

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
 Data File : BG057473.D
 Acq On : 19 May 2023 18:52
 Operator : CG/JU
 Sample : 02845-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP2

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-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057473.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.383	308	314	320	rBV	14934	23300	2.56%	0.471%
2	5.870	391	397	409	rBB	201178	328706	36.15%	6.649%
3	7.497	665	674	684	rBV	213891	373971	41.13%	7.565%
4	8.355	814	820	827	rBB	61243	102495	11.27%	2.073%
5	9.530	1012	1020	1032	rBB	122165	226754	24.94%	4.587%
6	11.192	1295	1303	1312	rVB	79211	141739	15.59%	2.867%
7	13.595	1705	1712	1720	rVB	381245	579223	63.70%	11.717%
8	14.282	1824	1829	1834	rBV2	42837	59717	6.57%	1.208%
9	14.911	1931	1936	1940	rBV2	17417	23020	2.53%	0.466%
10	14.970	1940	1946	1951	rBV	143479	218633	24.04%	4.423%
11	15.193	1979	1984	1989	rVB2	8898	12171	1.34%	0.246%
12	16.303	2165	2173	2181	rVB	47978	75640	8.32%	1.530%
13	16.415	2185	2192	2193	rBV2	13909	20831	2.29%	0.421%
14	16.450	2193	2198	2205	rVB	314825	472289	51.94%	9.554%
15	17.707	2406	2412	2418	rBV	190195	290522	31.95%	5.877%
16	18.547	2551	2555	2563	rBV	41886	68327	7.51%	1.382%
17	19.804	2765	2769	2776	rBV8	11460	27860	3.06%	0.564%
18	20.274	2844	2849	2855	rBV	722213	909316	100.00%	18.394%
19	20.427	2871	2875	2879	rVB2	8774	10551	1.16%	0.213%
20	21.038	2976	2979	2985	rBV5	5683	9825	1.08%	0.199%
21	21.408	3037	3042	3048	rVB	75302	102608	11.28%	2.076%
22	21.578	3066	3071	3080	rBV4	18796	47274	5.20%	0.956%
23	22.013	3139	3145	3152	rBV2	192077	317336	34.90%	6.419%
24	22.794	3272	3278	3283	rBV5	8452	15188	1.67%	0.307%
25	23.529	3400	3403	3412	rVB4	8456	16814	1.85%	0.340%
26	24.398	3545	3551	3558	rVB4	15055	31969	3.52%	0.647%
27	25.426	3718	3726	3729	rBV6	12691	29603	3.26%	0.599%
28	25.502	3731	3739	3754	rVB2	109542	319286	35.11%	6.459%
29	26.648	3924	3934	3943	rVB4	16312	48262	5.31%	0.976%
30	28.111	4171	4183	4192	rBV7	10534	40359	4.44%	0.816%

