

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
 Data File : BG055561.D
 Acq On : 11 Nov 2022 10:53
 Operator : CG/JU
 Sample : N5360-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20221113-COMP-12

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055561.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	13	rBV	230789	353194	6.87%	1.704%
2	5.326	340	347	360	rVB	138251	226992	4.41%	1.095%
3	5.796	420	427	441	rVB	1010352	1624251	31.58%	7.835%
4	7.400	692	700	713	rBV	951926	1674702	32.56%	8.078%
5	8.270	841	848	854	rBV	178910	307822	5.99%	1.485%
6	9.439	1038	1047	1056	rBV	546233	978121	19.02%	4.718%
7	11.096	1319	1329	1338	rBV	230702	420152	8.17%	2.027%
8	13.517	1733	1741	1748	rBV	1230839	1928258	37.49%	9.301%
9	14.886	1967	1974	1984	rVB	366537	575481	11.19%	2.776%
10	15.514	2062	2081	2082	rBV2	25436	97605	1.90%	0.471%
11	16.031	2143	2169	2170	rBV	70298	310734	6.04%	1.499%
12	16.366	2206	2226	2263	rBV2	1492043	5142737	100.00%	24.806%
13	16.754	2283	2292	2297	rBV2	18182	53725	1.04%	0.259%
14	17.624	2434	2440	2448	rVB	489715	743132	14.45%	3.584%
15	18.487	2582	2587	2598	rBV	79150	125649	2.44%	0.606%
