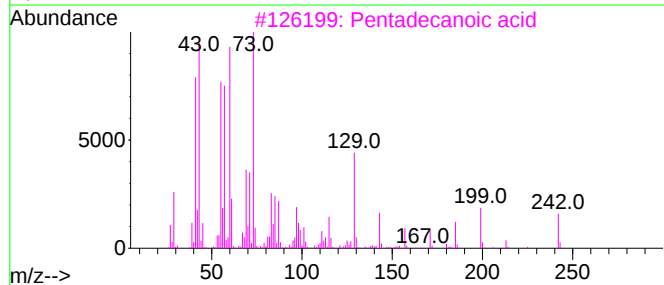
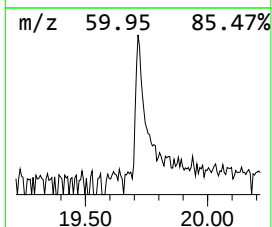
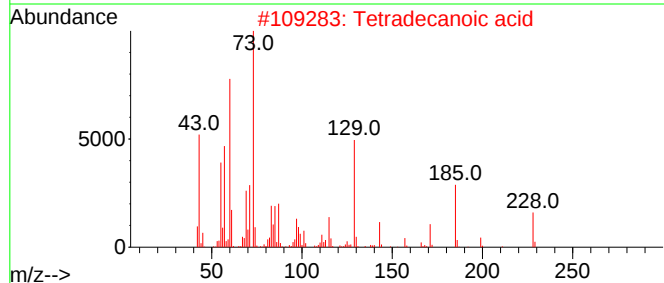
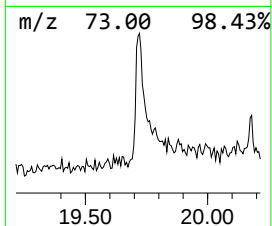
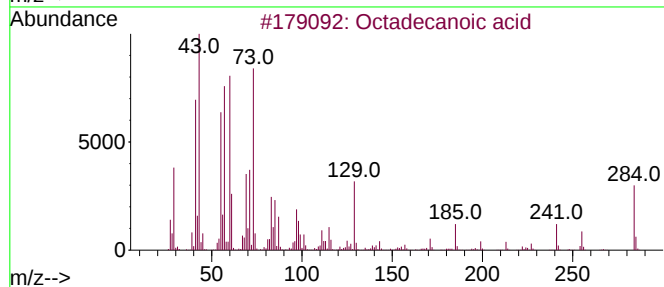
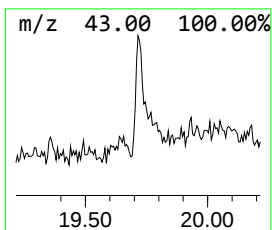
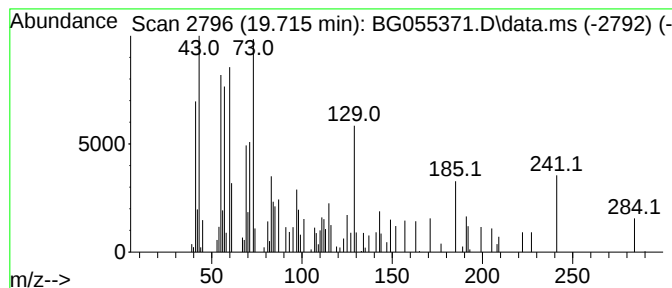
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.715	2.02 ng	51351	Phenanthrene-d10	17.606

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	50
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102922\
Data File : BG055371.D
Acq On : 29 Oct 2022 18:50
Operator : CG/JU
Sample : N5313-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-SE-QUARTER