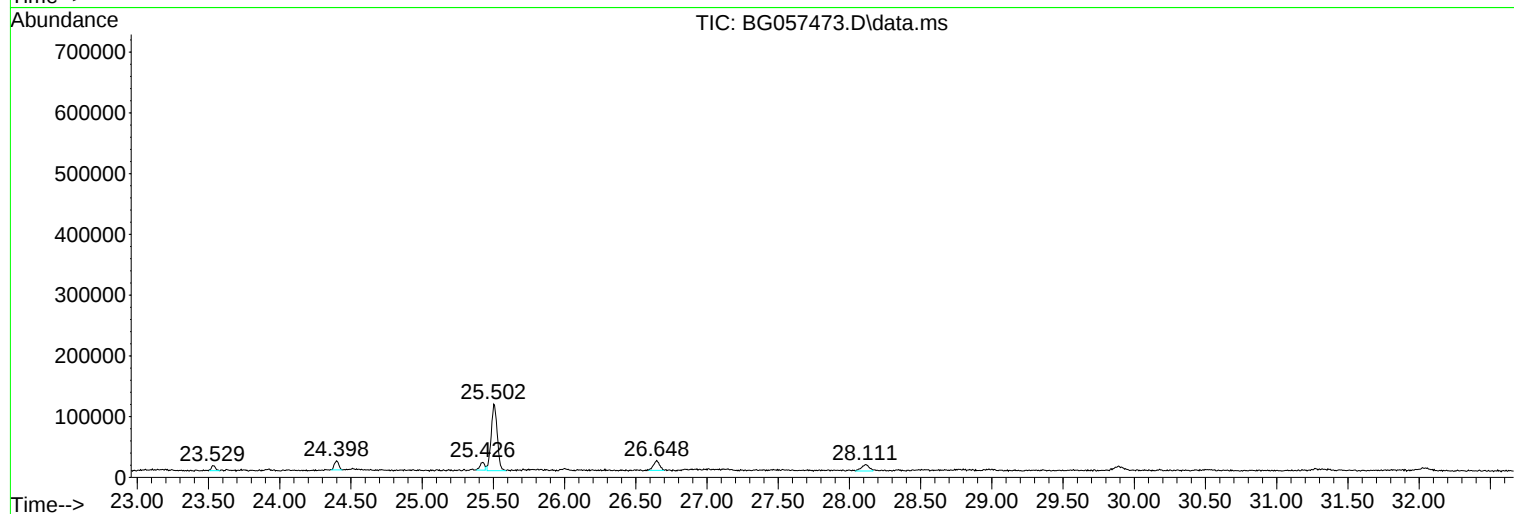
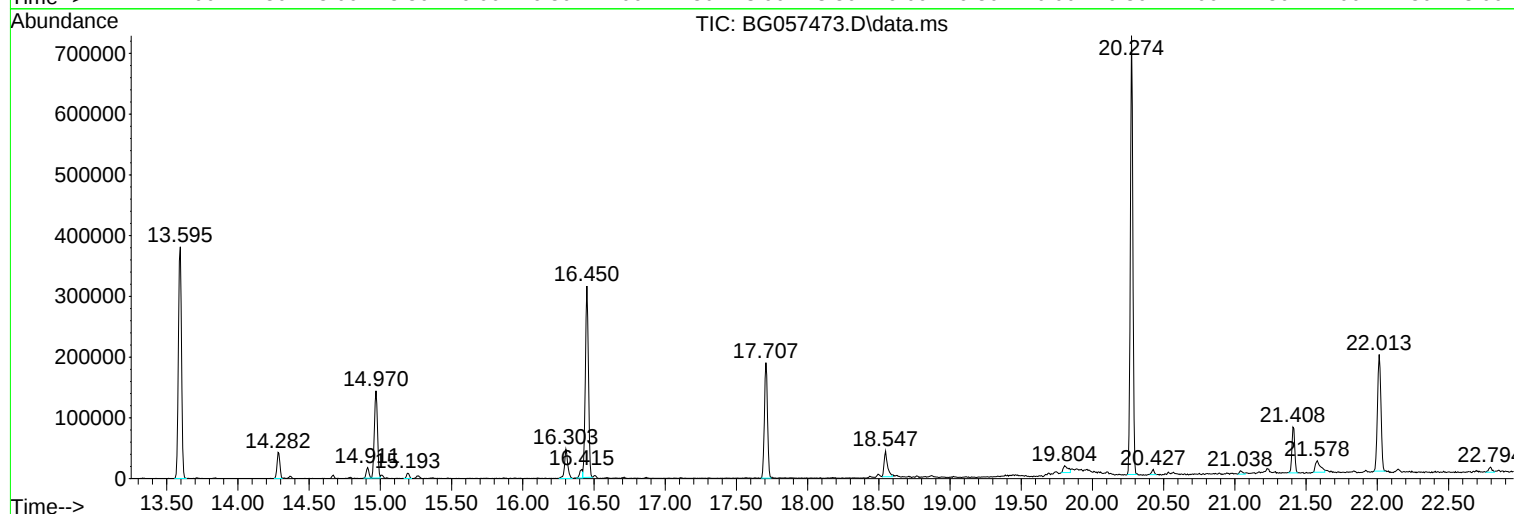
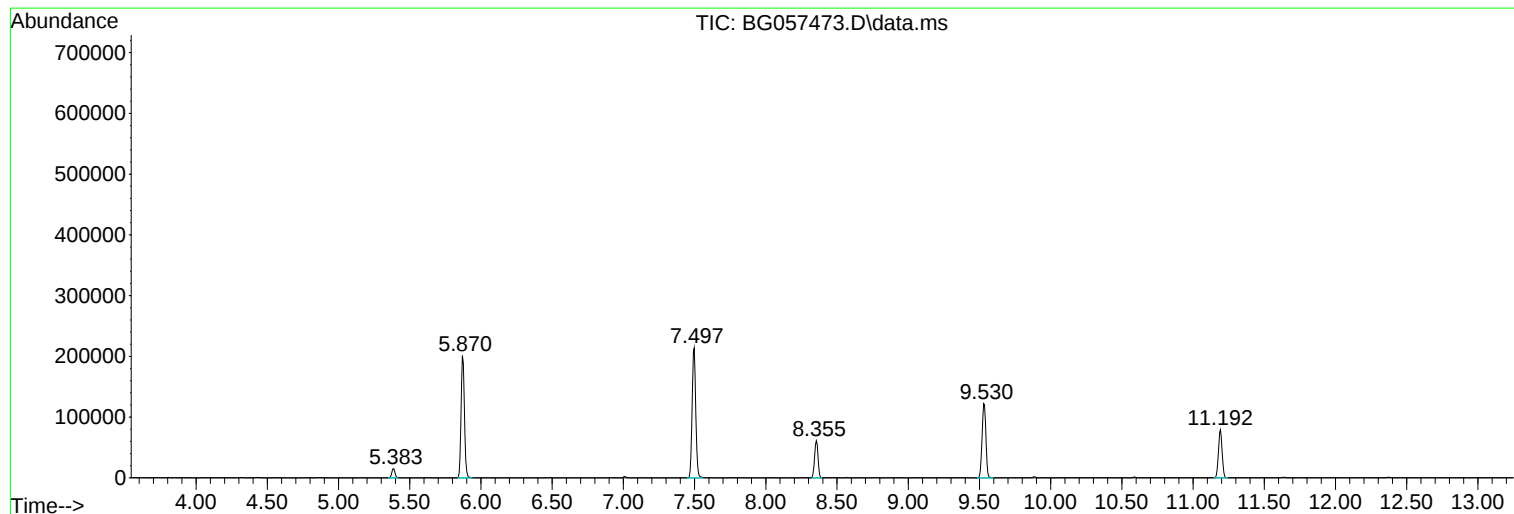
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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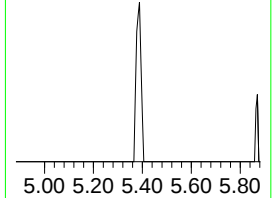
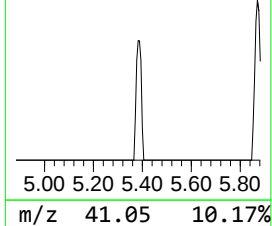
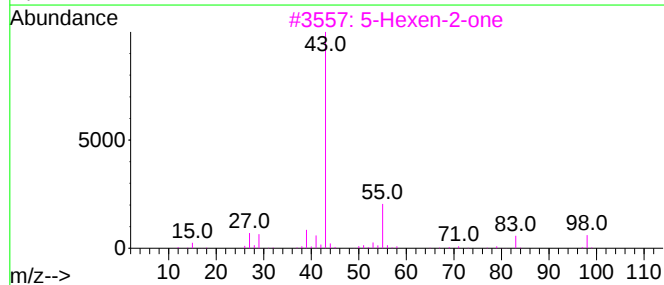
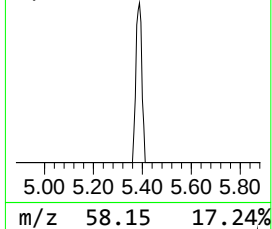
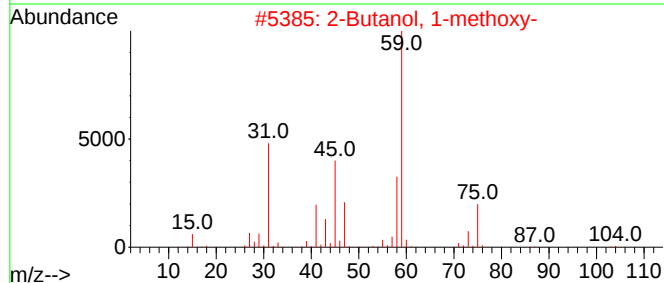
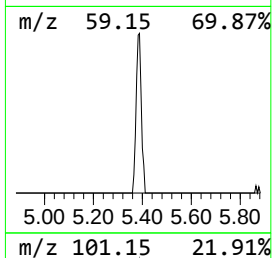
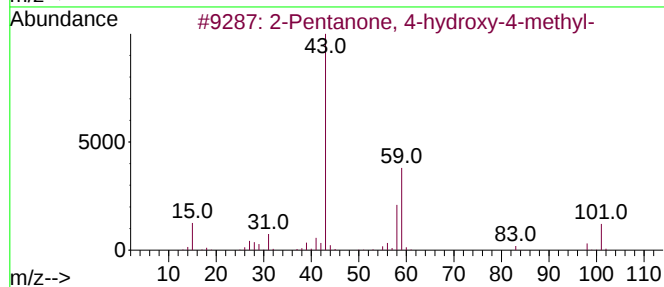
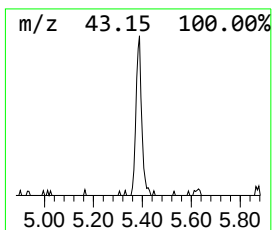
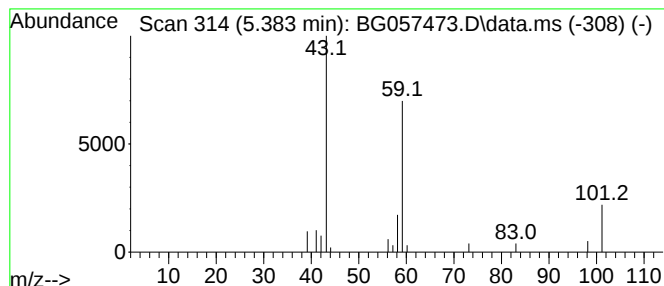
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.383	4.55 ng	23300	1,4-Dichlorobenzene-d4	8.355

