

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
 Data File : BG048327.D
 Acq On : 4 Mar 2021 14:01
 Operator : CG/JU
 Sample : M1545-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MH-5

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-BG021021.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048327.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.688	394	400	412	rBV	367308	613514	16.74%	4.008%
2	7.309	669	676	688	rBV	207378	421206	11.49%	2.752%
3	8.102	805	811	820	rBV	142731	247217	6.74%	1.615%
4	9.277	1003	1011	1024	rBV	486851	949936	25.91%	6.206%
5	10.923	1284	1291	1301	rVB	166017	330523	9.02%	2.159%
6	13.355	1698	1705	1717	rVB	1223457	2019082	55.08%	13.191%
7	14.183	1842	1846	1855	rBV3	15181	37976	1.04%	0.248%
8	14.736	1934	1940	1952	rVB	303247	491116	13.40%	3.208%
9	16.234	2187	2195	2206	rBV	1259509	1945757	53.08%	12.712%
10	16.968	2317	2320	2325	rVB3	29730	44110	1.20%	0.288%
11	17.156	2336	2352	2353	rBV2	63243	191150	5.21%	1.249%
12	17.380	2379	2390	2392	rBV2	93574	250850	6.84%	1.639%
13	17.485	2402	2408	2413	rVB	383169	577879	15.76%	3.775%
14	17.585	2413	2425	2426	rBV	232590	532851	14.54%	3.481%
15	17.791	2455	2460	2477	rVB2	182445	356427	9.72%	2.329%
16	18.138	2515	2519	2523	rBV7	28558	39708	1.08%	0.259%
17	18.772	2623	2627	2636	rVB7	17421	38281	1.04%	0.250%
18	19.101	2676	2683	2690	rBV	82179	136580	3.73%	0.892%
19	19.842	2804	2809	2816	rVB5	38235	82105	2.24%	0.536%
20	20.082	2844	2850	2856	rBV	2839601	3665858	100.00%	23.949%
21	20.688	2948	2953	2961	rVB3	51450	100095	2.73%	0.654%
22	20.846	2977	2980	2986	rBV5	50886	71346	1.95%	0.466%
23	21.334	3057	3063	3066	rBV4	28923	65416	1.78%	0.427%
24	21.375	3066	3070	3072	rBV4	47615	68243	1.86%	0.446%
25	21.469	3082	3086	3091	rVB	111132	158518	4.32%	1.036%
26	21.534	3093	3097	3104	rVB4	51760	103782	2.83%	0.678%
27	21.763	3130	3136	3144	rVB2	463235	779795	21.27%	5.094%
28	23.666	3455	3460	3469	rVB5	33436	85832	2.34%	0.561%
29	25.059	3686	3697	3708	rVB2	286681	901822	24.60%	5.892%

