

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
 Data File : BG057013.D
 Acq On : 6 Apr 2023 15:30
 Operator : CG/JU
 Sample : 02209-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PSC-124055

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-BG033023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057013.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.442	317	324	334	rBB	158153	246959	33.01%	4.934%
2	5.924	399	406	414	rBV	241846	395976	52.93%	7.910%
3	7.545	674	682	692	rBB	312192	544372	72.77%	10.875%
4	8.409	822	829	835	rBV2	52567	89937	12.02%	1.797%
5	9.584	1022	1029	1039	rBB	199144	357356	47.77%	7.139%
6	11.246	1304	1312	1320	rBB	66883	119462	15.97%	2.386%
7	11.411	1335	1340	1349	rVB	12097	19497	2.61%	0.389%
8	13.649	1713	1721	1728	rVB	389765	583678	78.02%	11.660%
9	15.023	1944	1955	1964	rVB2	111202	177018	23.66%	3.536%
10	16.357	2176	2182	2187	rVB	15627	23598	3.15%	0.471%
11	16.498	2200	2206	2213	rBV	320049	469478	62.76%	9.379%
12	17.620	2392	2397	2400	rBV	7859	10892	1.46%	0.218%
13	17.714	2408	2413	2415	rBV3	8942	11036	1.48%	0.220%
14	17.761	2415	2421	2430	rVB	147043	232020	31.02%	4.635%
15	18.078	2471	2475	2480	rBV	9416	12643	1.69%	0.253%
16	18.378	2521	2526	2531	rBV	29185	38424	5.14%	0.768%
17	18.431	2531	2535	2544	rVV7	12889	29689	3.97%	0.593%
18	18.501	2544	2547	2551	rVB	9142	11406	1.52%	0.228%