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	23	
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9	
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9	



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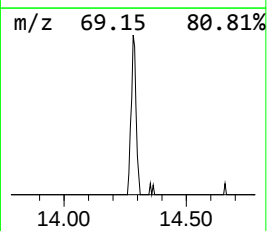
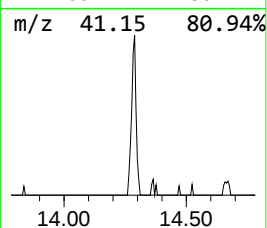
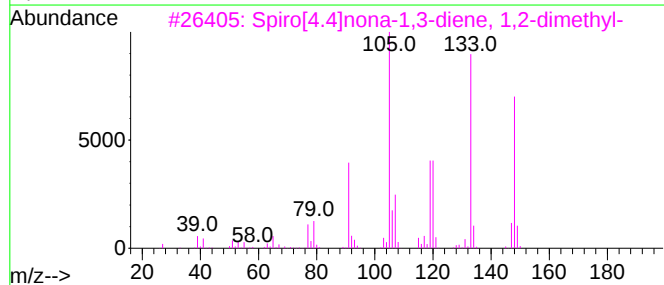
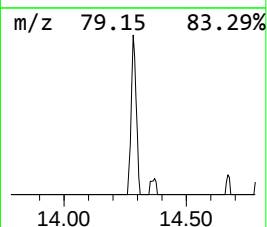
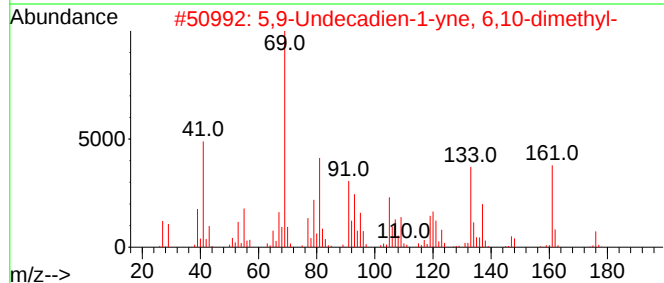
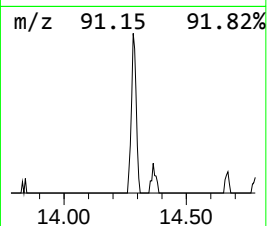
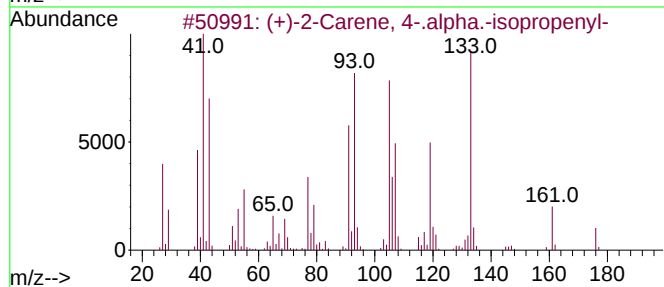
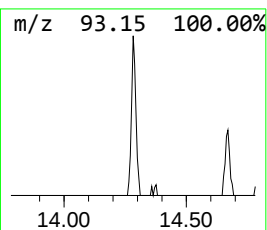
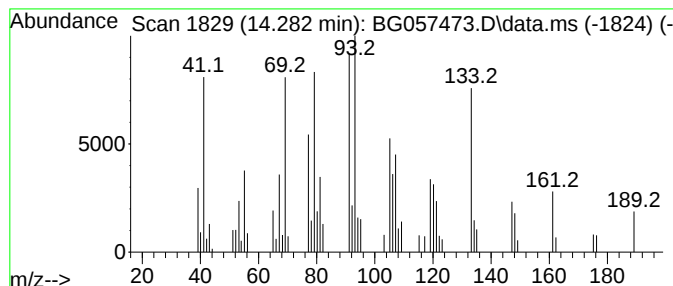
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Peak Number 2 unknown14.282 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.282	5.46 ng	59717	Acenaphthene-d10	14.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Carene, 4-.alpha.-isopropenyl-	176	C13H20	1000151-26-0	38		
2	5,9-Undecadien-1-yne, 6,10-dimethyl-	176	C13H20	100451-98-7	25		
3	Spiro[4.4]nona-1,3-diene, 1,2-dimethyl-	148	C11H16	1000163-57-6	18		
4	Bicyclo[2.2.1]heptane, 2-cyclopropyl-	176	C13H20	1000159-45-7	18		
5	1,7-Octadiene, 2,7-dimethyl-3,6-diene	162	C12H18	016714-60-6	11		