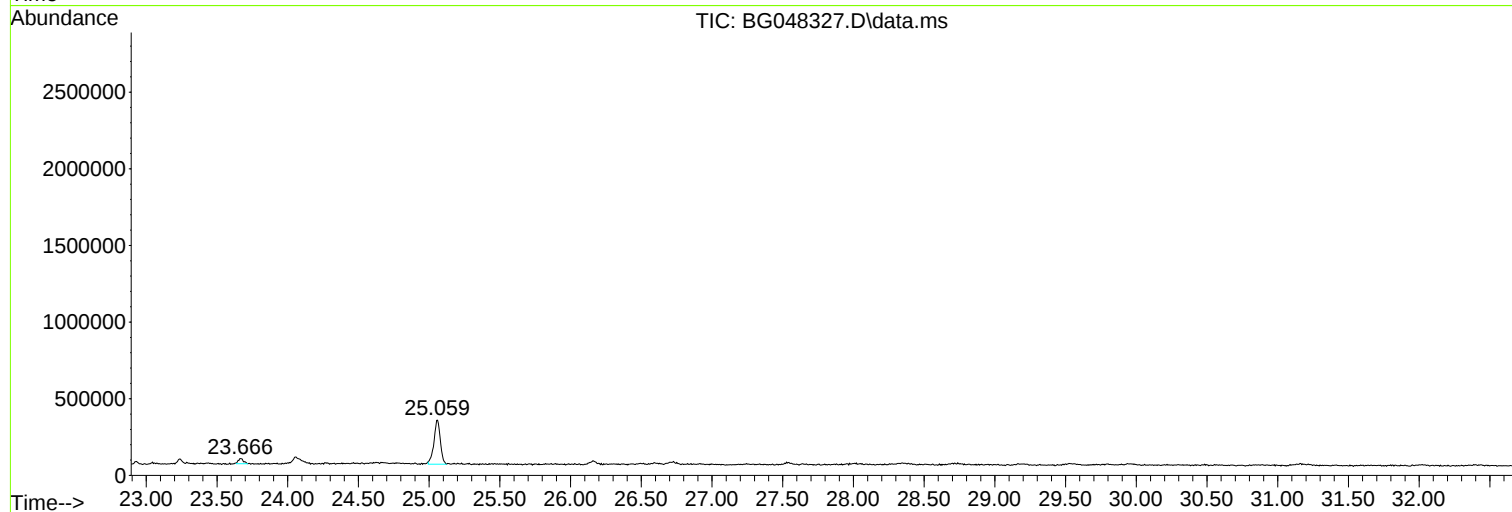
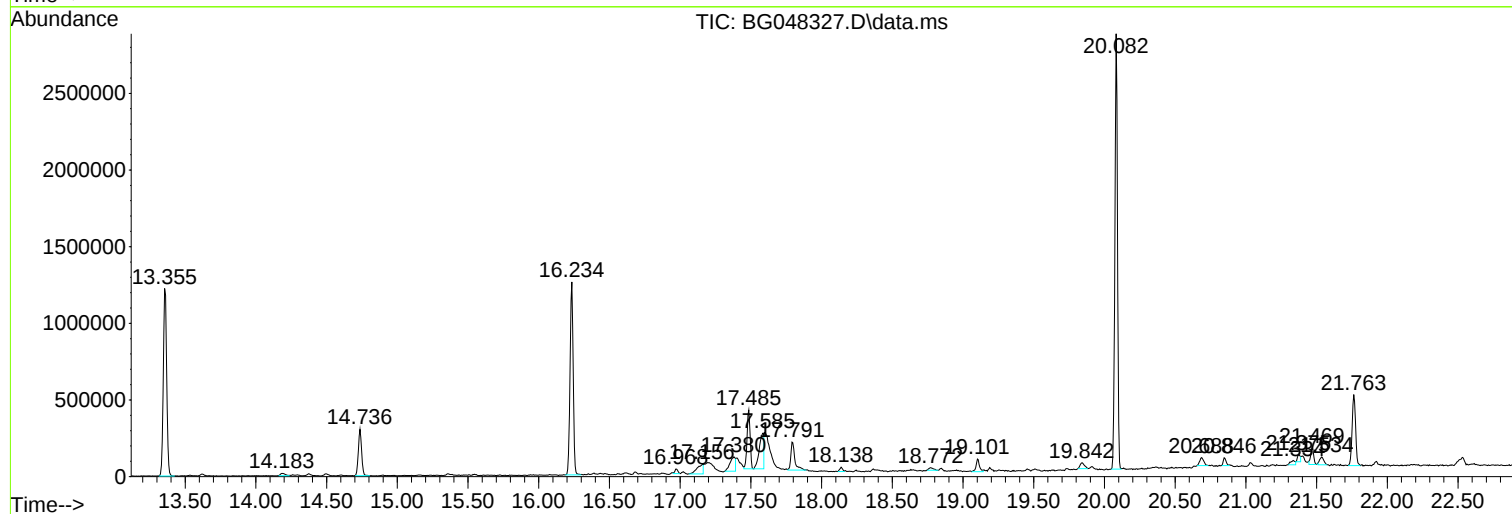
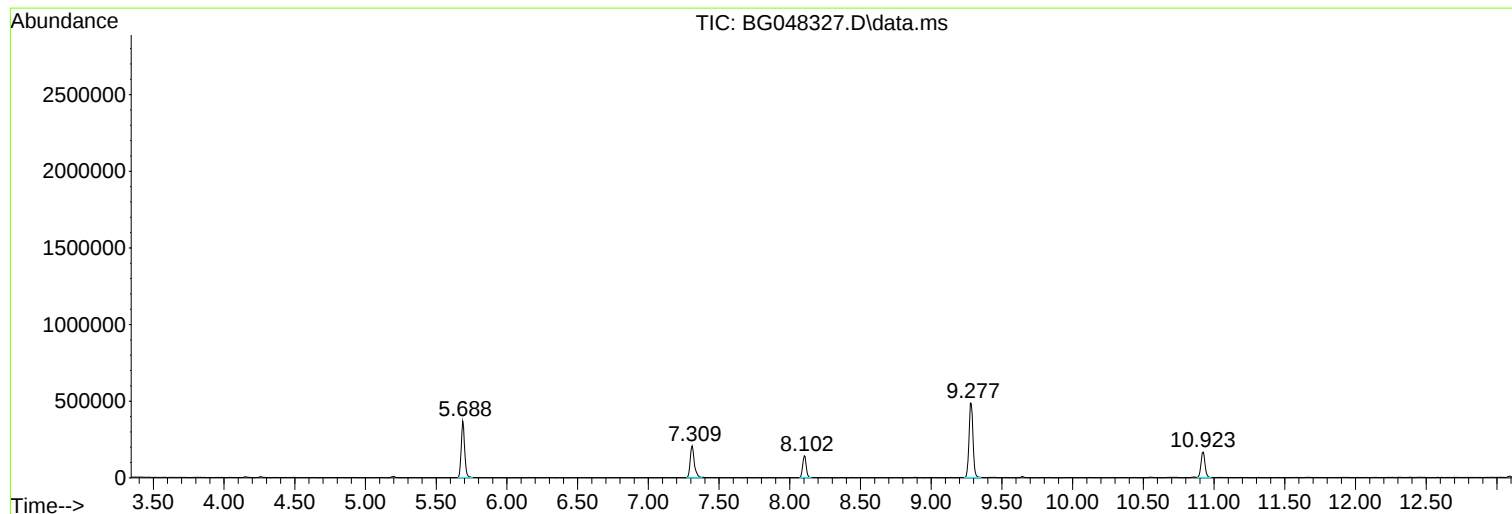
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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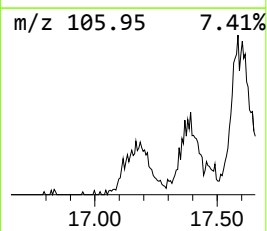
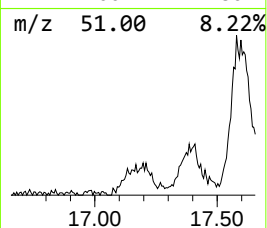
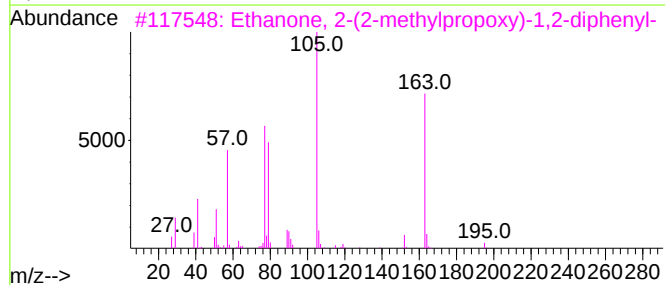
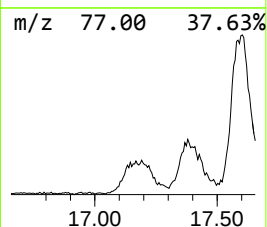
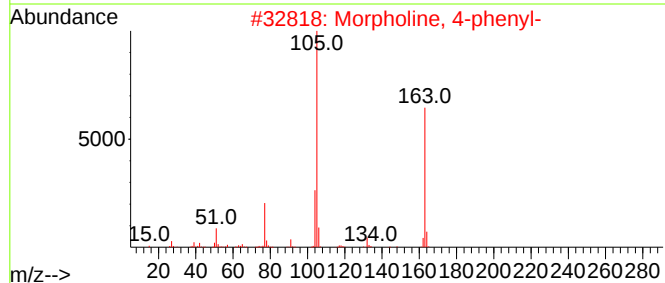
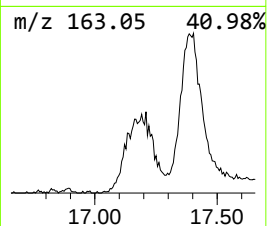
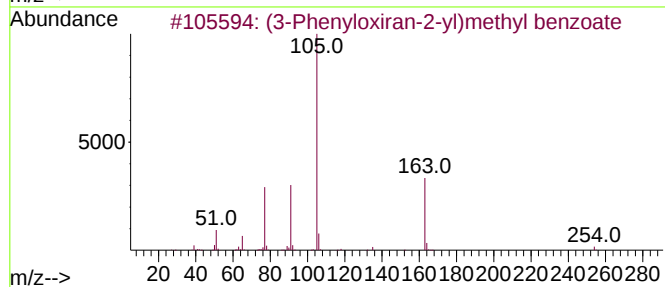
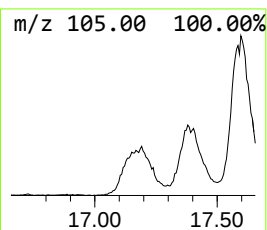
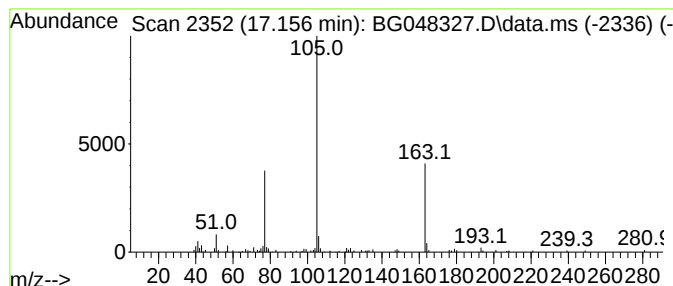
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TIC Library : C:\Database\NIST11.L
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Peak Number 1 (3-Phenyloxiran-2-yl)methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.156	6.62 ng	191150	Phenanthrene-d10	17.485