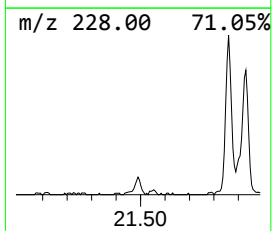
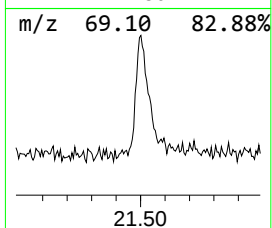
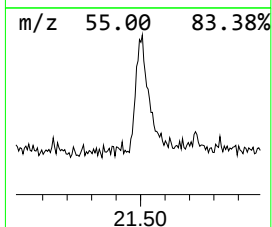
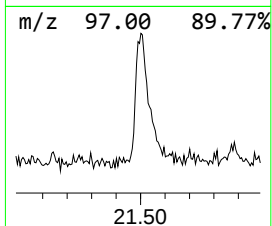
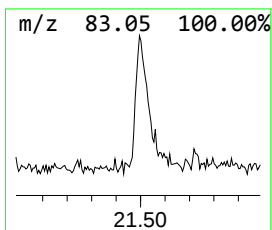
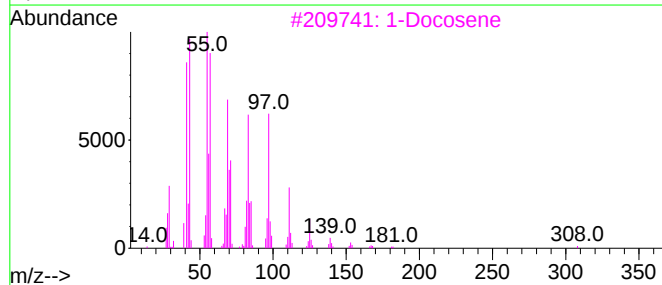
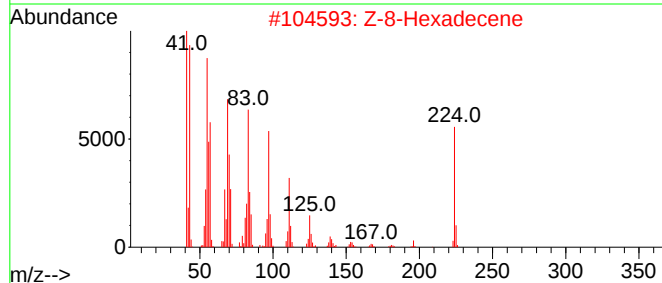
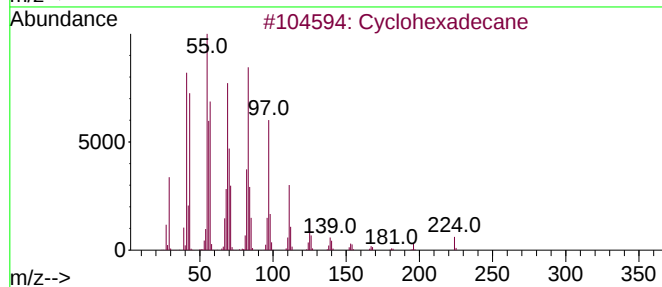
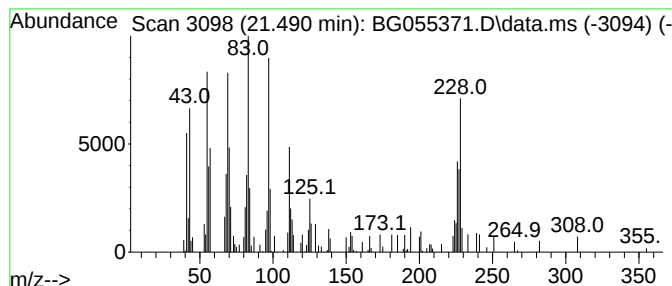
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.490	2.08 ng	66638	Chrysene-d12	21.878

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	86
2			Z-8-Hexadecene	224	C16H32	1000130-87-5	64
3			1-Docosene	308	C22H44	001599-67-3	64
4			Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1010164-49-7	62
5			Trichloroacetic acid, 4-hexadecy...	386	C18H33Cl3O2	1000282-92-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102922\
Data File : BG055371.D
Acq On : 29 Oct 2022 18:50
Operator : CG/JU
Sample : N5313-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-SE-QUARTER