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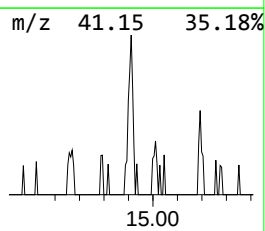
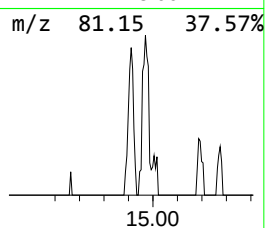
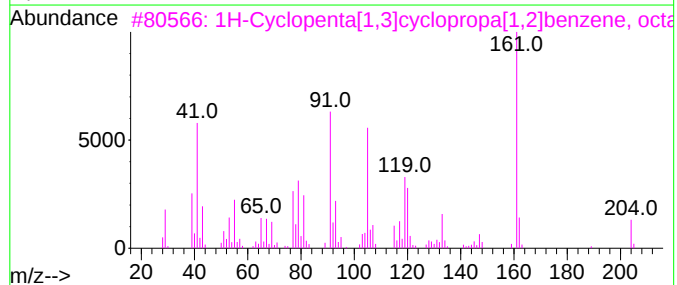
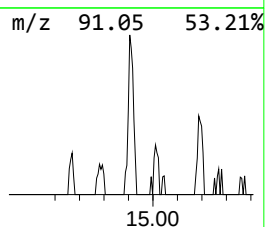
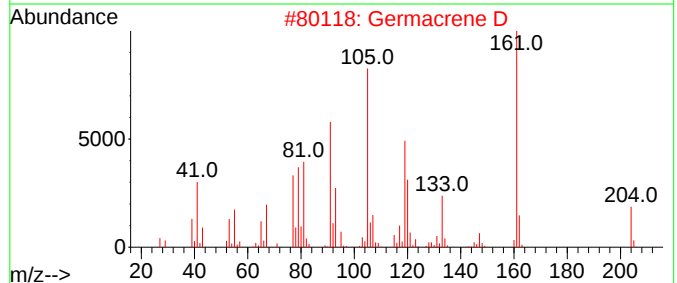
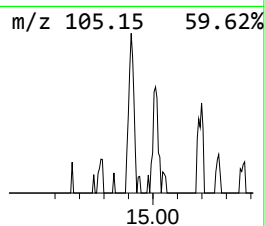
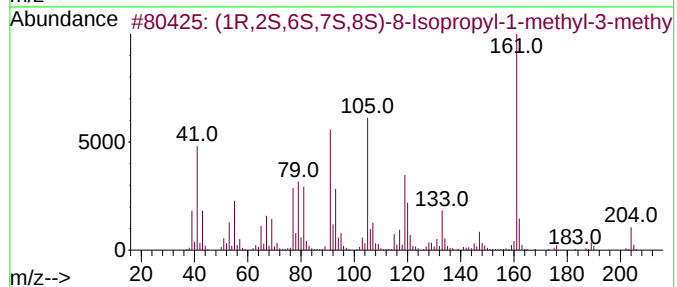
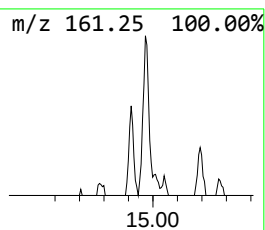
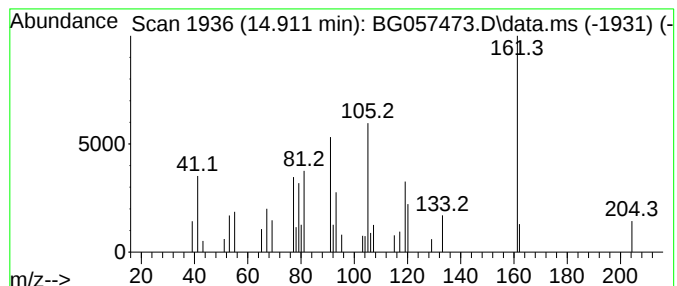
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Peak Number 3 (1R,2S,6S,7S,8S)-8-Isopropy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.911	2.11 ng	23020	Acenaphthene-d10	14.970

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	97
2		Germacrene D	204	C15H24	023986-74-5	96
3		1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	94
4		(+)-epi-Bicyclosesquiphellandrene	204	C15H24	054274-73-6	87
5		cis-Muurolo-4(15),5-diene	204	C15H24	157477-72-0	87



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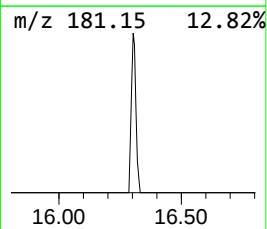
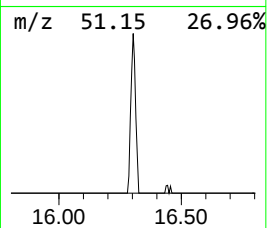
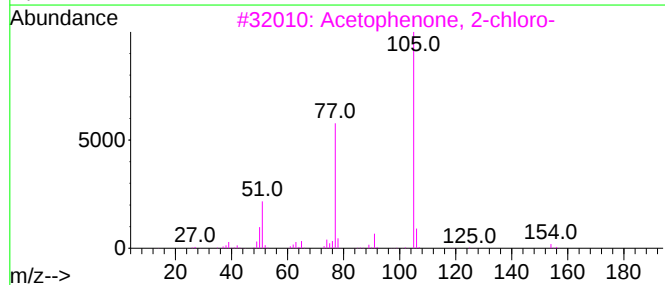
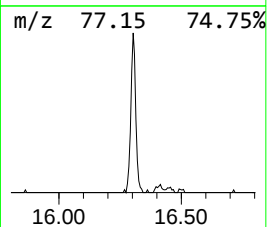
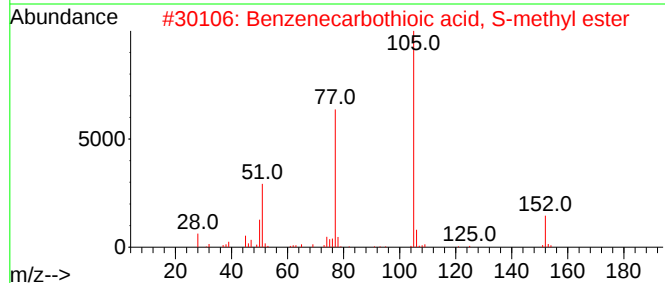
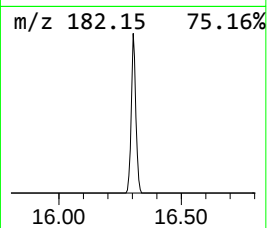
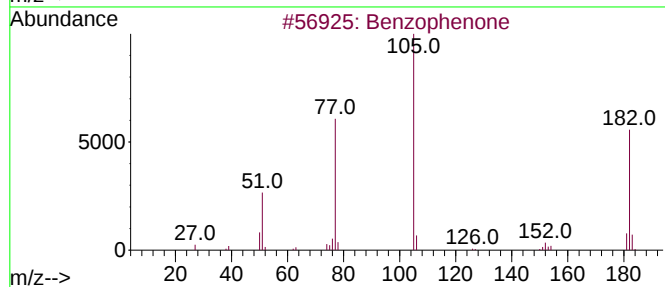
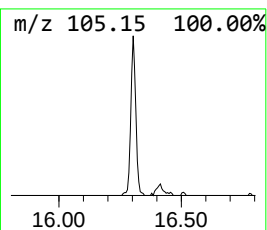
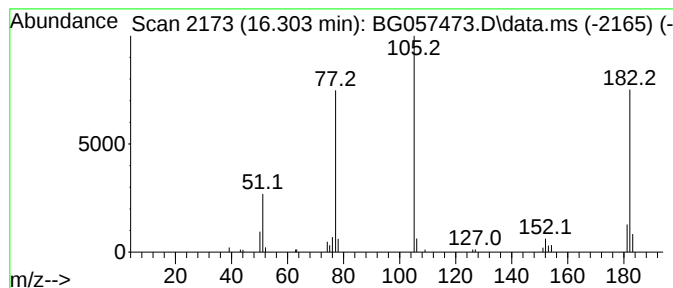
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Peak Number 4 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.303	6.92 ng	75640	Acenaphthene-d10	14.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
5			.beta.-Benzilmonoxime	225	C14H11NO2	014090-77-8	43