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	56
2		Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	50
3		Ethanone, 2-(2-methylpropoxy)-1,...	268	C18H20O2	022499-12-3	45
4		Benzamide, N-propyl-	163	C10H13NO	010546-70-0	45
5		1,3-Dibenzoyl-4-benzylidene-5-ox...	412	C24H16N2O3S	083800-62-8	35



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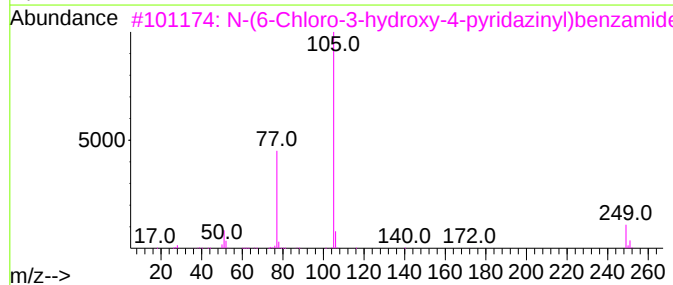
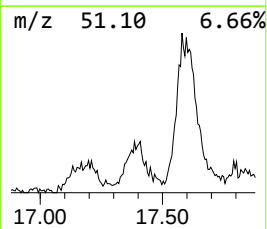
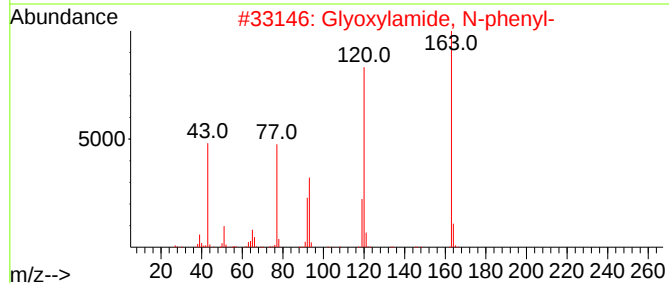
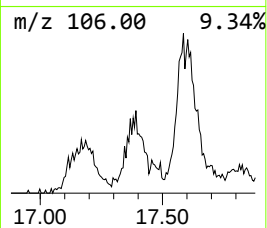
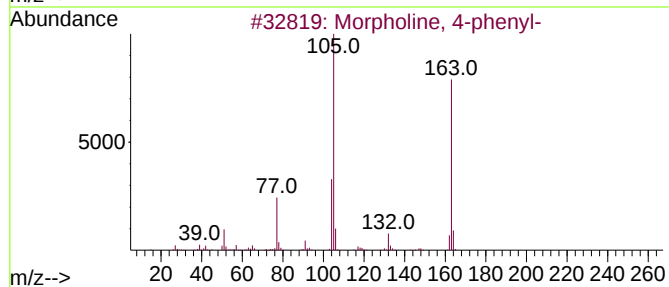
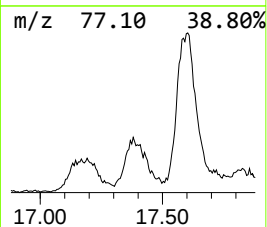
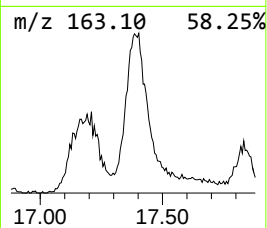
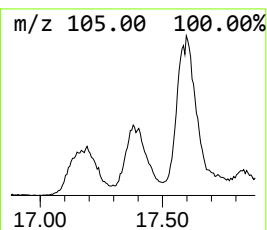
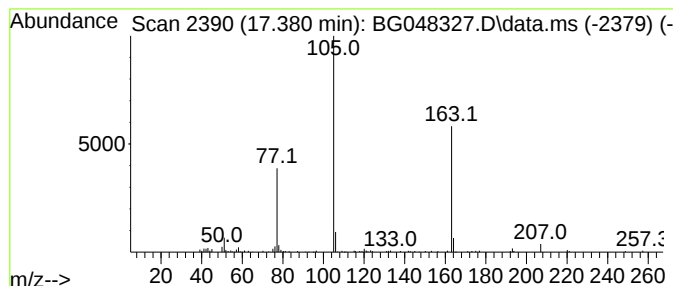
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Peak Number 2 Morpholine, 4-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.380	8.68 ng	250850	Phenanthrene-d10	17.485