16	19.604	2768	2777	2785	rBV4	35754	98567	1.92%	0.475%
17	19.745	2798	2801	2810	rBV	46560	70817	1.38%	0.342%
18	20.215	2875	2881	2887	rBV	2248426	2913362	56.65%	14.053%
19	20.567	2937	2941	2949	rVB3	31227	63736	1.24%	0.307%
20	21.496	3093	3099	3101	rBV3	37263	73711	1.43%	0.356%
21	21.531	3101	3105	3114	rVV2	128599	277522	5.40%	1.339%
22	21.625	3116	3121	3128	rVB	319133	479022	9.31%	2.311%
23	21.925	3165	3172	3183	rVB	561525	963613	18.74%	4.648%
24	22.765	3311	3315	3324	rVB2	28330	55608	1.08%	0.268%
25	24.369	3582	3588	3595	rVB3	33634	74899	1.46%	0.361%
26	25.344	3744	3754	3775	rVB	333230	1098533	21.36%	5.299%

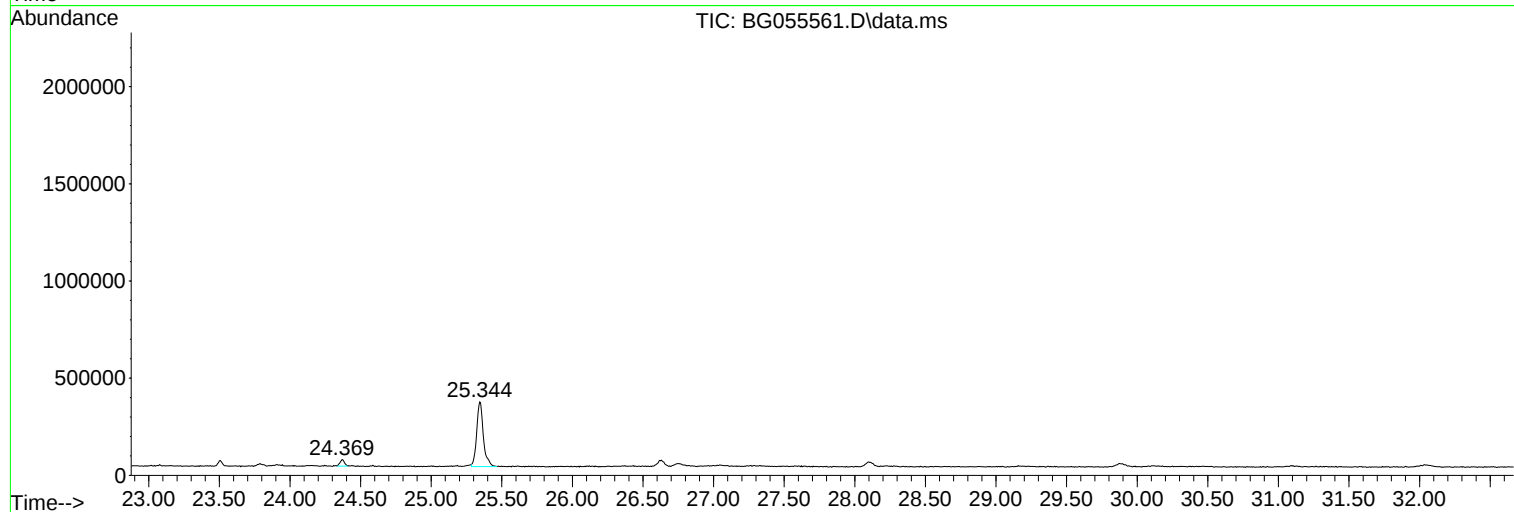
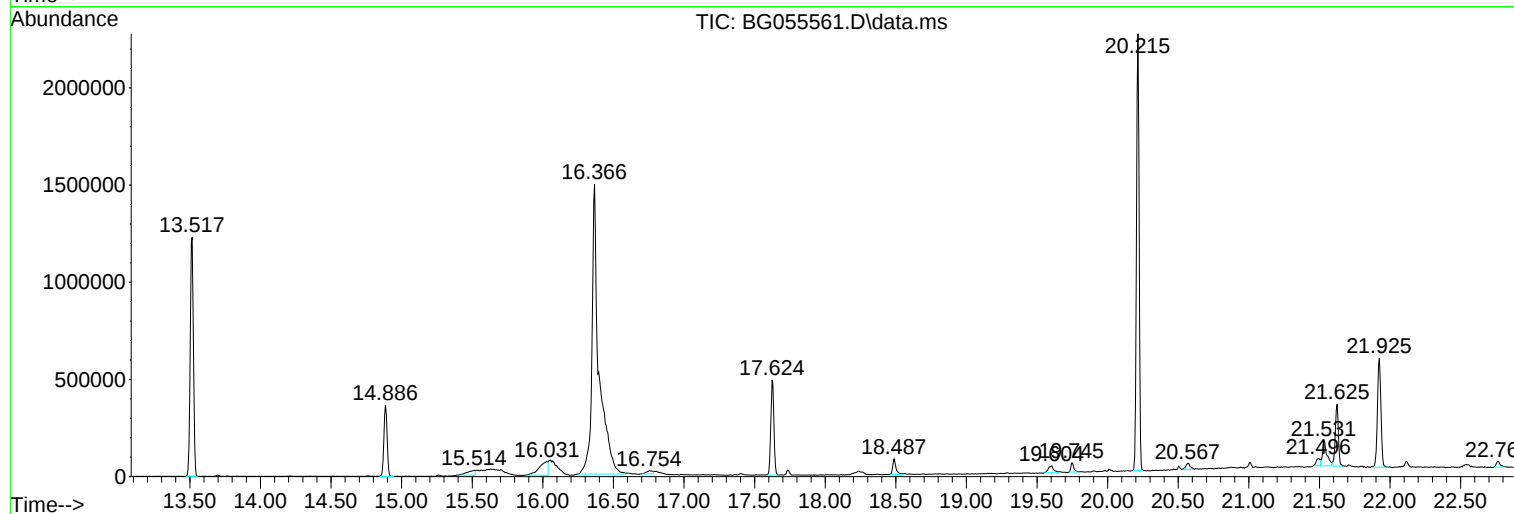
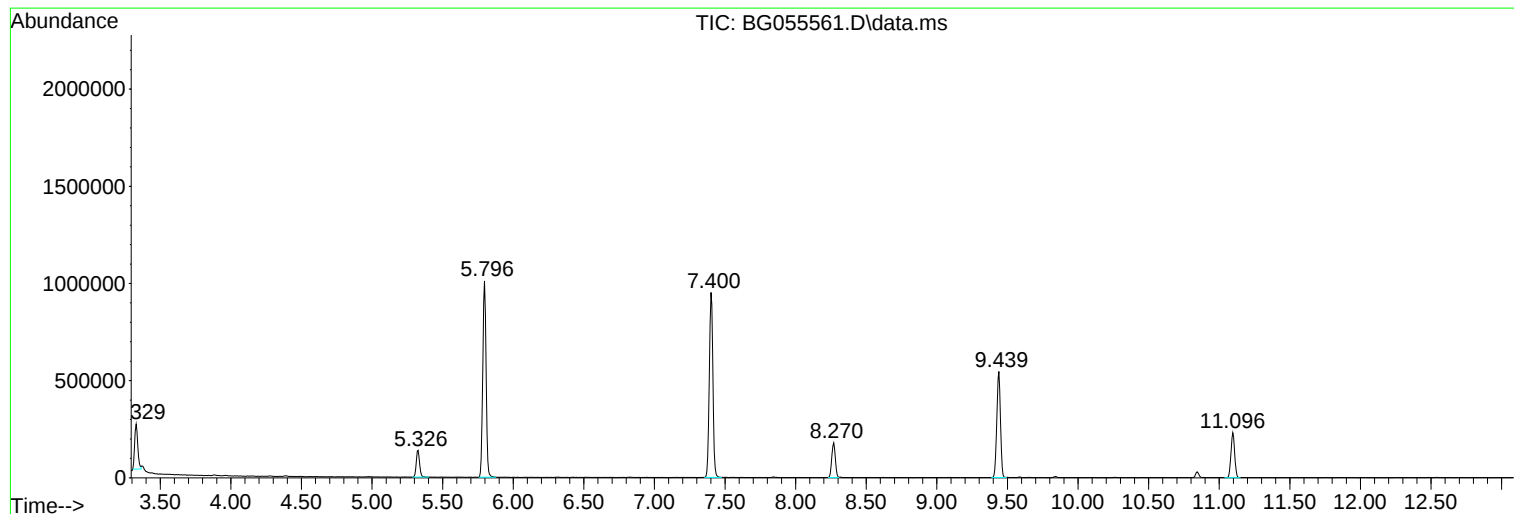
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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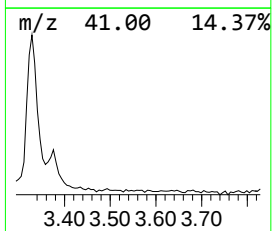
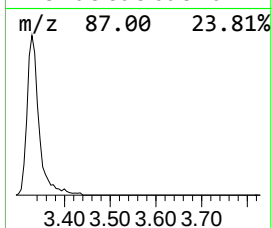
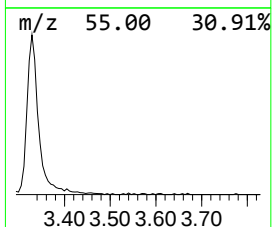
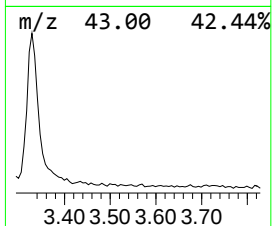
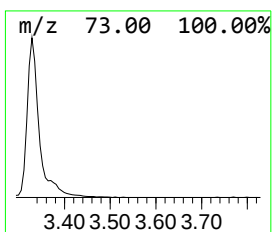
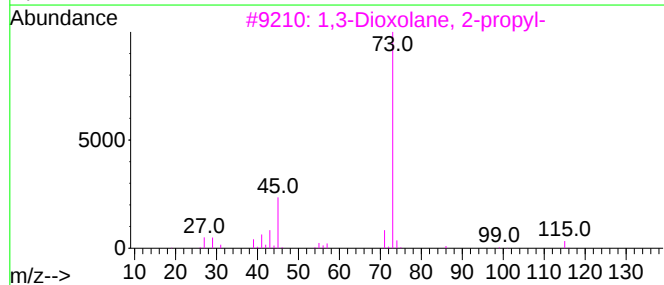