19	18.595	2558	2563	2570	rBV4	53221	85183	11.39%	1.702%
20	18.801	2593	2598	2602	rBV	13699	18328	2.45%	0.366%
21	19.071	2637	2644	2648	rBV	32546	42774	5.72%	0.854%
22	19.846	2773	2776	2781	rBV6	12835	15443	2.06%	0.309%
23	19.911	2783	2787	2790	rVB5	6869	9529	1.27%	0.190%
24	20.122	2817	2823	2825	rBV6	12395	20016	2.68%	0.400%
25	20.211	2834	2838	2841	rBV6	7572	13509	1.81%	0.270%
26	20.328	2852	2858	2866	rBV	576840	748068	100.00%	14.944%
27	20.522	2887	2891	2893	rBV5	9704	14629	1.96%	0.292%
28	20.598	2901	2904	2907	rVB5	8274	9090	1.22%	0.182%
29	20.810	2936	2940	2943	rBV5	6287	10206	1.36%	0.204%
30	20.980	2964	2969	2971	rBV5	10987	19036	2.54%	0.380%
31	21.568	3066	3069	3074	rVB6	13447	20487	2.74%	0.409%
32	21.638	3077	3081	3087	rVV3	35161	54985	7.35%	1.098%
33	22.073	3150	3155	3165	rVB	140106	251061	33.56%	5.015%
34	22.613	3245	3247	3255	rVB8	9181	16548	2.21%	0.331%
35	22.895	3290	3295	3297	rBV6	7804	12868	1.72%	0.257%
36	25.621	3747	3759	3769	rVB2	80545	270544	36.17%	5.405%

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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-BG033023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

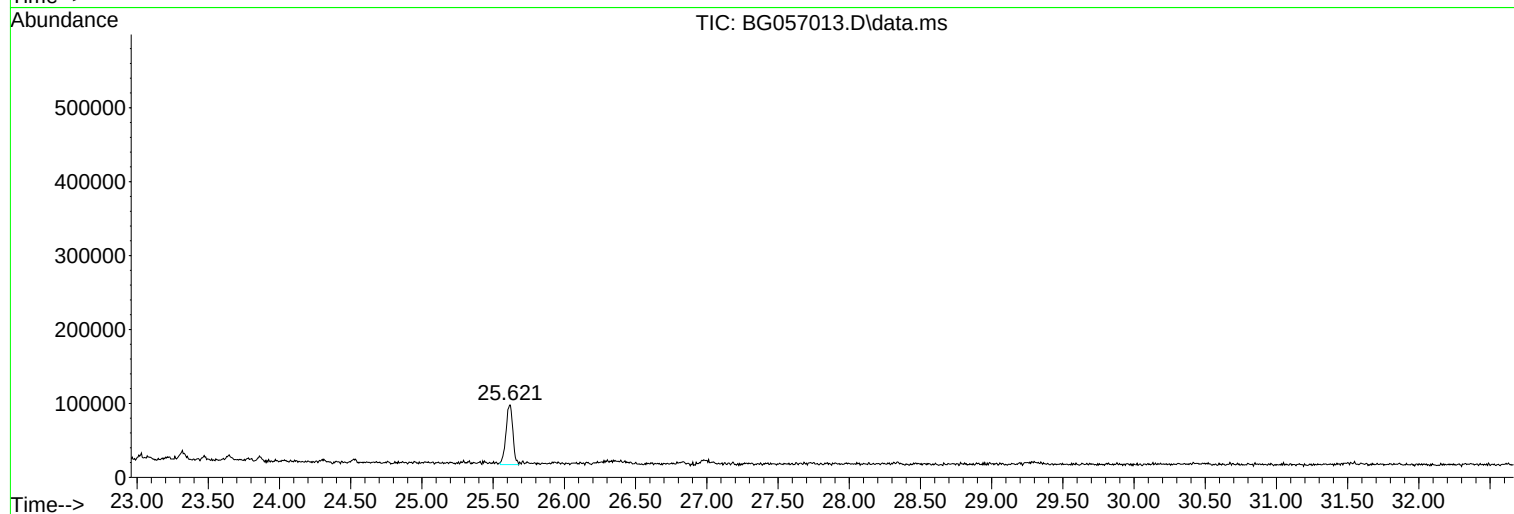
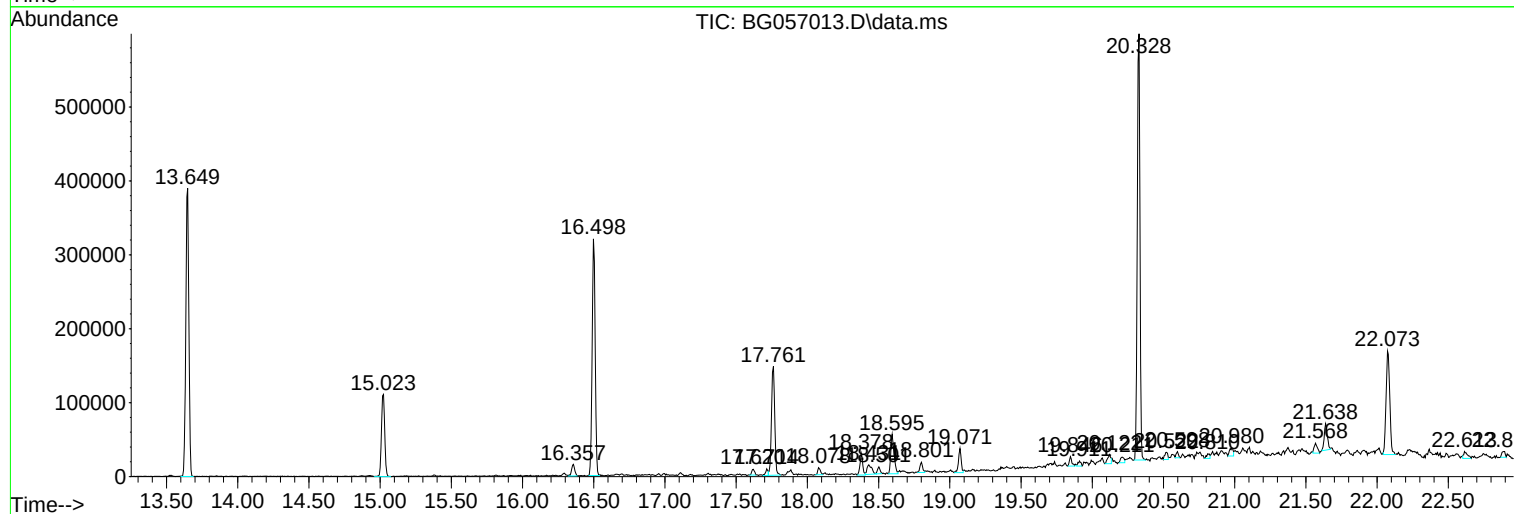
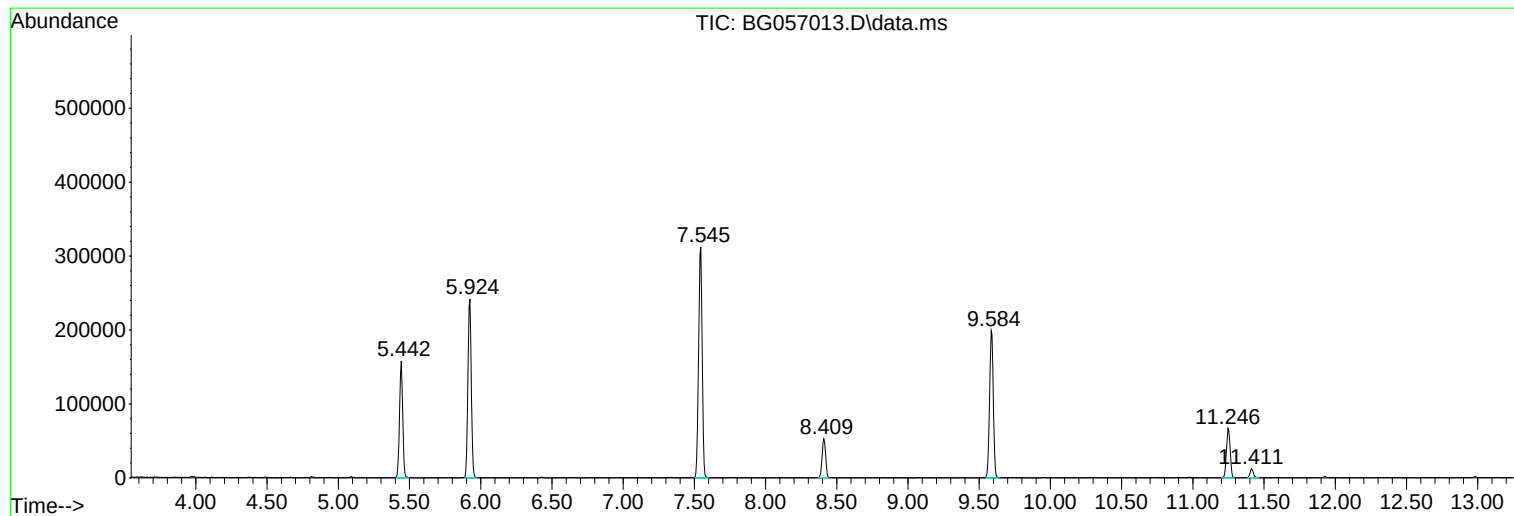