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
3			N-(6-Chloro-3-hydroxy-4-pyridazi...	249	C11H8ClN3O2	117892-39-4	43
4			Hippuric-benzaldehyde azalactone	249	C16H11NO2	000842-74-0	43
5			Methanone, (4-bromo-5-methyl-2-n...	357	C12H8BrN03S2	1000274-00-2	38



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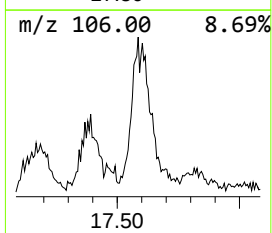
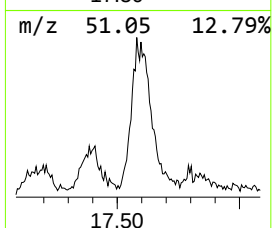
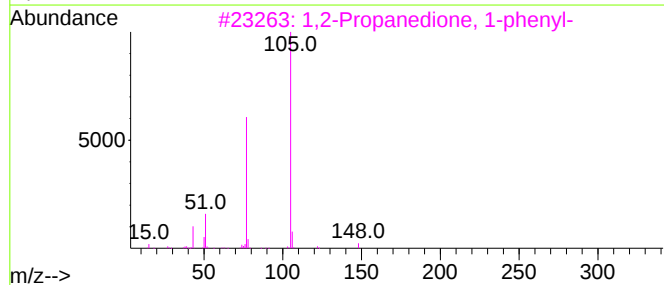
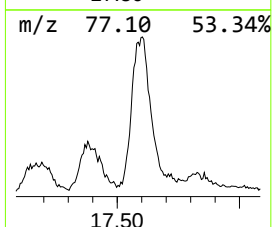
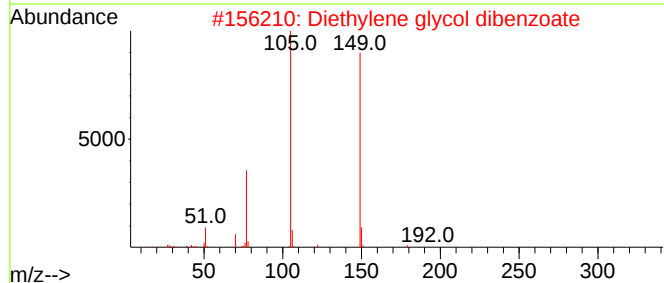
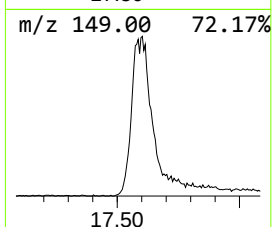
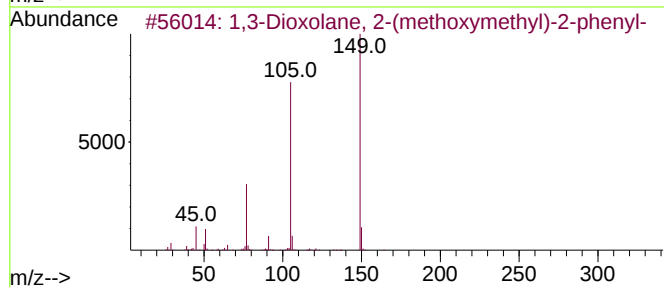
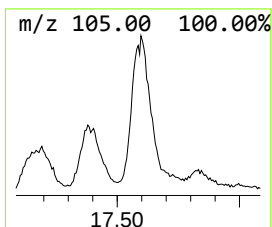
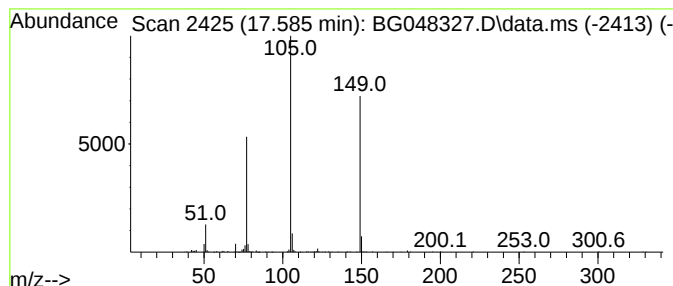
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Peak Number 3 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.585	18.44 ng	532851	Phenanthrene-d10	17.485	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	78
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	50
3	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
4	4,5-Bis(benzoylthio)-1,2-dithiol...	406	C17H10O2S5	082504-65-2	47
5	Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	47