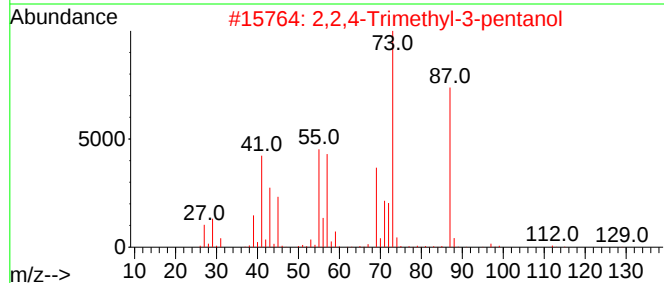
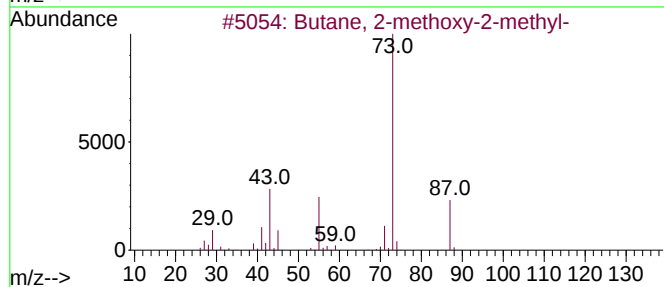
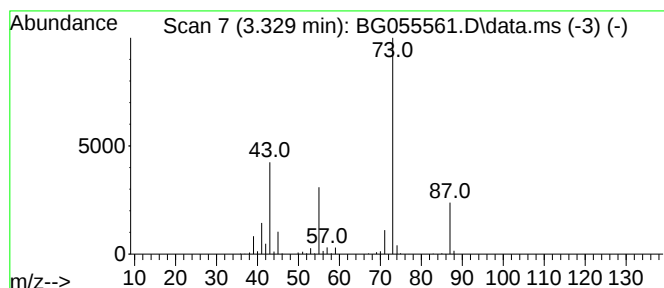
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.329	22.95 ng	353194	1,4-Dichlorobenzene-d4	8.270

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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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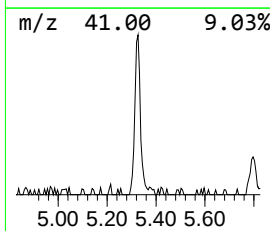
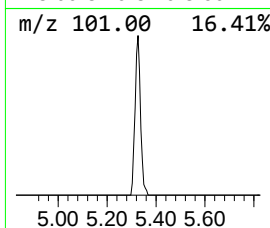
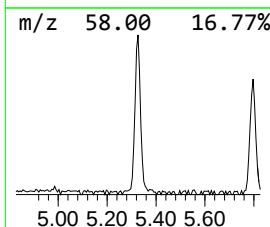
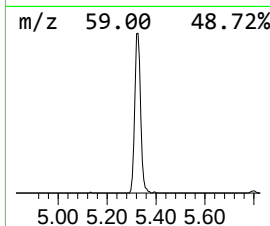
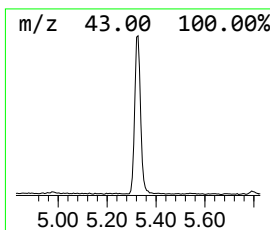
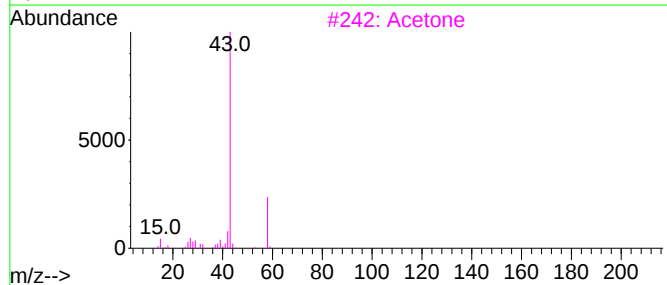
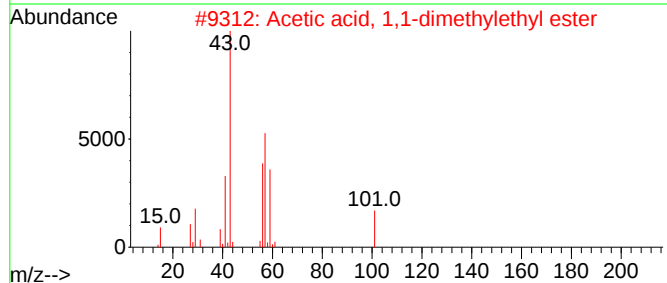
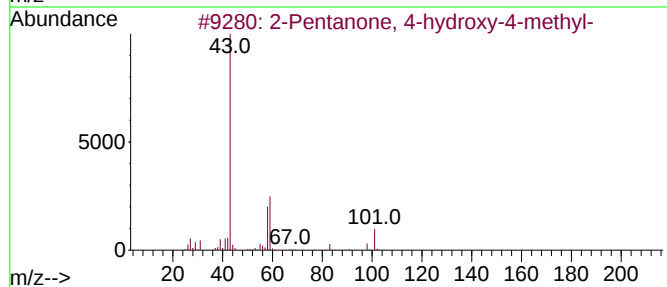
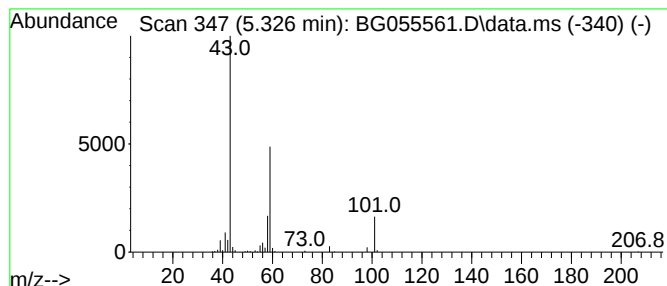
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.326	14.75 ng	226992	1,4-Dichlorobenzene-d4	8.270

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	38
3		Acetone	58	C3H6O	000067-64-1	22
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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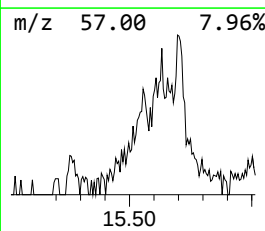
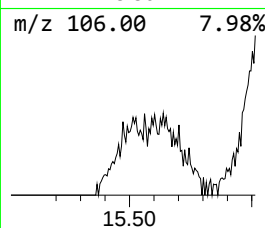