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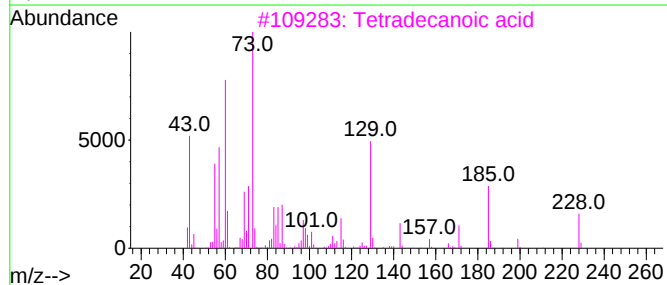
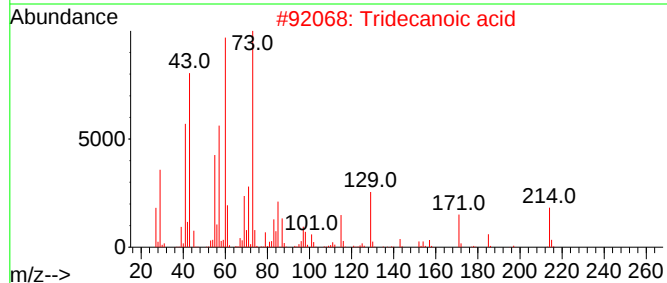
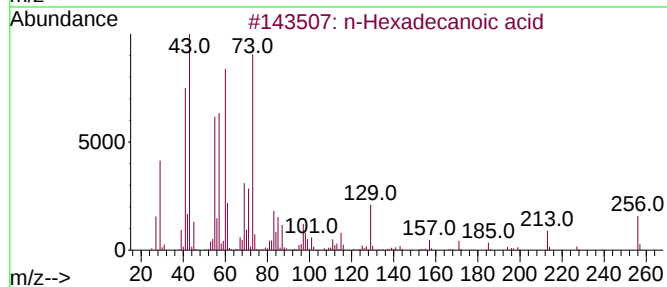
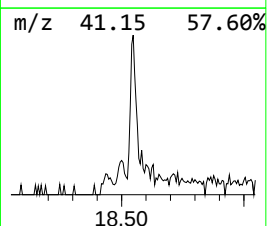
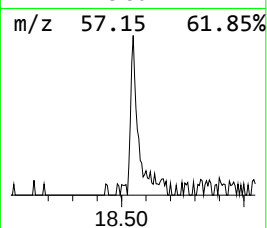
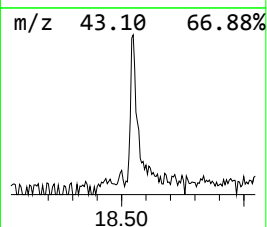
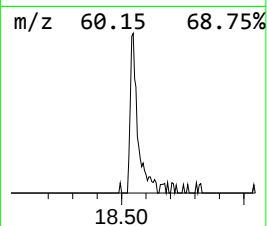
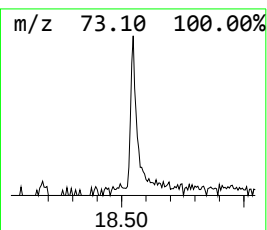
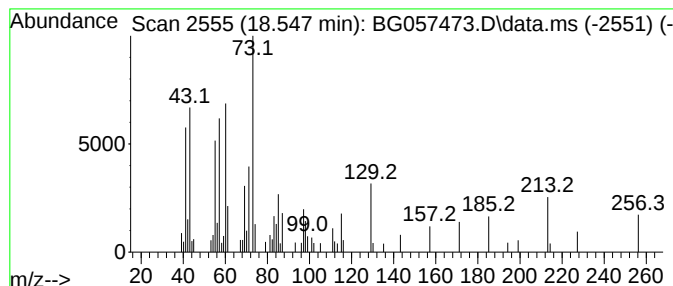
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.547	4.70 ng	68327	Phenanthrene-d10	17.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5			Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	30