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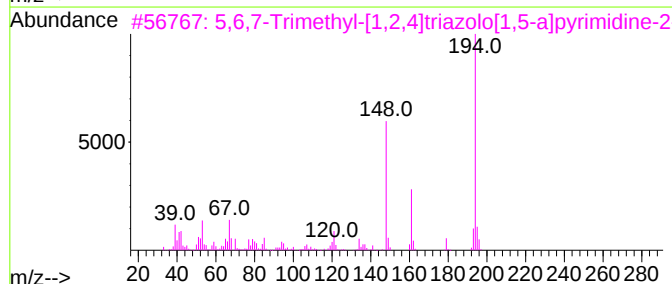
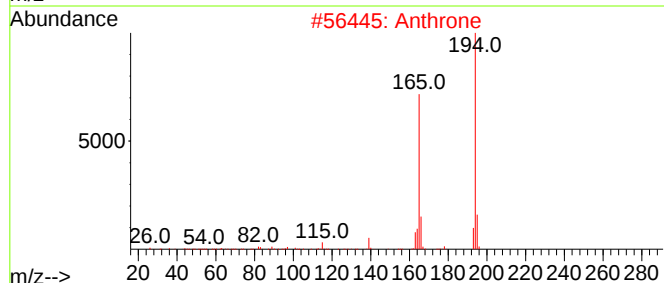
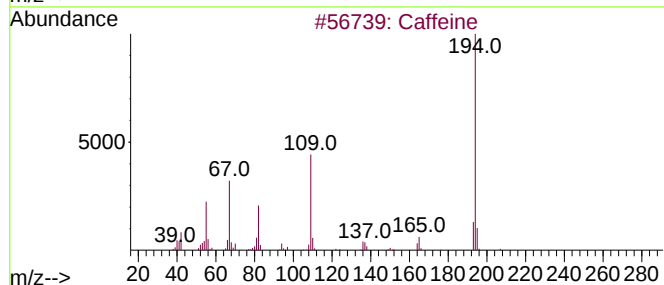
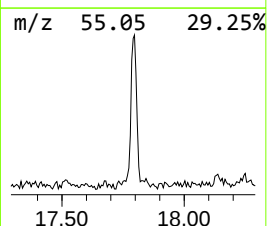
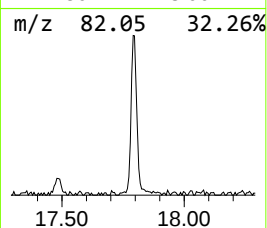
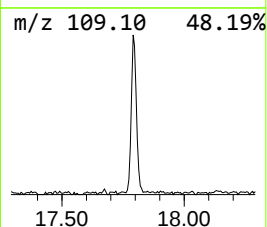
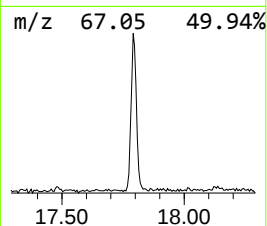
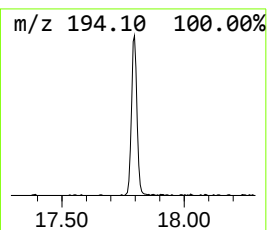
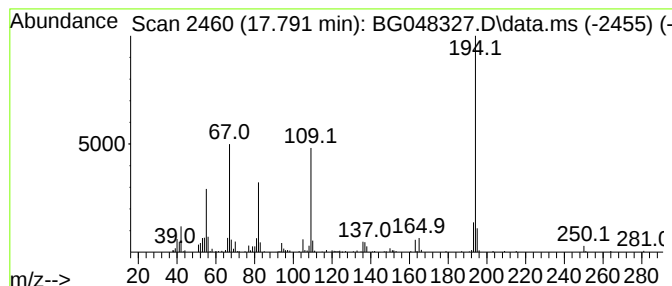
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Peak Number 4 Caffeine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.791	12.34 ng	356427	Phenanthrene-d10	17.485

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caffeine	194	C8H10N4O2	000058-08-2	95
2			Anthrone	194	C14H10O	000090-44-8	35
3			5,6,7-Trimethyl-[1,2,4]triazolo[...]	194	C8H10N4S	1000300-21-6	35
4			6-Amino-1,3-dimethyl-1,6-dihydro...	194	C8H10N4O2	1000301-21-5	32
5			Benzenamine, N,N'-methanetetrayl...	194	C13H10N2	000622-16-2	27



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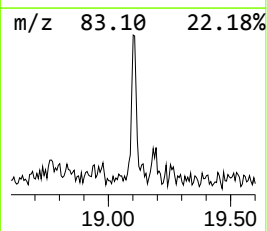
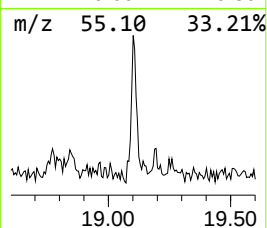
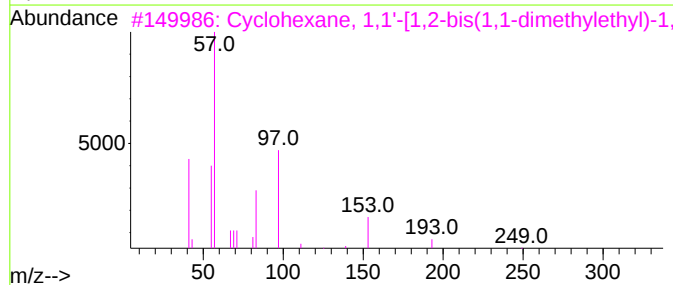
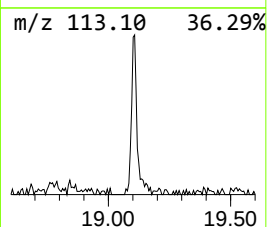
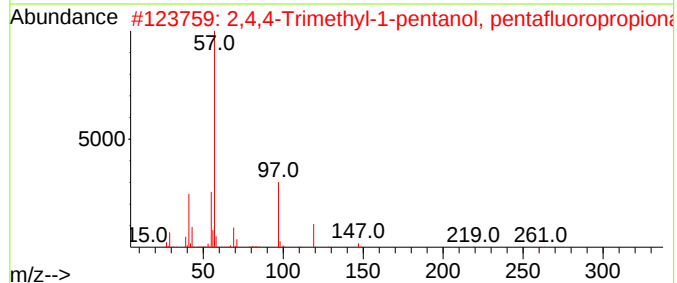
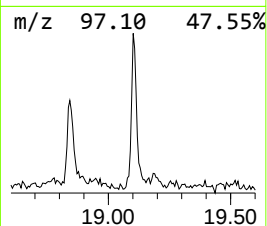
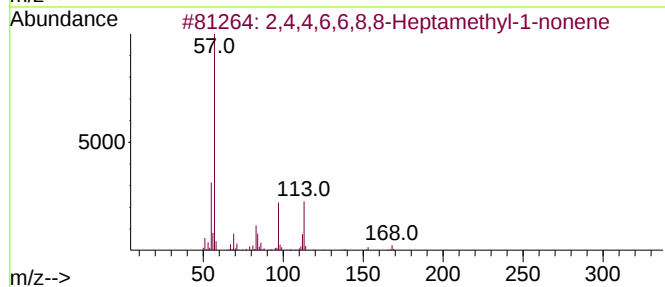
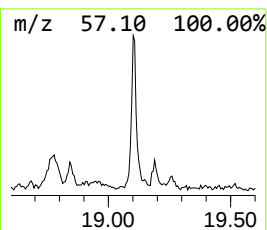
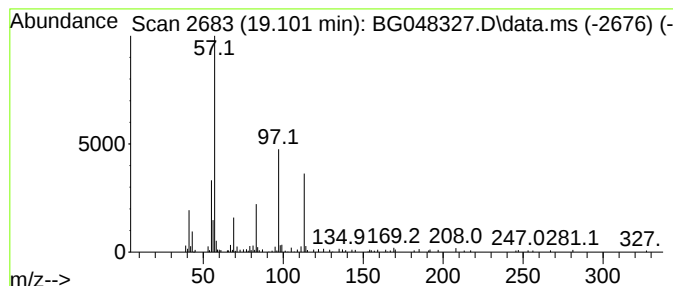
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Peak Number 5 unknown19.10 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.101	4.73 ng	136580	Phenanthrene-d10	17.485