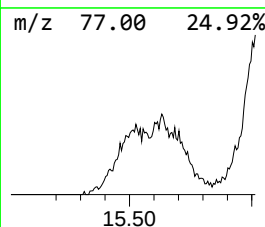
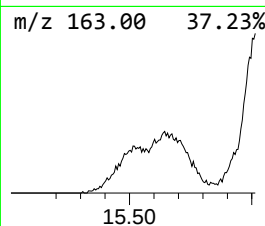
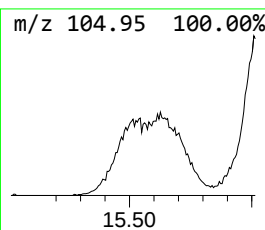
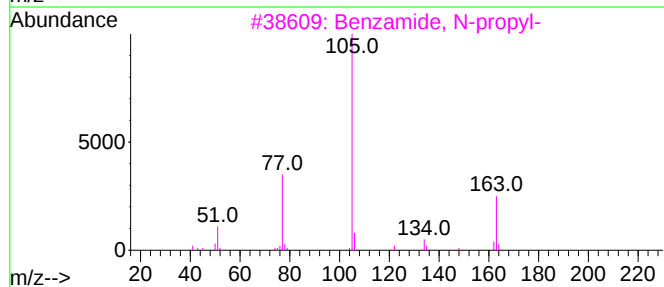
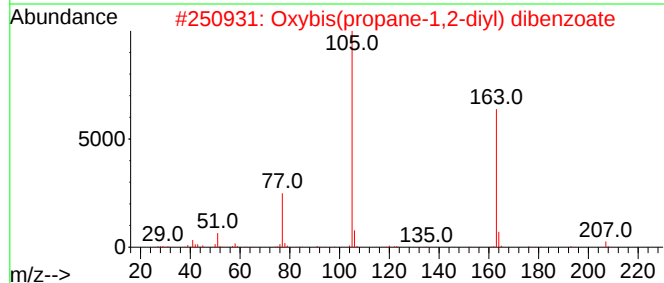
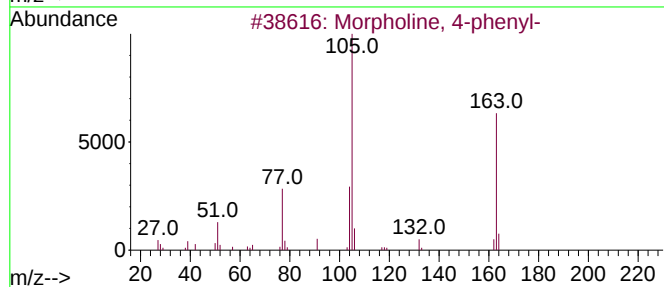
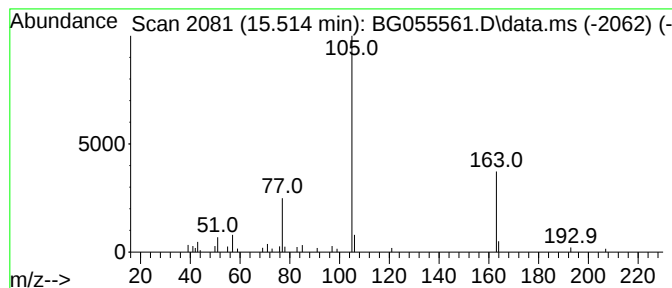
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Morpholine, 4-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.514	3.39 ng	97605	Acenaphthene-d10	14.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
3			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
4			(1-Oxa-2-aza-spiro[2.5]oct-2-yl)...	217	C13H15NO2	002289-83-0	43
5			Phenylglyoxylic acid, 2-methylbu...	220	C13H16O3	1010453-46-2	43



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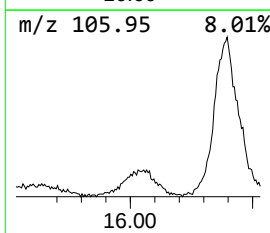
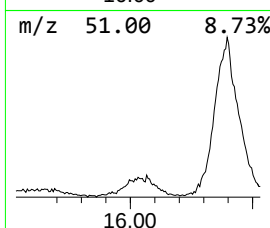
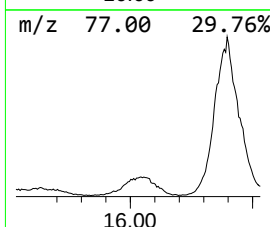
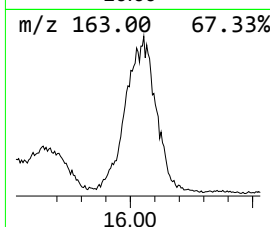
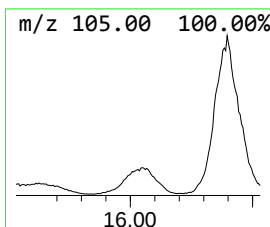
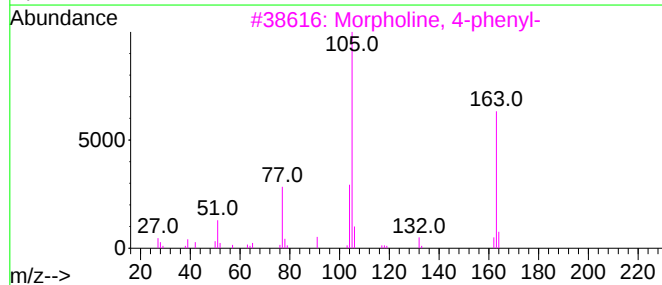
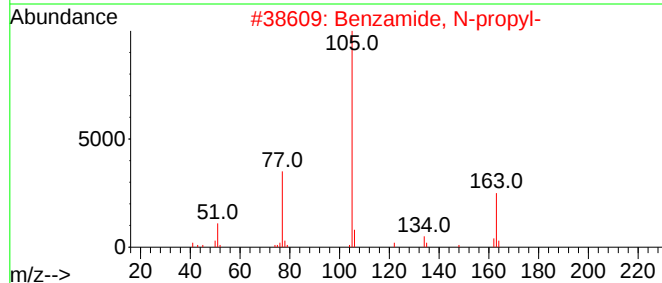
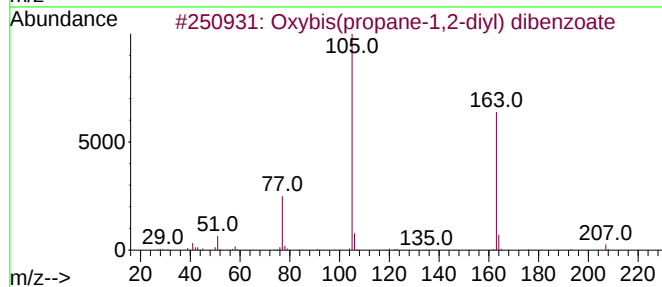
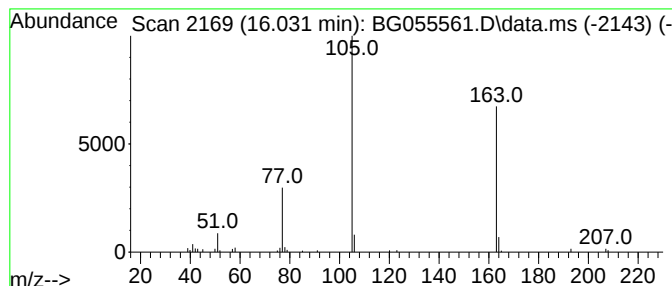