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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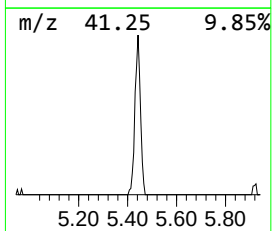
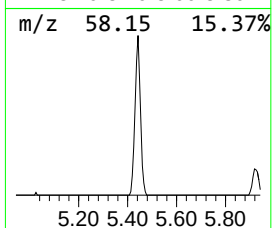
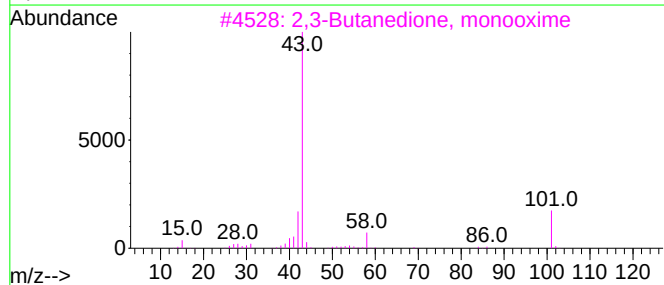
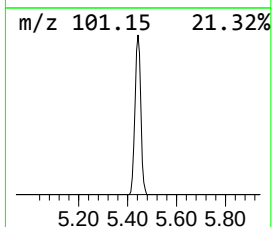
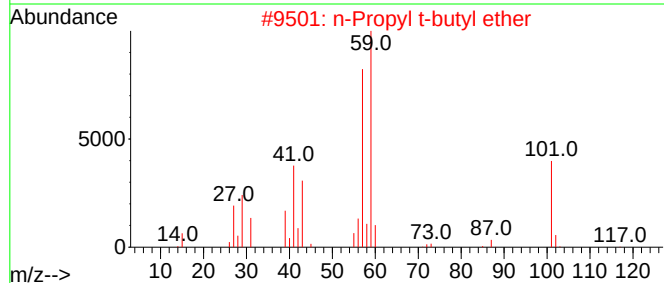
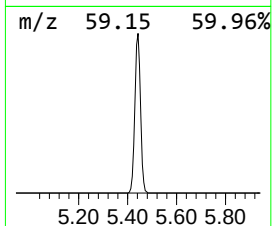
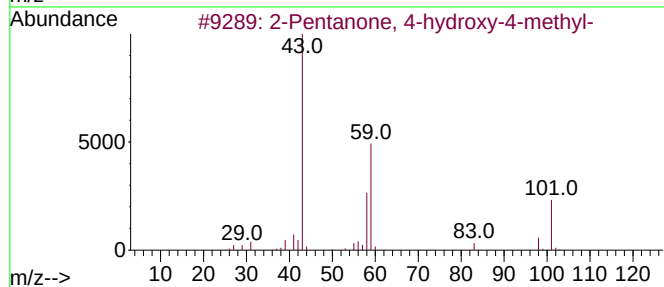
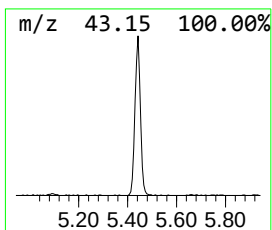
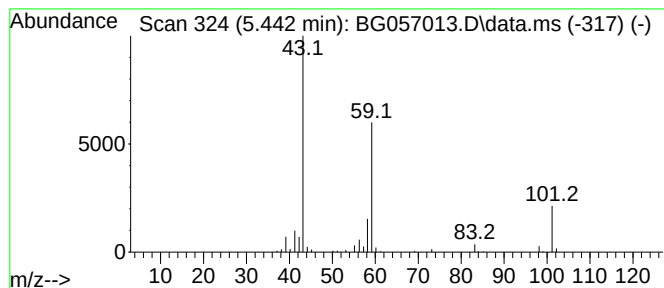
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.442	54.92 ng	246959	1,4-Dichlorobenzene-d4			8.415
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	n-Propyl t-butyl ether		116	C7H16O	1000334-81-9	33
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	25
4	1,3-Dioxolane-2-methanol, 2,4-di...		132	C6H12O3	053951-43-2	25
5	1,2-Butanediol		90	C4H10O2	000584-03-2	17



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Instrument :
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ClientSampleId :
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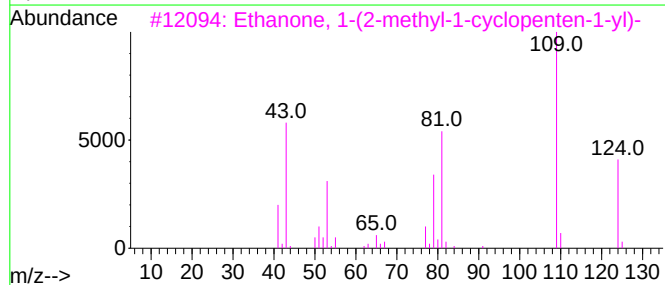
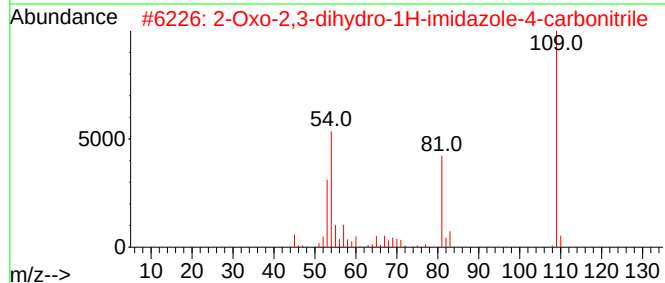
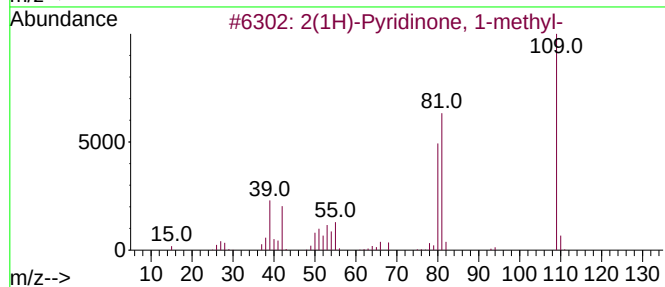
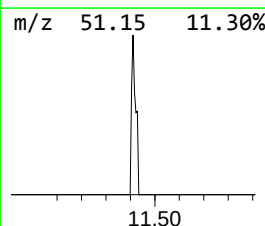
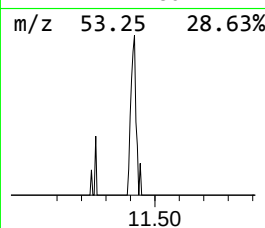
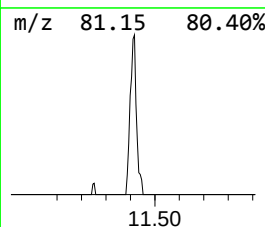
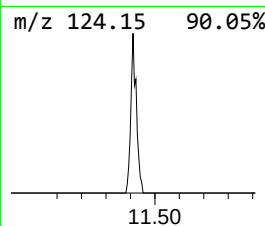
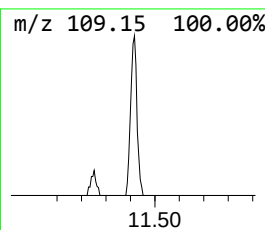