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	43		
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	38		
3	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	33		
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	32		
5	Pentane, 2,2,4-trimethyl-4-nitro-	159	C8H17NO2	005342-78-9	32		



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ALS Vial : 6 Sample Multiplier: 1

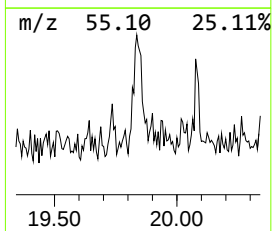
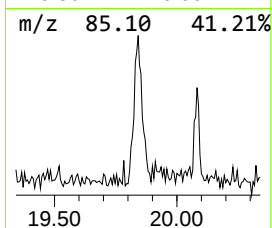
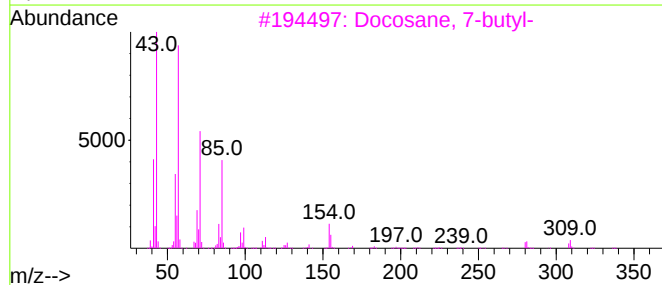
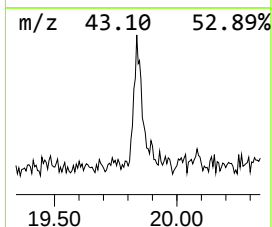
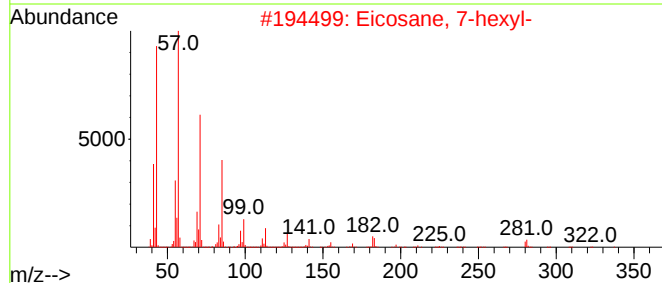
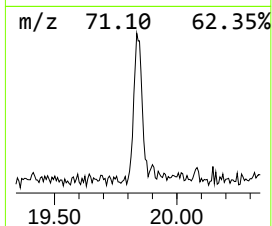
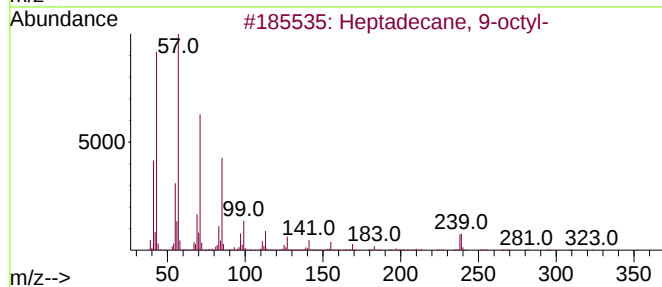
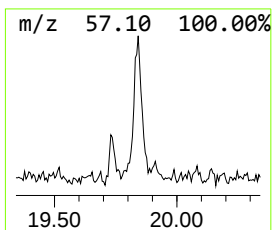
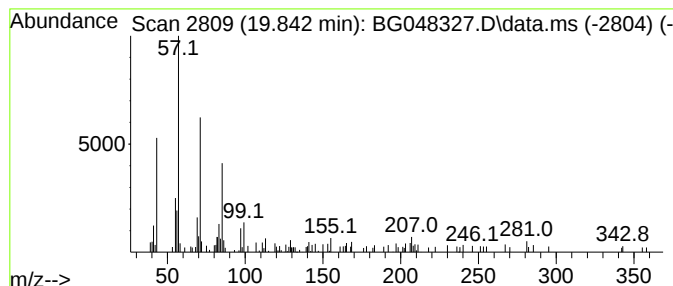
Instrument :
BNA_G
ClientSampleId :
MH-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.842	2.11 ng	82105	Chrysene-d12		21.763	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	86
2	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	86
3	Docosane, 7-butyl-		366	C26H54	055282-15-0	86
4	Eicosane		282	C20H42	000112-95-8	86
5	Heptadecane		240	C17H36	000629-78-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048327.D
Acq On : 4 Mar 2021 14:01
Operator : CG/JU
Sample : M1545-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-5