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Peak Number 4 Oxybis(propene-1,2-diyl) di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.032	10.80 ng	310734	Acenaphthene-d10	14.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	90
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	78
3			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	78
4			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
5			.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	43



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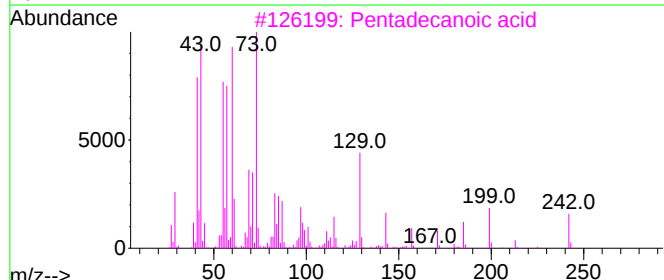
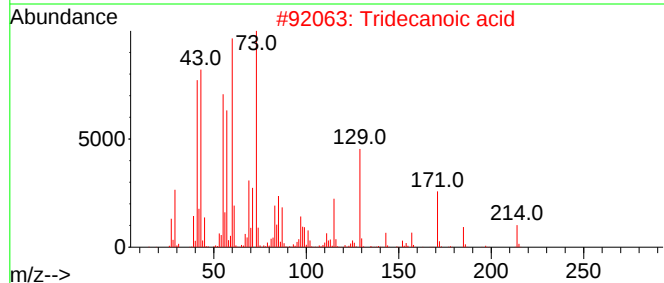
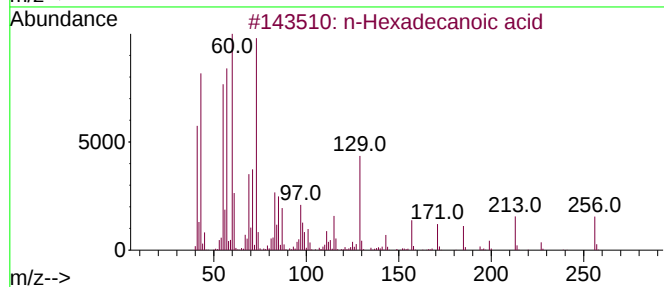
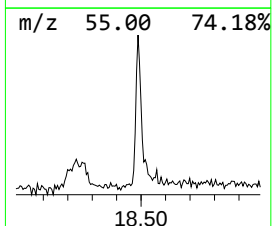
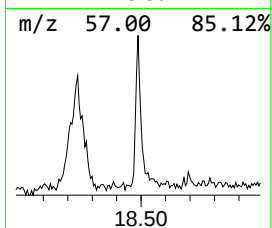
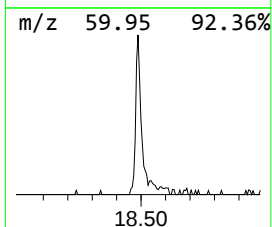
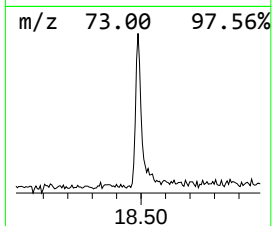
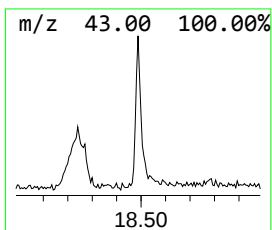
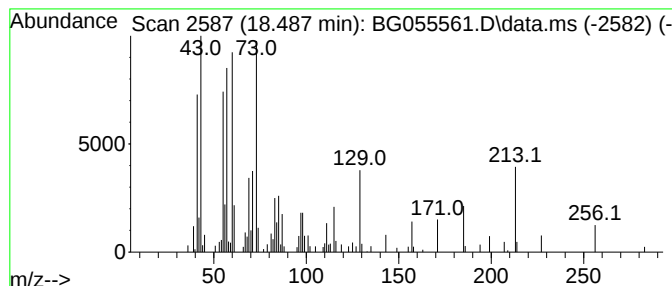
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.487	3.38 ng	125649	Phenanthrene-d10	17.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Undecanoic acid	186	C11H22O2	000112-37-8	50