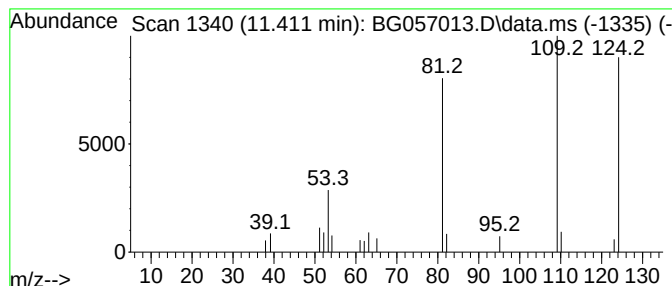
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown11.411 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.411	3.26 ng	19497	Naphthalene-d8	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyridinone, 1-methyl-		109	C6H7NO		000694-85-9	47
2	2-Oxo-2,3-dihydro-1H-imidazole-4...		109	C4H3N3O		1000294-08-6	37
3	Ethanone, 1-(2-methyl-1-cyclopenten...		124	C8H12O		003168-90-9	32
4	Phenol, 3-amino-		109	C6H7NO		000591-27-5	27
5	Phenol, o-amino-		109	C6H7NO		000095-55-6	27



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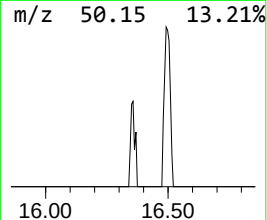
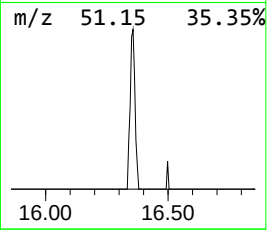
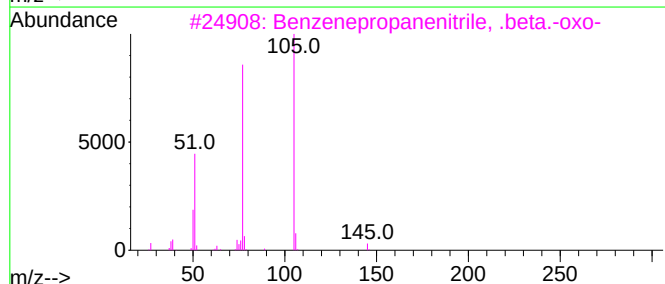
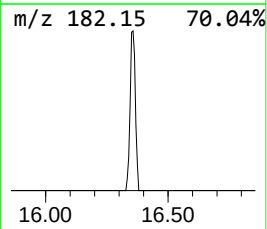
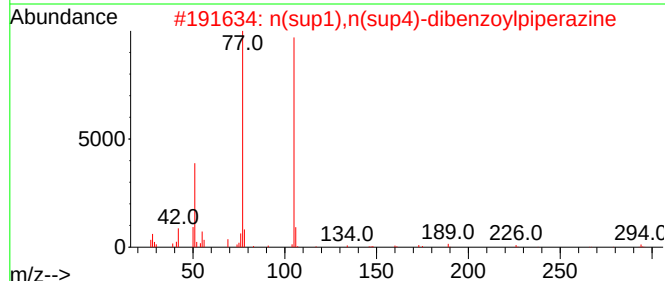
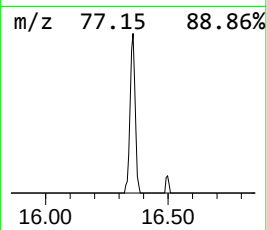
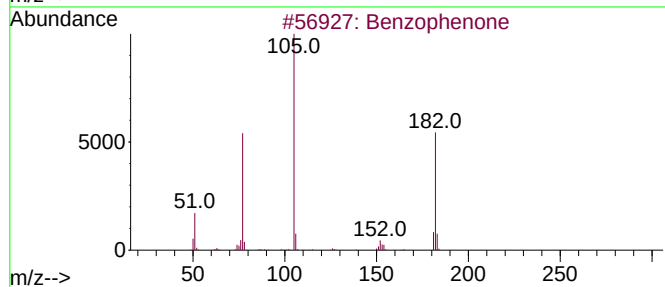
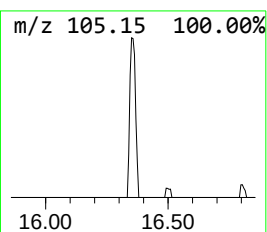
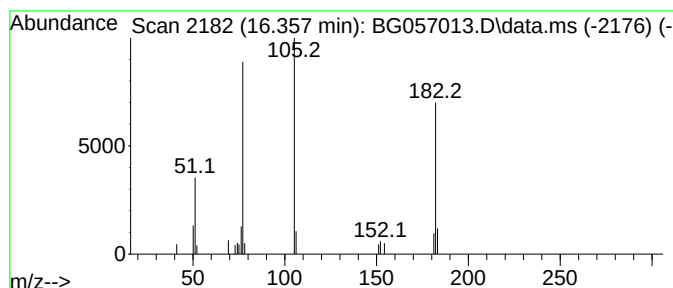
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.357	2.67 ng	23598	Acenaphthene-d10	15.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	94
2	n(sup1),n(sup4)-dibenzoylpiperazine	294	C18H18N2O2	006091-41-4	50
3	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	50
5	S-Benzoyl-N-(p-nitrobenzylidene)...	286	C14H10N2O3S	139776-09-3	50