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TP2

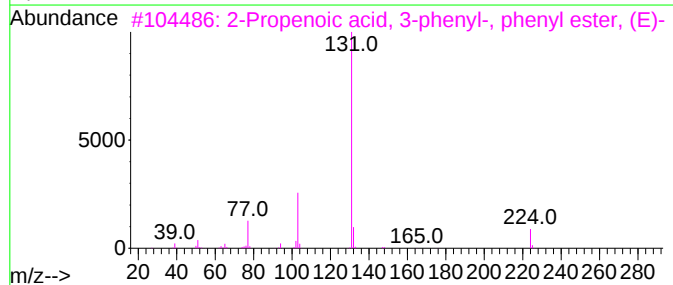
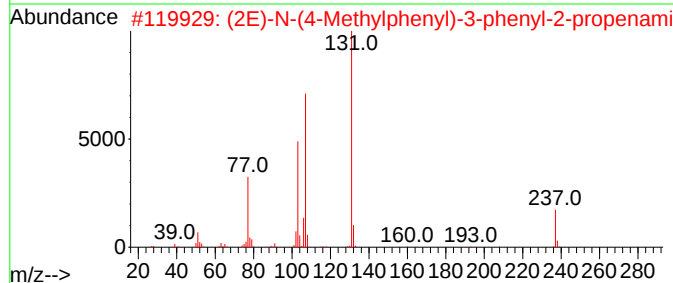
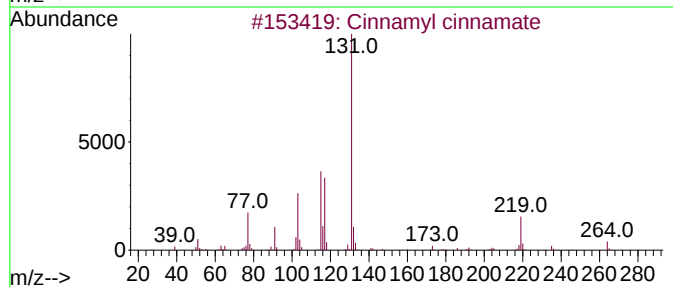
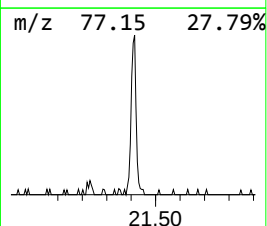
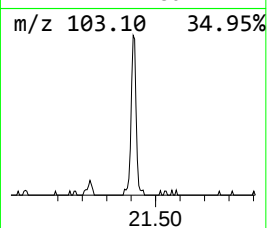
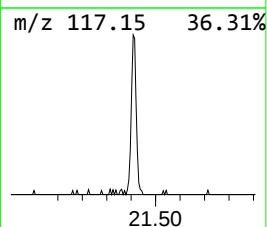
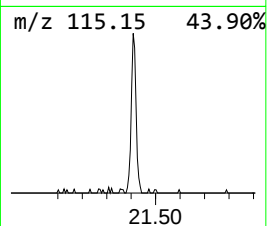
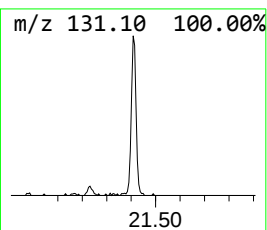
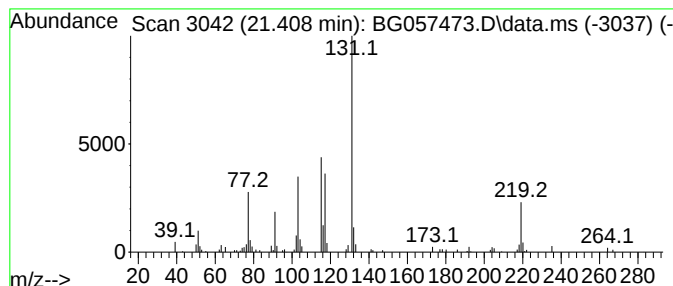
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.408	6.47 ng	102608	Chrysene-d12	22.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			(2E)-N-(4-Methylphenyl)-3-phenyl...	237	C16H15NO	134430-88-9	46
3			2-Propenoic acid, 3-phenyl-, phe...	224	C15H12O2	025695-77-6	43
4			1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	43
5			trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057473.D
Acq On : 19 May 2023 18:52
Operator : CG/JU
Sample : 02845-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

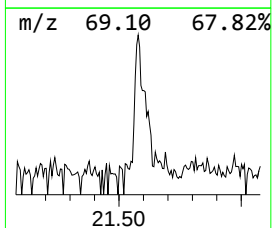
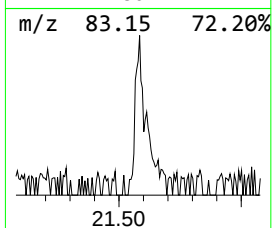
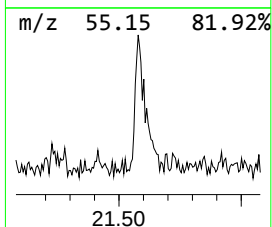
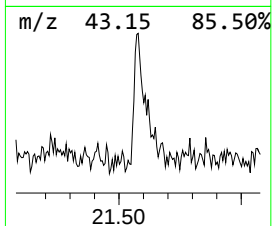
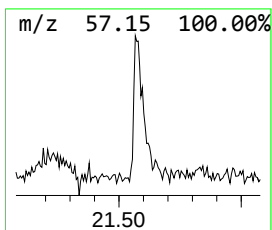
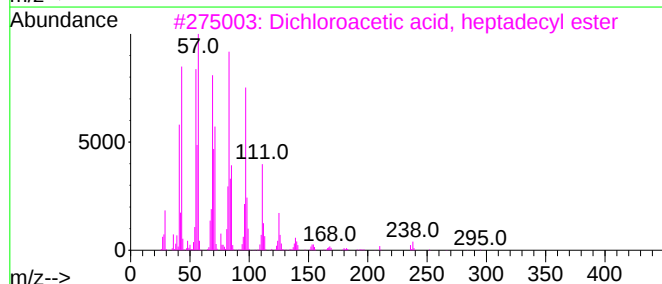
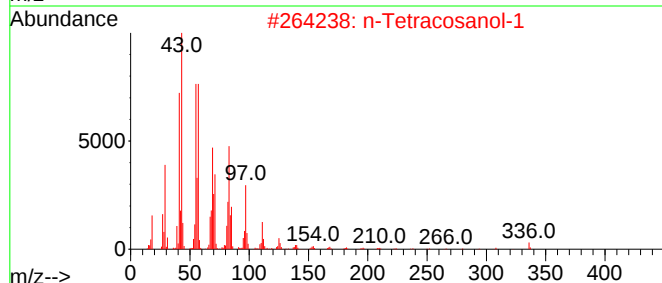
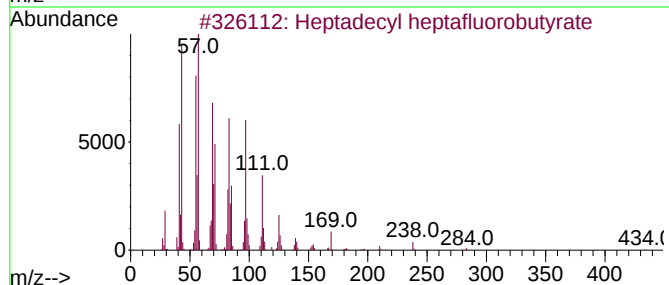
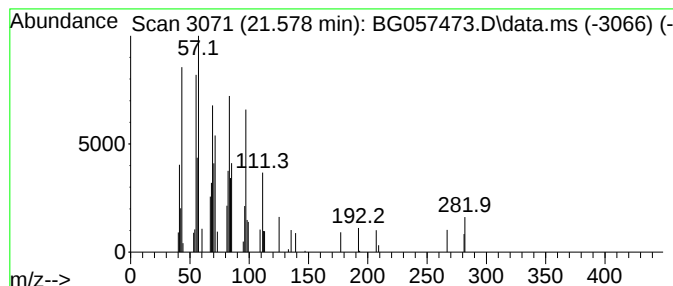
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.578	2.98 ng	47274	Chrysene-d12	22.013	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
5	1-Heptacosanol	396	C27H56O	002004-39-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057473.D
Acq On : 19 May 2023 18:52
Operator : CG/JU
Sample : 02845-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