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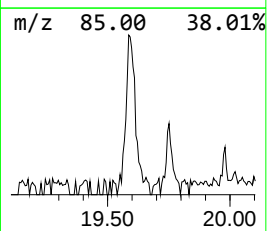
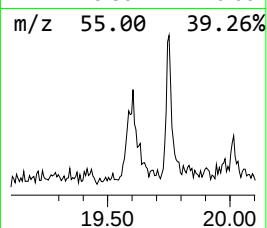
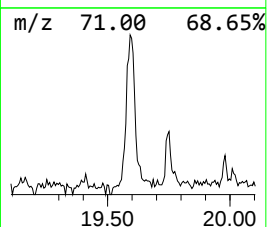
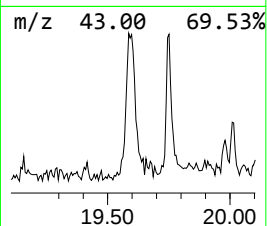
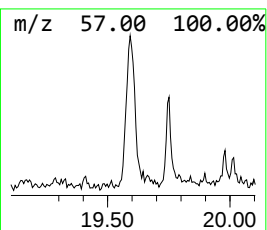
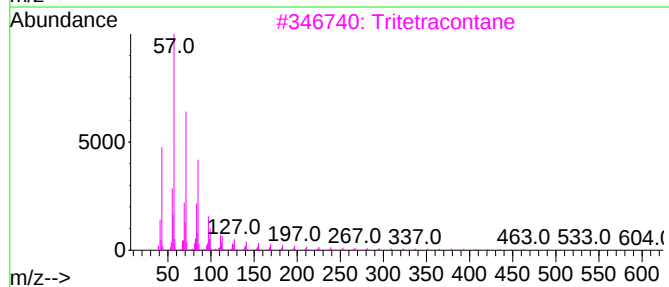
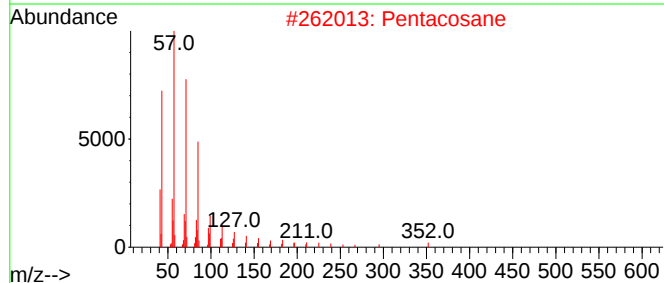
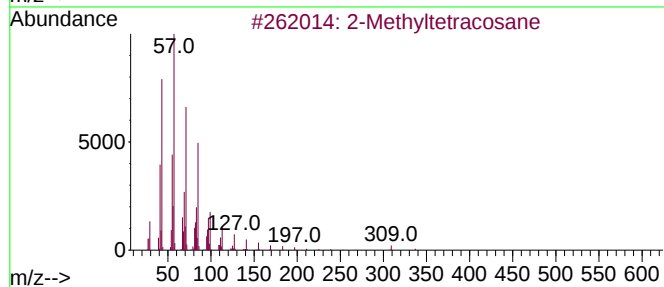
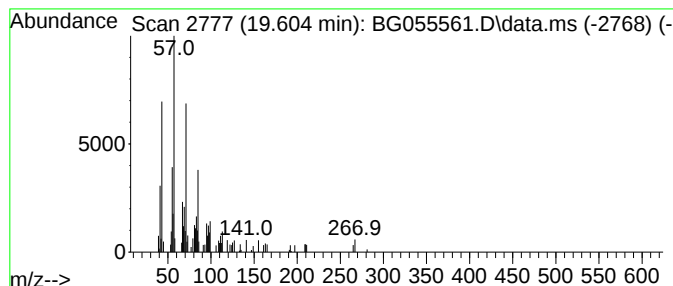
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Methyltetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.604	2.65 ng	98567	Phenanthrene-d10	17.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyltetracosane	352	C25H52	001560-78-7	76
2			Pentacosane	352	C25H52	000629-99-2	68
3			Tritetracontane	605	C43H88	007098-21-7	62
4			Heptacosane	380	C27H56	000593-49-7	62
5			Tetratetracontane	619	C44H90	007098-22-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055561.D
Acq On : 11 Nov 2022 10:53
Operator : CG/JU
Sample : N5360-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

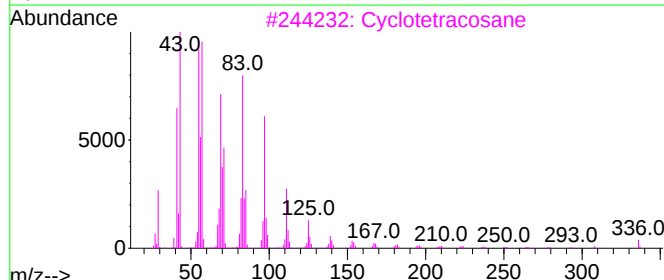
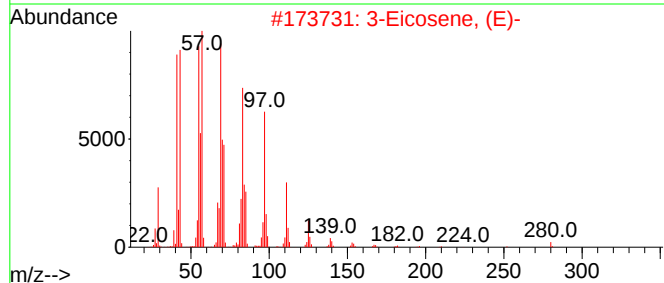
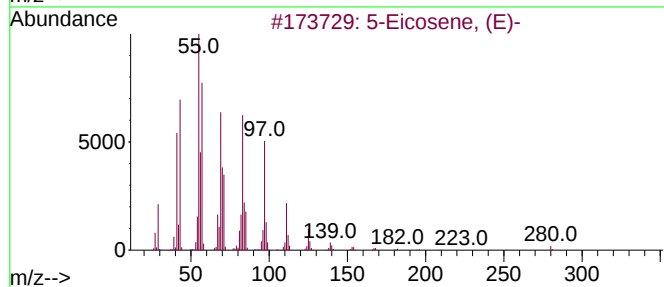