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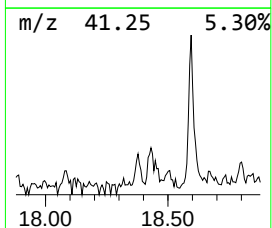
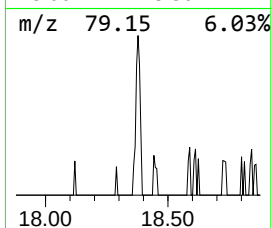
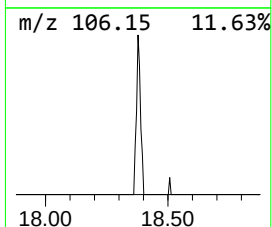
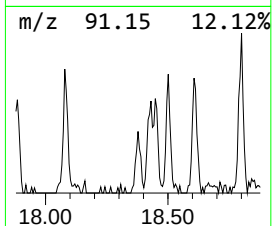
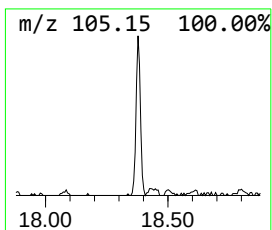
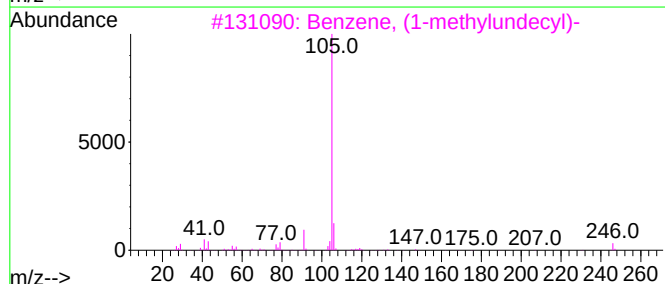
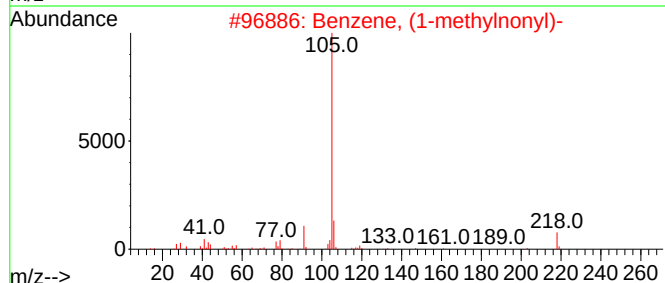
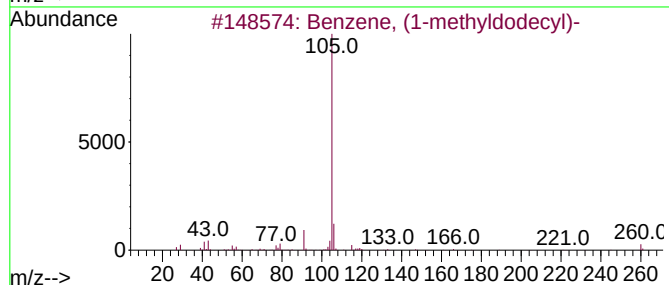
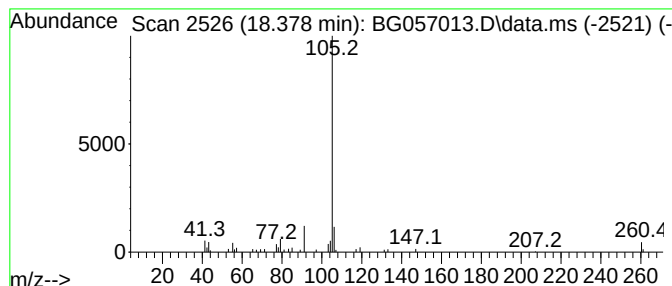
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzene, (1-methyldodecyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.378	3.31 ng	38424	Phenanthrene-d10	17.761

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	87
2		Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	59
3		Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	59
4		Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	59
5		Benzene, (2-ethenyl-1,4,4-trimet...	216	C16H24	074810-76-7	50



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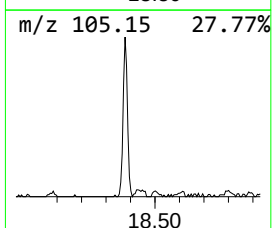
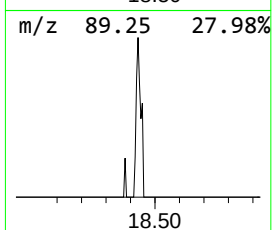
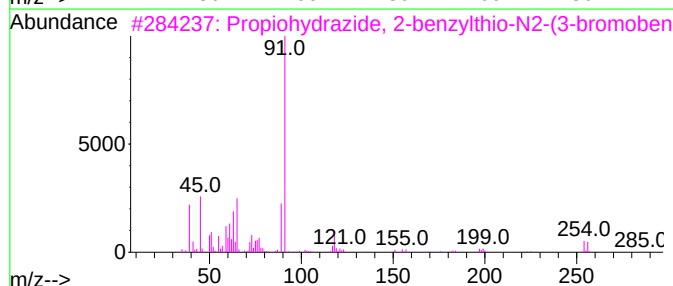
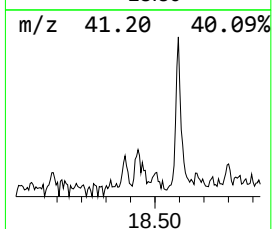
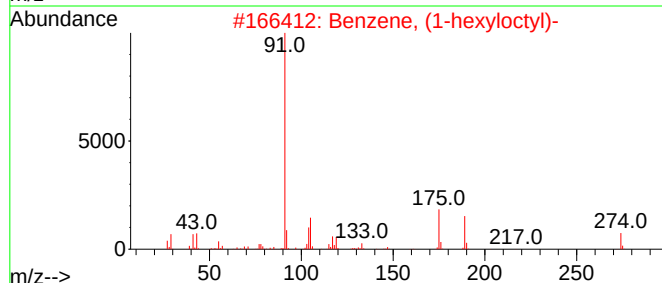
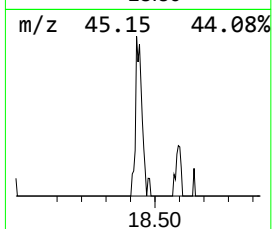
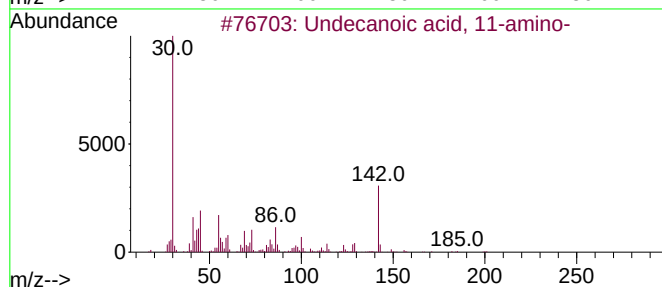
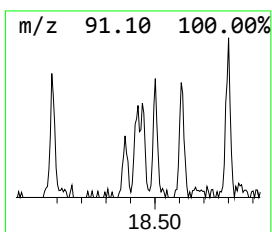
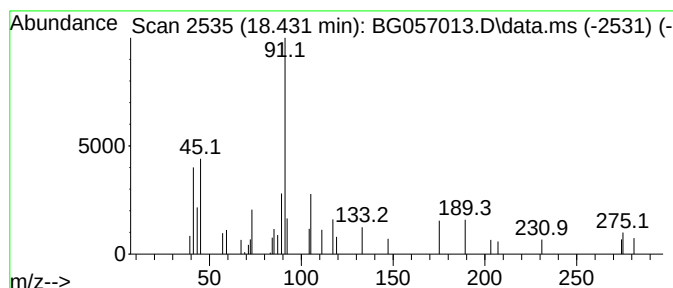