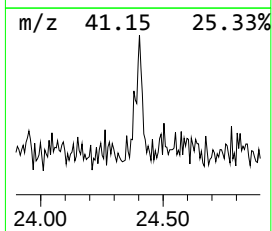
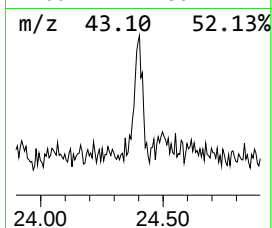
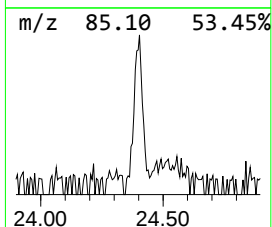
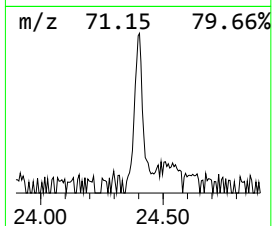
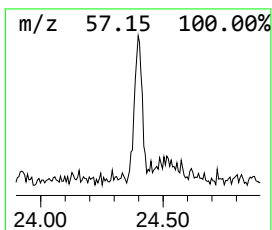
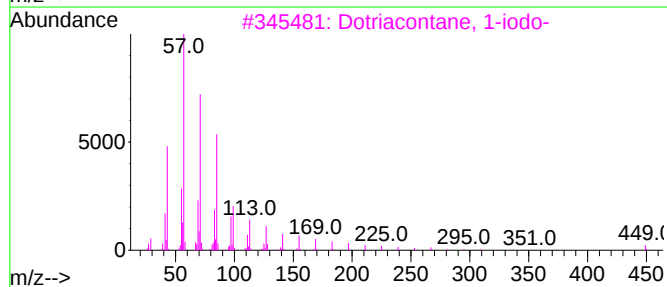
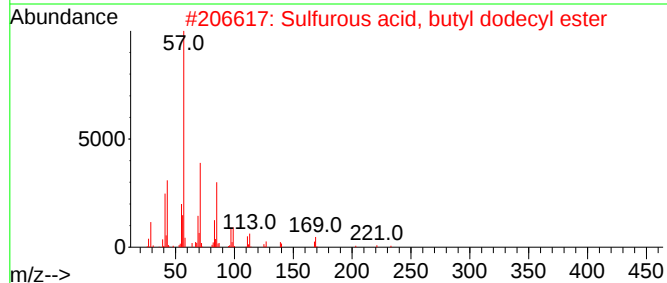
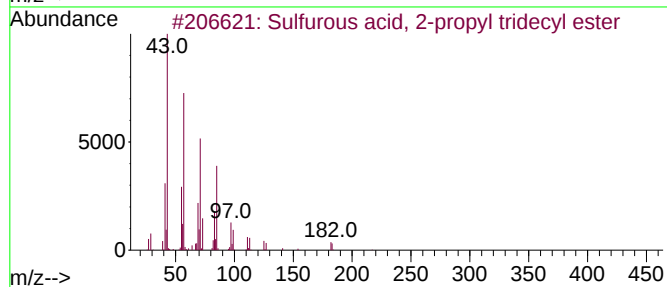
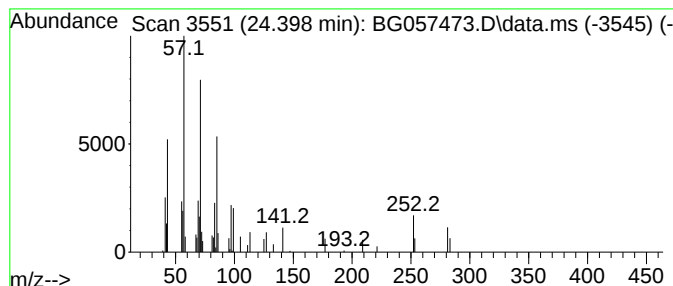
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Sulfurous acid, 2-propyl tr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.398	2.00 ng	31969	Perylene-d12	25.502	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	72
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	64
3	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	64
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	59
5	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057473.D
Acq On : 19 May 2023 18:52
Operator : CG/JU
Sample : 02845-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP2

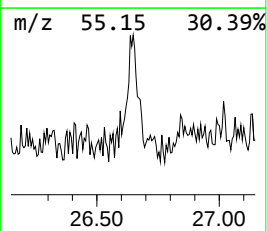
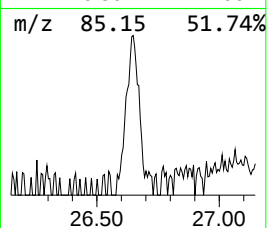
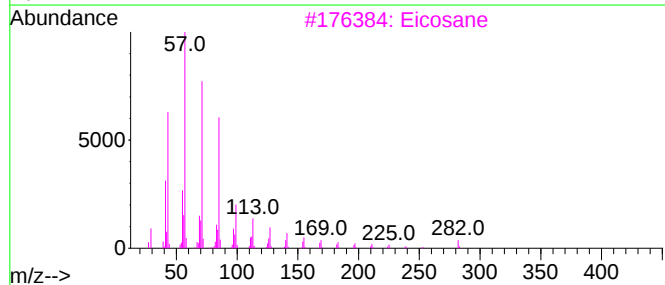
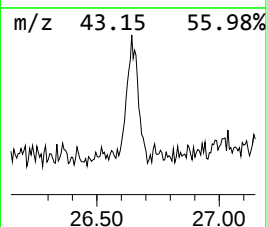
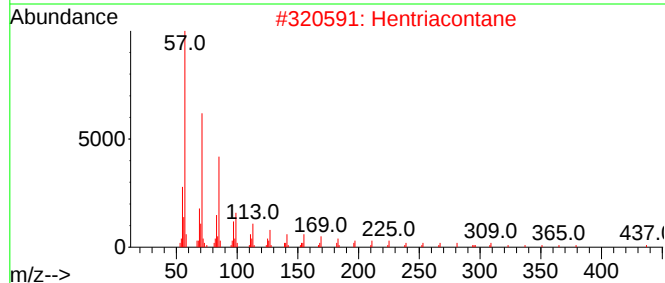
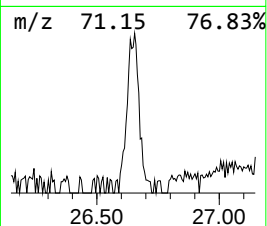
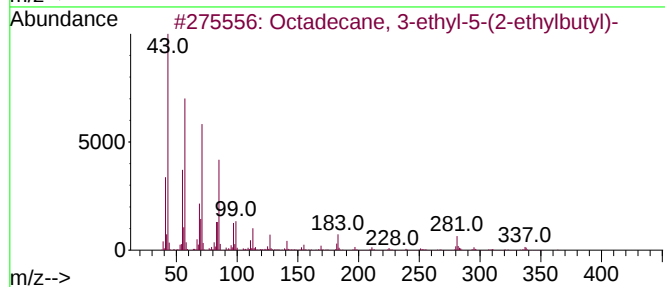
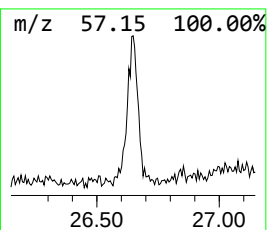
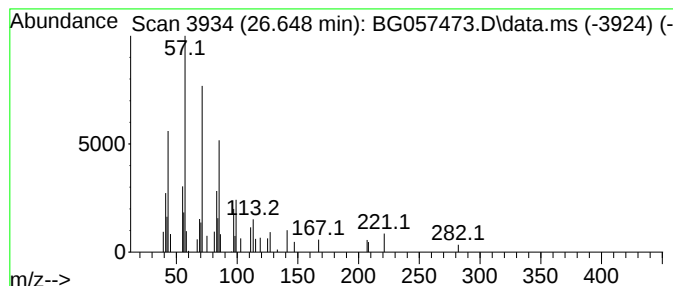
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane, 3-ethyl-5-(2-et... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.648	3.02 ng	48262	Perylene-d12	25.502