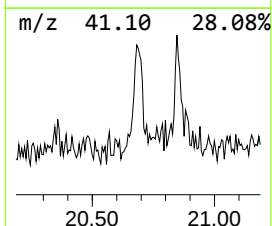
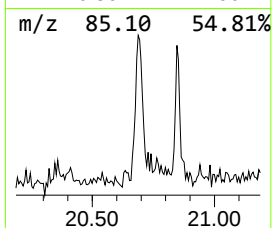
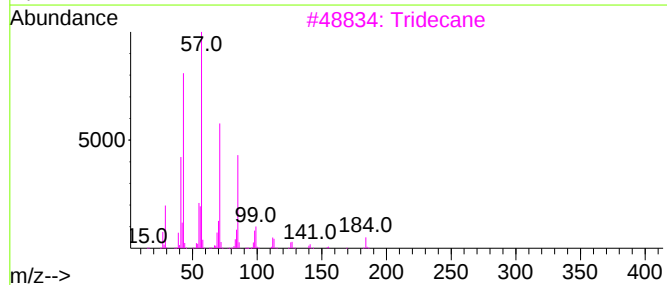
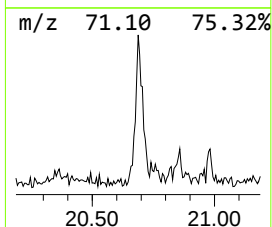
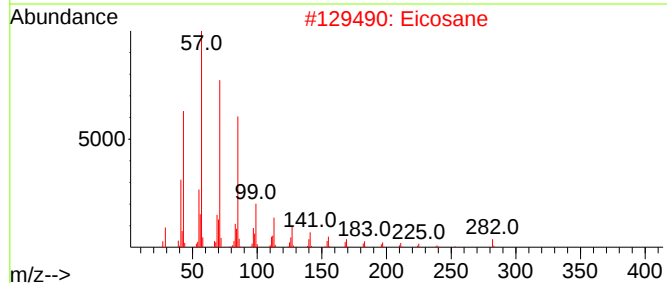
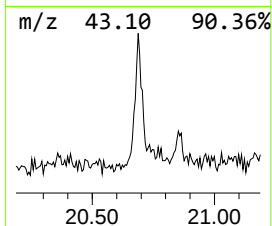
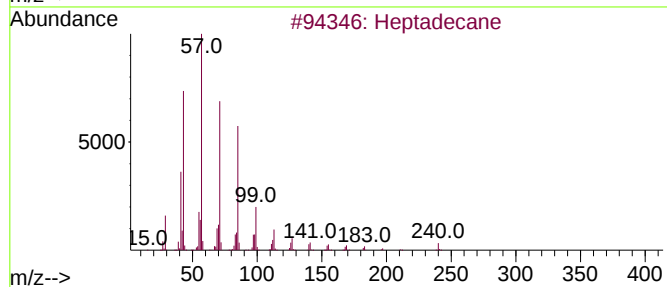
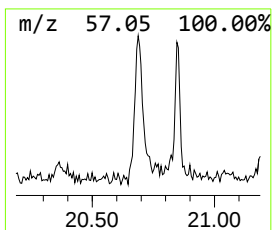
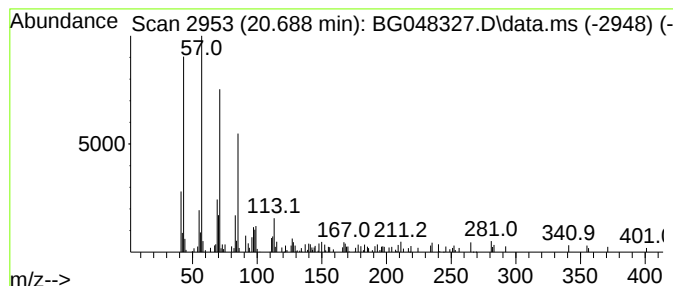
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.688	2.57 ng	100095	Chrysene-d12	21.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	80
2		Eicosane	282	C20H42	000112-95-8	74
3		Tridecane	184	C13H28	000629-50-5	72
4		Octacosane	394	C28H58	000630-02-4	72
5		Nonadecane	268	C19H40	000629-92-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048327.D
Acq On : 4 Mar 2021 14:01
Operator : CG/JU
Sample : M1545-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

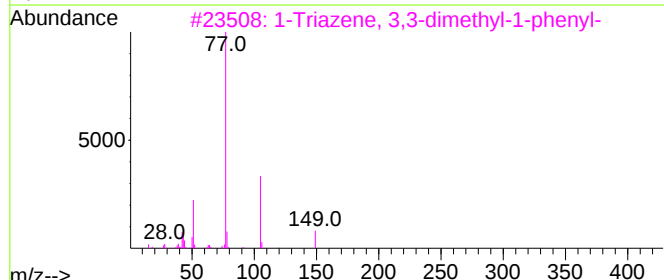
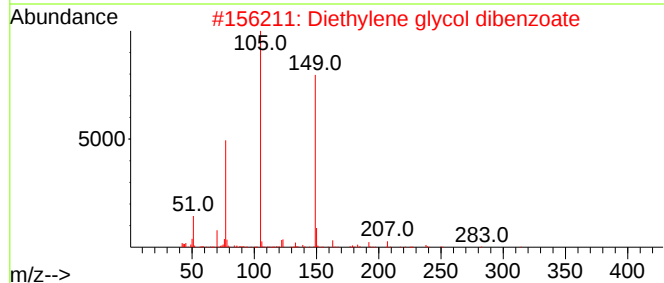
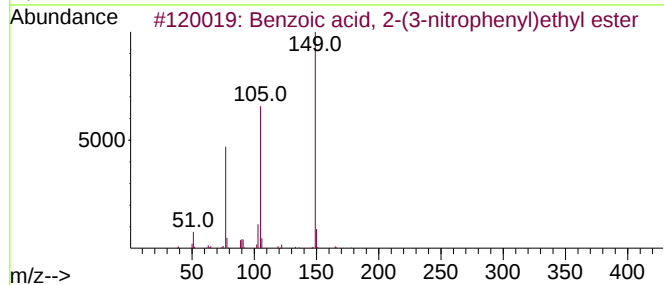
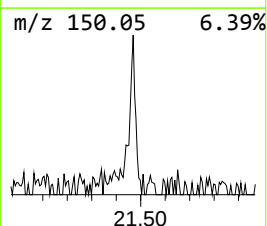
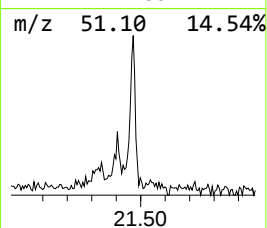
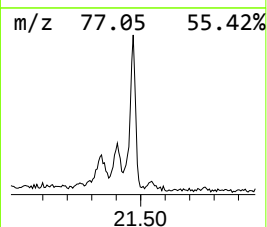
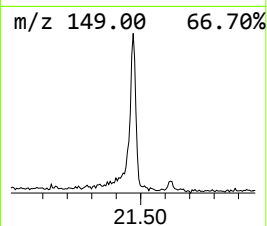
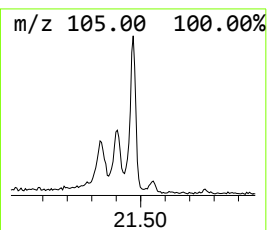
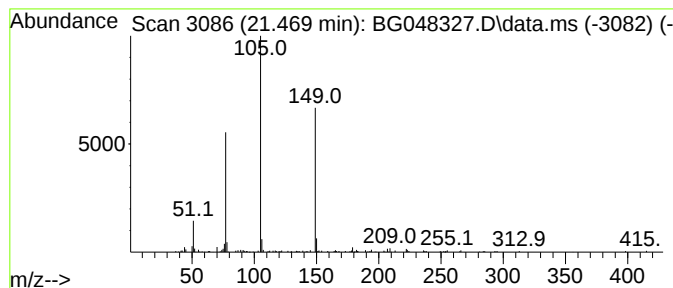
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzoic acid, 2-(3-nitrophe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.469	4.07 ng	158518	Chrysene-d12	21.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
3	1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	64
4	2(3H)-Furanone, 3-[(4-nitropheny...	293	C17H11NO4	054833-77-1	49
5	1,2,5-Benzothiadiazol, 4-benzamido-	255	C13H9N3OS	339302-44-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048327.D
Acq On : 4 Mar 2021 14:01
Operator : CG/JU
Sample : M1545-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-5