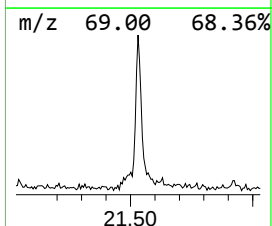
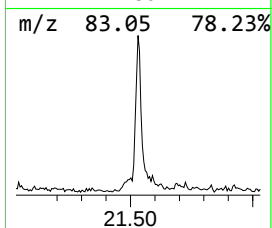
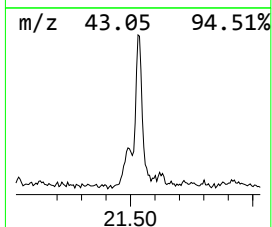
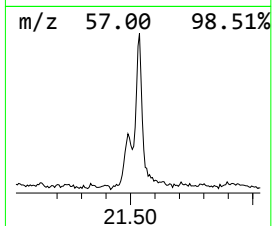
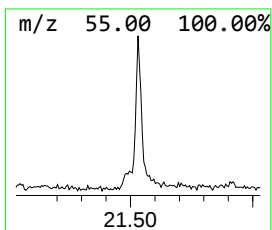
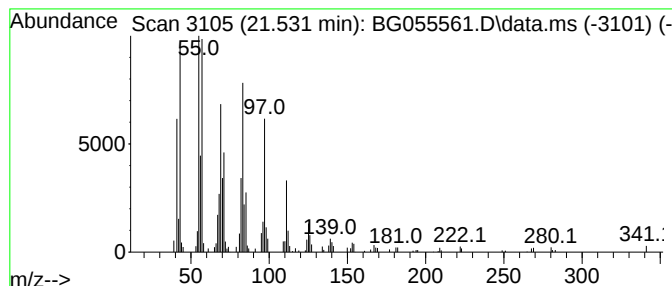
Instrument :
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ClientSampleId :
20221113-COMP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.531	5.76 ng	277522	Chrysene-d12	21.925	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
3	Cyclotetracosane	336	C24H48	000297-03-0	94
4	1-Docosene	308	C22H44	001599-67-3	94
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055561.D
Acq On : 11 Nov 2022 10:53
Operator : CG/JU
Sample : N5360-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221113-COMP-12

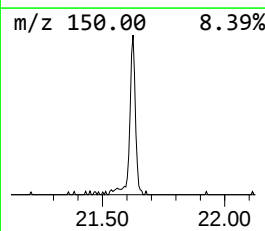
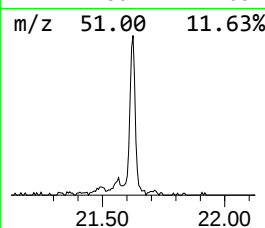
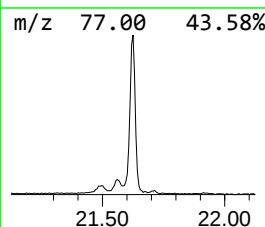
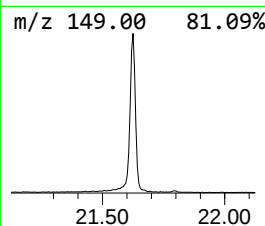
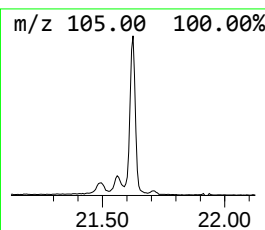
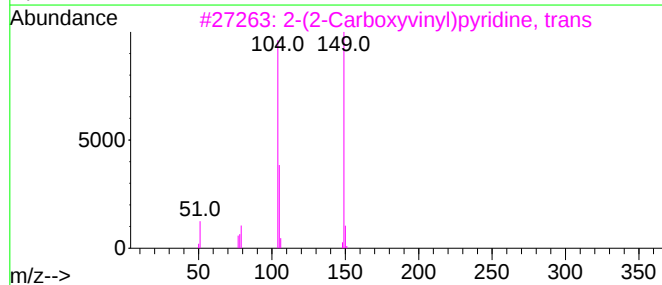
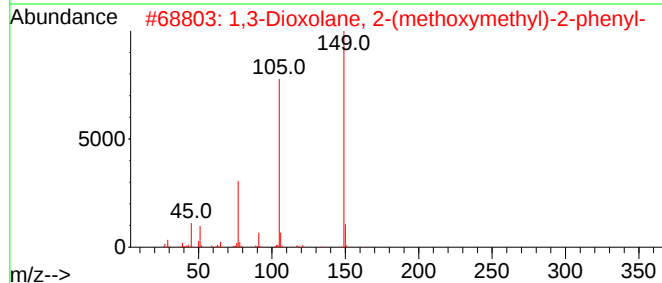
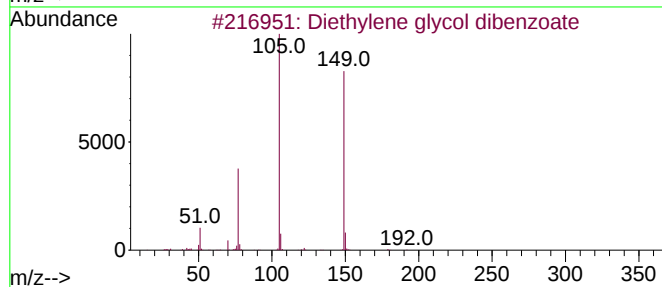