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown18.431 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.431	2.56 ng	29689	Phenanthrene-d10	17.761

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid, 11-amino-	201	C11H23NO2	002432-99-7	16
2			Benzene, (1-hexyloctyl)-	274	C20H34	004534-54-7	10
3			Propiohydrazide, 2-benzylthio-N2...	376	C17H17BrN2OS	1000295-67-3	9
4			Hydrazinecarboxylic acid, ethyl ...	104	C3H8N2O2	004114-31-2	7
5			Adenosine, 2-methyl-	281	C11H15N5O4	016526-56-0	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
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Acq On : 6 Apr 2023 15:30
Operator : CG/JU
Sample : 02209-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

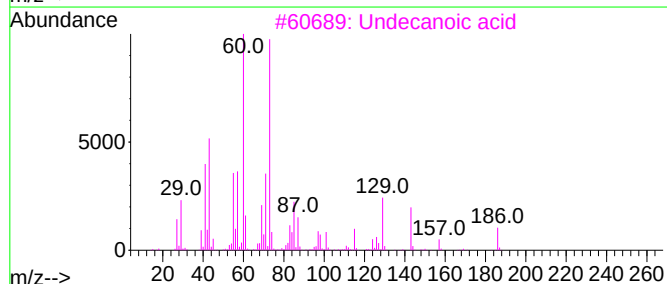
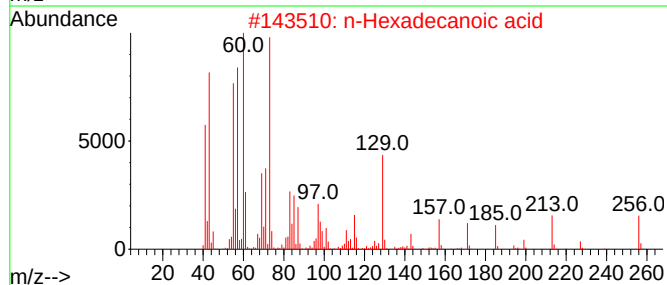
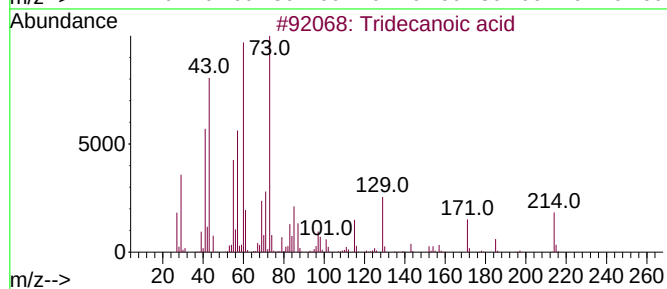
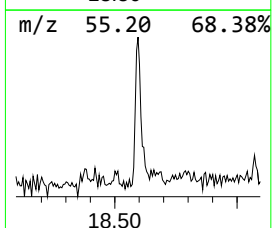
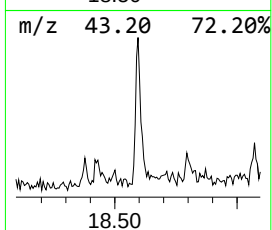
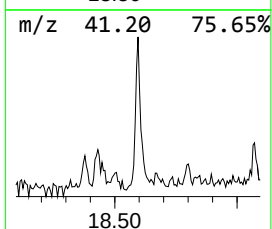
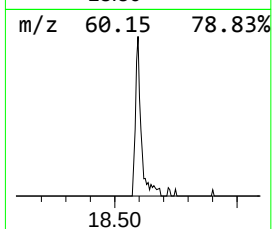
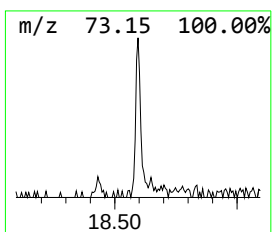
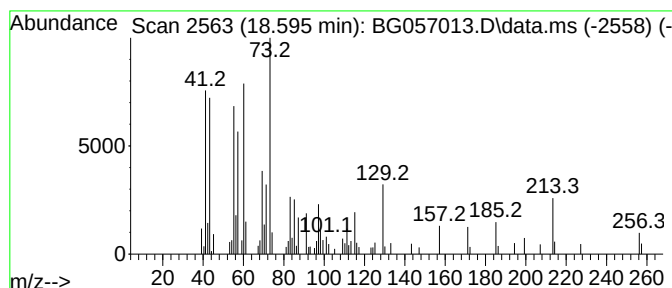
Instrument :
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ClientSampleId :
PSC-124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.595	7.34 ng	85183	Phenanthrene-d10		17.761	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tridecanoic acid		214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	93