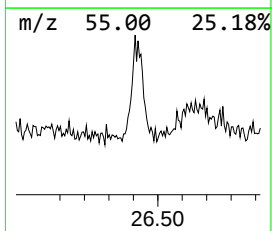
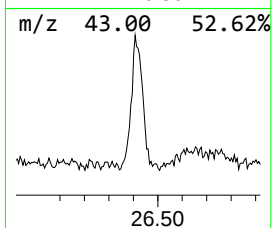
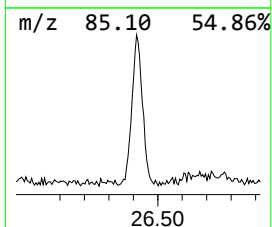
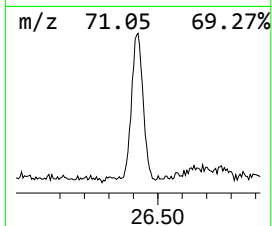
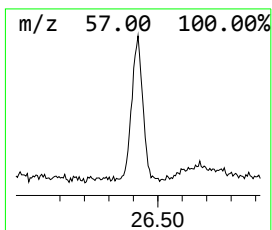
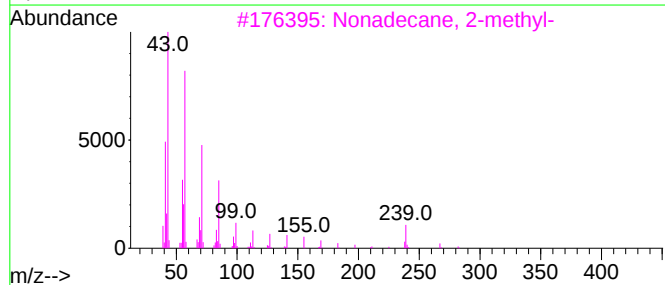
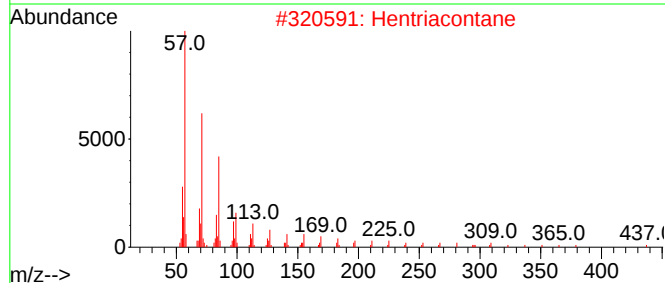
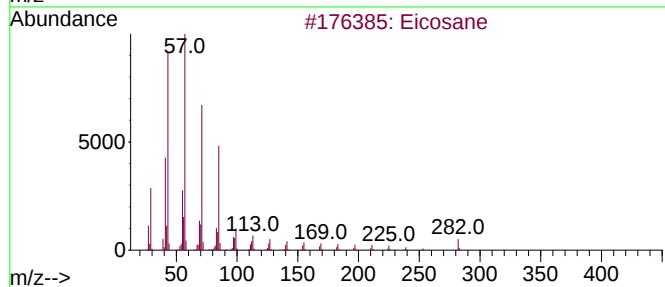
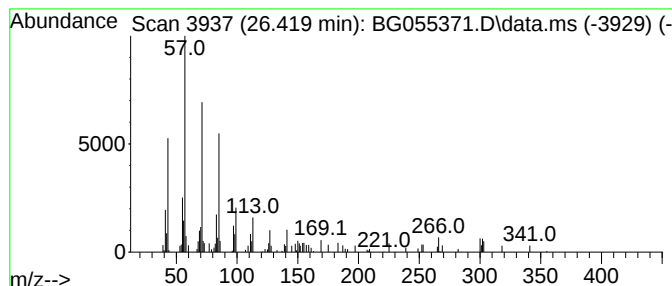
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.419	3.40 ng	102213	Perylene-d12	25.273

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	83
2			Hentriacontane	437	C31H64	000630-04-6	81
3			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	81
4			Hexacosane	366	C26H54	000630-01-3	81
5			Tetracosane	338	C24H50	000646-31-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102922\
Data File : BG055371.D
Acq On : 29 Oct 2022 18:50
Operator : CG/JU
Sample : N5313-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-SE-QUARTER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.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
Propane, 1,1-di...	3.323	2.4	ng	21982	1	8.258	183427	20.0
2-Pentanone, 4-...	5.303	11.1	ng	101342	1	8.258	183427	20.0
.alpha.-Pinene	6.924	6.3	ng	57310	1	8.258	183427	20.0
Ethanol, 2-(2-b...	10.832	4.1	ng	56816	2	11.090	275876	20.0
n-Hexadecanoic ...	18.464	3.9	ng	99129	4	17.606	509390	20.0
Octadecanoic acid	19.715	2.0	ng	51351	4	17.606	509390	20.0
Cyclohexadecane	21.490	2.1	ng	66638	5	21.878	641627	20.0
Eicosane	26.419	3.4	ng	102213	6	25.273	601939	20.0