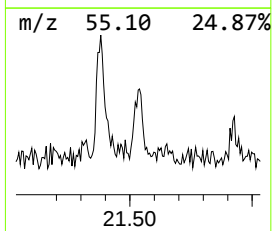
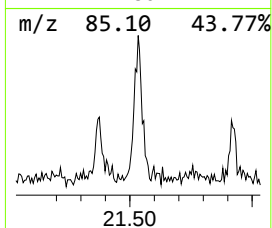
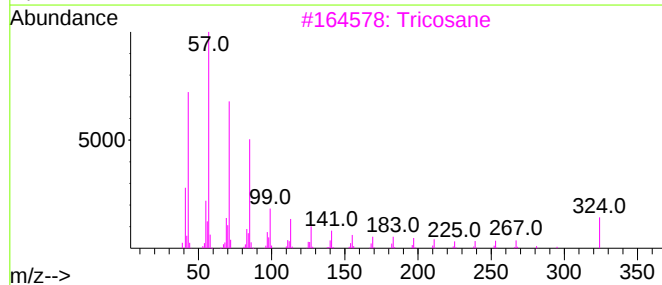
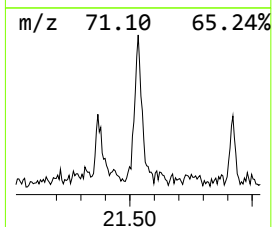
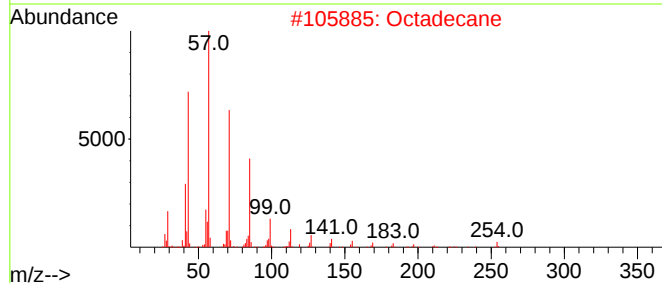
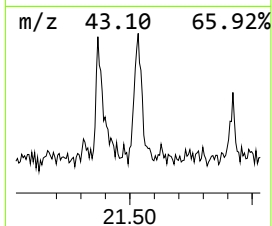
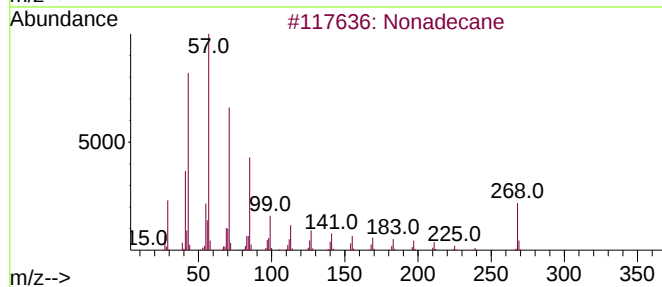
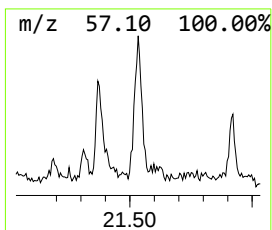
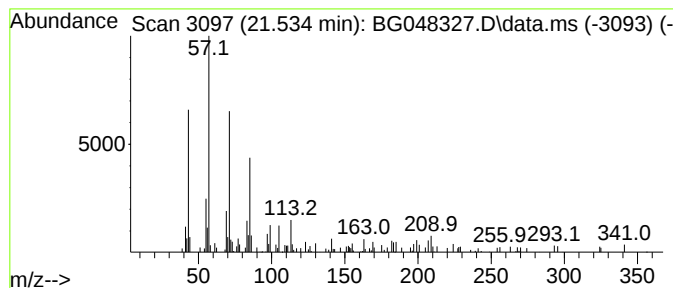
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.534	2.66 ng	103782	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	94
2			Octadecane	254	C18H38	000593-45-3	91
3			Tricosane	324	C23H48	000638-67-5	87
4			Docosane	310	C22H46	000629-97-0	83
5			Heneicosane	296	C21H44	000629-94-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048327.D
Acq On : 4 Mar 2021 14:01
Operator : CG/JU
Sample : M1545-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(3-Phenyloxiran...	17.156	6.6	ng	191150	4	17.485	577879	20.0
Morpholine, 4-p...	17.380	8.7	ng	250850	4	17.485	577879	20.0
1,3-Dioxolane, ...	17.585	18.4	ng	532851	4	17.485	577879	20.0
Caffeine	17.791	12.3	ng	356427	4	17.485	577879	20.0
unknown19.10	19.101	4.7	ng	136580	4	17.485	577879	20.0
Heptadecane, 9-...	19.842	2.1	ng	82105	5	21.763	779795	20.0
Heptadecane	20.688	2.6	ng	100095	5	21.763	779795	20.0
Benzoic acid, 2...	21.469	4.1	ng	158518	5	21.763	779795	20.0
Nonadecane	21.534	2.7	ng	103782	5	21.763	779795	20.0