3	Undecanoic acid		186	C11H22O2	000112-37-8	70
4	n-Decanoic acid		172	C10H20O2	000334-48-5	60
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057013.D
Acq On : 6 Apr 2023 15:30
Operator : CG/JU
Sample : 02209-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

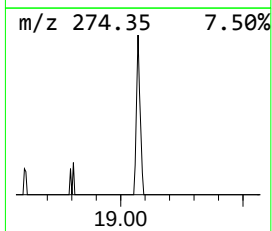
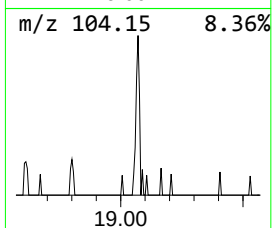
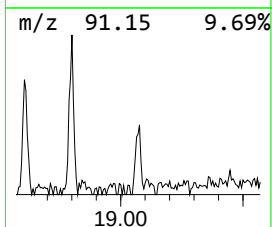
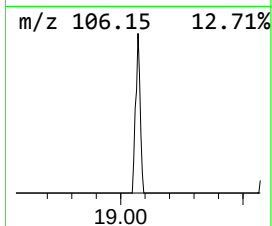
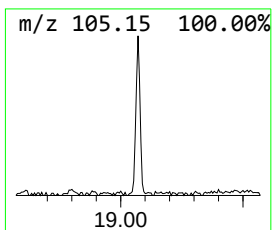
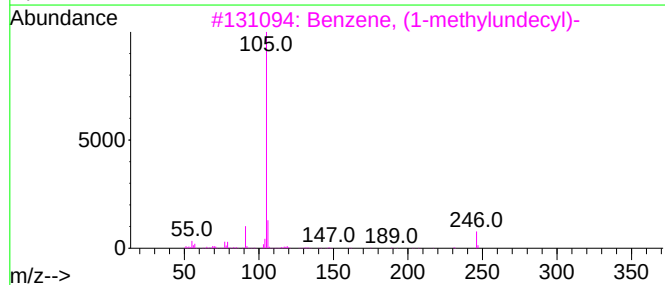
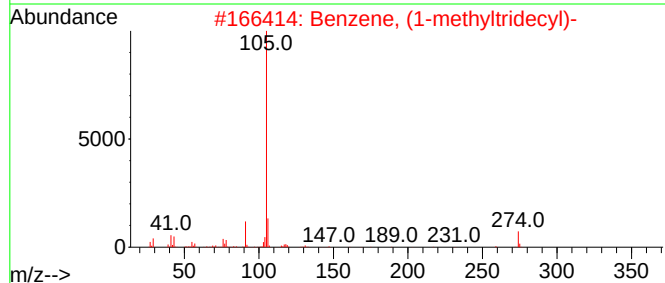
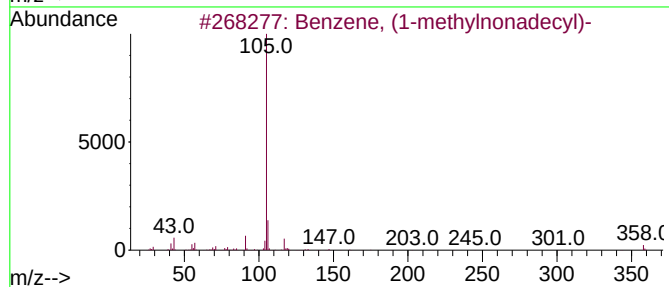
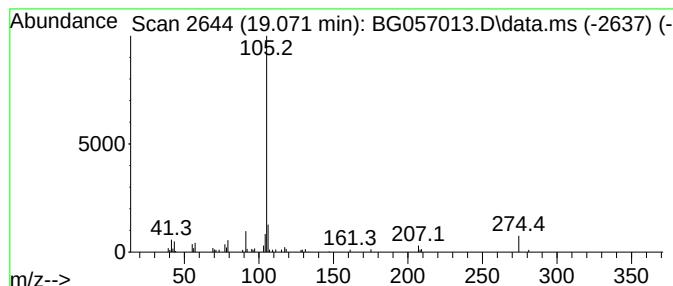
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, (1-methylnonadecyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.071	3.69 ng	42774	Phenanthrene-d10	17.761

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methylnonadecyl)-	358	C26H46	002398-66-5	53
2			Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	53
3			Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	53
4			Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	53
5			Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057013.D
Acq On : 6 Apr 2023 15:30
Operator : CG/JU
Sample : 02209-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

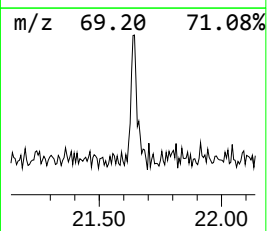