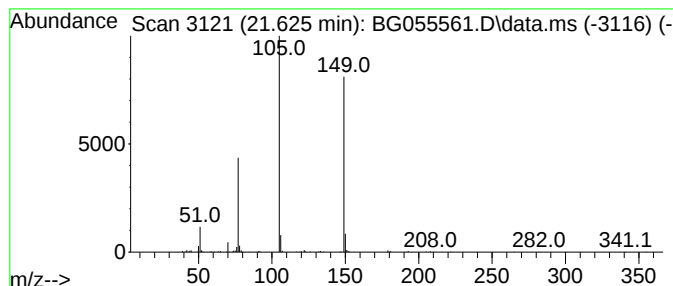
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.625	9.94 ng	479022	Chrysene-d12	21.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	91
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49
4			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
5			N-(5-Pyrimidinyl)benzamide	199	C11H9N3O	103854-65-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055561.D
Acq On : 11 Nov 2022 10:53
Operator : CG/JU
Sample : N5360-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221113-COMP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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
Butane, 2-metho...	3.329	22.9	ng	353194	1	8.270	307822	20.0
2-Pentanone, 4-...	5.326	14.8	ng	226992	1	8.270	307822	20.0
Morpholine, 4-p...	15.514	3.4	ng	97605	3	14.886	575481	20.0
Oxybis(propane-...	16.032	10.8	ng	310734	3	14.886	575481	20.0
n-Hexadecanoic ...	18.487	3.4	ng	125649	4	17.624	743132	20.0
2-Methyltetraco...	19.604	2.6	ng	98567	4	17.624	743132	20.0
5-Eicosene, (E)-	21.531	5.8	ng	277522	5	21.925	963613	20.0
Diethylene glyc...	21.625	9.9	ng	479022	5	21.925	963613	20.0