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	90
2			Hentriacontane	437	C31H64	000630-04-6	90
3			Eicosane	282	C20H42	000112-95-8	87
4			Isopropyl tetradecyl ether	256	C17H36O	1000406-34-0	86
5			Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057473.D
Acq On : 19 May 2023 18:52
Operator : CG/JU
Sample : 02845-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

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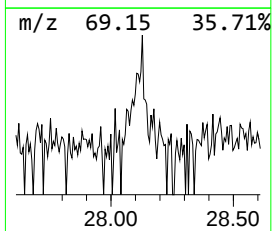
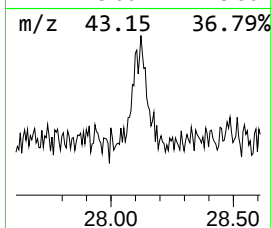
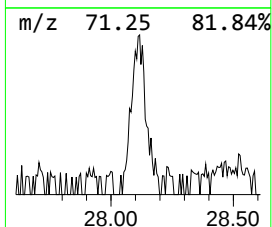
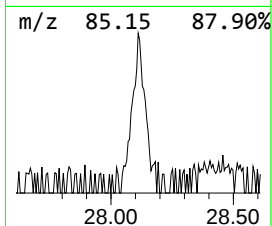
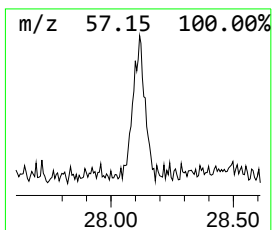
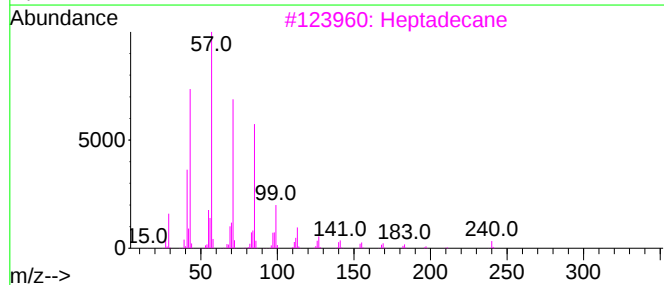
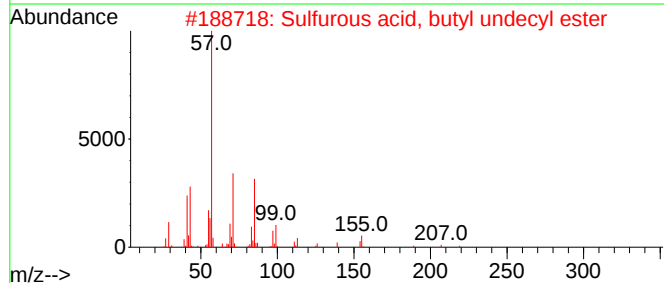
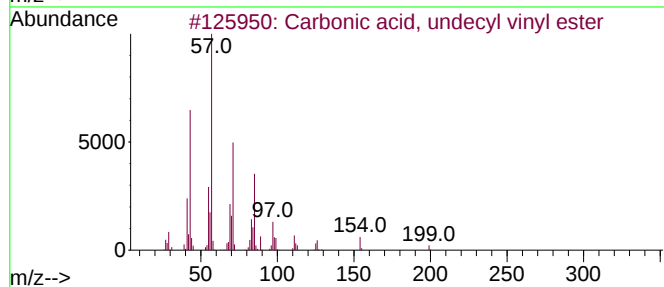
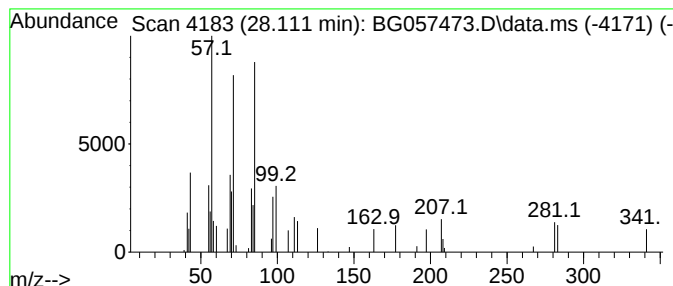
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Carbonic acid, undecyl vinyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.111	2.53 ng	40359	Perylene-d12	25.502

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	72
2			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	64
3			Heptadecane	240	C17H36	000629-78-7	59
4			Dotriacontane	451	C32H66	000544-85-4	59
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057473.D
Acq On : 19 May 2023 18:52
Operator : CG/JU
Sample : 02845-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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
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unknown14.282	14.282	5.5	ng	59717	3	14.970	218633	20.0
(1R,2S,6S,7S,8S...	14.911	2.1	ng	23020	3	14.970	218633	20.0
Benzophenone	16.303	6.9	ng	75640	3	14.970	218633	20.0
n-Hexadecanoic ...	18.547	4.7	ng	68327	4	17.707	290522	20.0
Cinnamyl cinnamate	21.408	6.5	ng	102608	5	22.013	317336	20.0
Heptadecyl hept...	21.578	3.0	ng	47274	5	22.013	317336	20.0
Sulfurous acid,...	24.398	2.0	ng	31969	6	25.502	319286	20.0
Octadecane, 3-e...	26.648	3.0	ng	48262	6	25.502	319286	20.0
Carbonic acid, ...	28.111	2.5	ng	40359	6	25.502	319286	20.0