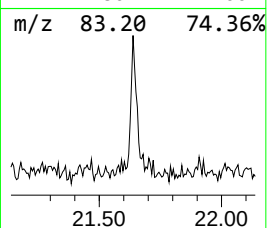
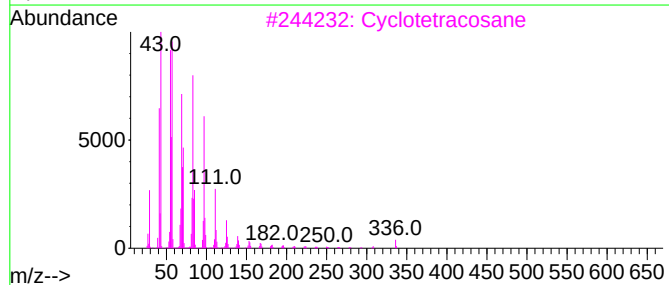
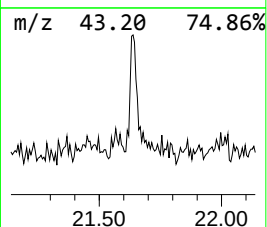
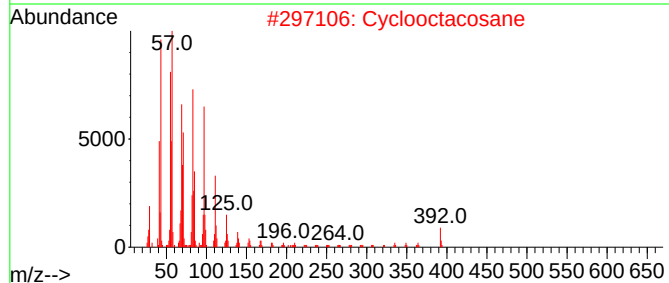
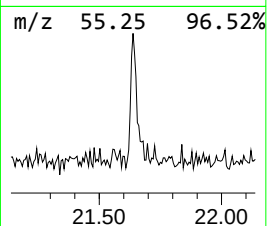
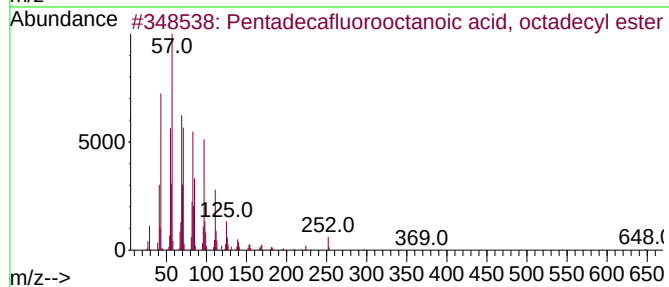
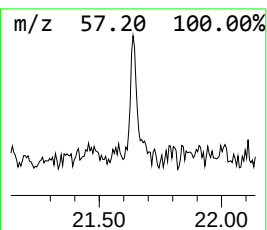
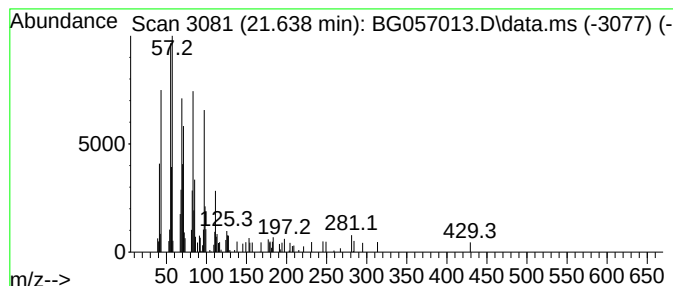
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.638	4.38 ng	54985	Chrysene-d12	22.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2			Cyclooctacosane	392	C28H56	000297-24-5	90
3			Cyclotetracosane	336	C24H48	000297-03-0	87
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5			1-Hexacosanol	382	C26H54O	000506-52-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057013.D
Acq On : 6 Apr 2023 15:30
Operator : CG/JU
Sample : 02209-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.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
2-Pentanone, 4-...	5.442	54.9	ng	246959	1	8.415	89937	20.0
unknown11.411	11.411	3.3	ng	19497	2	11.246	119462	20.0
Benzophenone	16.357	2.7	ng	23598	3	15.024	177018	20.0
Benzene, (1-met...	18.378	3.3	ng	38424	4	17.761	232020	20.0
unknown18.431	18.431	2.6	ng	29689	4	17.761	232020	20.0
Tridecanoic acid	18.595	7.3	ng	85183	4	17.761	232020	20.0
Benzene, (1-met...	19.071	3.7	ng	42774	4	17.761	232020	20.0
Pentadecafluoro...	21.638	4.4	ng	54985	5	22.073	251061	20.0