

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
 Data File : BG057479.D
 Acq On : 19 May 2023 23:00
 Operator : CG/JU
 Sample : 02848-20
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP6

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: BG057479.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	309	314	323	rBB2	14662	21881	2.18%	0.367%
2	5.871	391	397	410	rBB	218977	354704	35.32%	5.955%
3	7.011	586	591	596	rBV	14101	20822	2.07%	0.350%
4	7.498	667	674	684	rBV	236462	406000	40.43%	6.816%
5	8.356	814	820	827	rVB2	59948	101281	10.08%	1.700%
6	9.531	1012	1020	1031	rBV	139160	247849	24.68%	4.161%
7	11.193	1294	1303	1312	rBB	78093	139826	13.92%	2.347%
8	13.596	1704	1712	1719	rBV	416116	648163	64.54%	10.881%
9	13.837	1749	1753	1758	rVB2	8024	11070	1.10%	0.186%
10	14.283	1824	1829	1834	rBV2	43566	61128	6.09%	1.026%
11	14.365	1839	1843	1848	rBV	10339	13359	1.33%	0.224%
12	14.912	1930	1936	1940	rBV	117635	162424	16.17%	2.727%
13	14.970	1940	1946	1951	rVV	137781	217020	21.61%	3.643%
14	15.194	1979	1984	1990	rVB2	22459	29967	2.98%	0.503%
15	15.264	1990	1996	2001	rBV5	8755	12971	1.29%	0.218%
16	16.304	2165	2173	2178	rBV2	40661	63394	6.31%	1.064%
17	16.410	2184	2191	2193	rBV3	15766	26704	2.66%	0.448%
18	16.451	2193	2198	2204	rVV	328523	505108	50.29%	8.480%
19	16.504	2204	2207	2214	rVB5	9132	14247	1.42%	0.239%
20	16.786	2250	2255	2260	rBV2	7368	12038	1.20%	0.202%
21	17.708	2405	2412	2423	rBV	188714	285881	28.47%	4.799%
22	18.548	2549	2555	2562	rBV2	37574	59808	5.96%	1.004%
23	19.799	2765	2768	2777	rBV5	7658	15382	1.53%	0.258%
24	20.275	2843	2849	2855	rBV	810330	1004316	100.00%	16.860%
25	21.227	3008	3011	3017	rVB4	13189	17415	1.73%	0.292%
26	21.415	3036	3043	3050	rVB	318007	456805	45.48%	7.669%
27	21.573	3065	3070	3082	rBV4	23154	59054	5.88%	0.991%
28	22.014	3135	3145	3153	rBV	192924	319692	31.83%	5.367%
29	22.795	3273	3278	3281	rBV3	10581	15449	1.54%	0.259%
30	24.399	3541	3551	3561	rBV2	55195	133586	13.30%	2.243%
31	25.421	3719	3725	3730	rBV5	10834	24295	2.42%	0.408%
32	25.503	3730	3739	3751	rVB2	99447	294636	29.34%	4.946%
33	26.649	3925	3934	3944	rVB2	43799	132991	13.24%	2.233%
34	28.117	4176	4184	4194	rVB2	8815	32330	3.22%	0.543%
35	29.886	4475	4485	4492	rBV6	9999	35207	3.51%	0.591%

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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-BG042723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

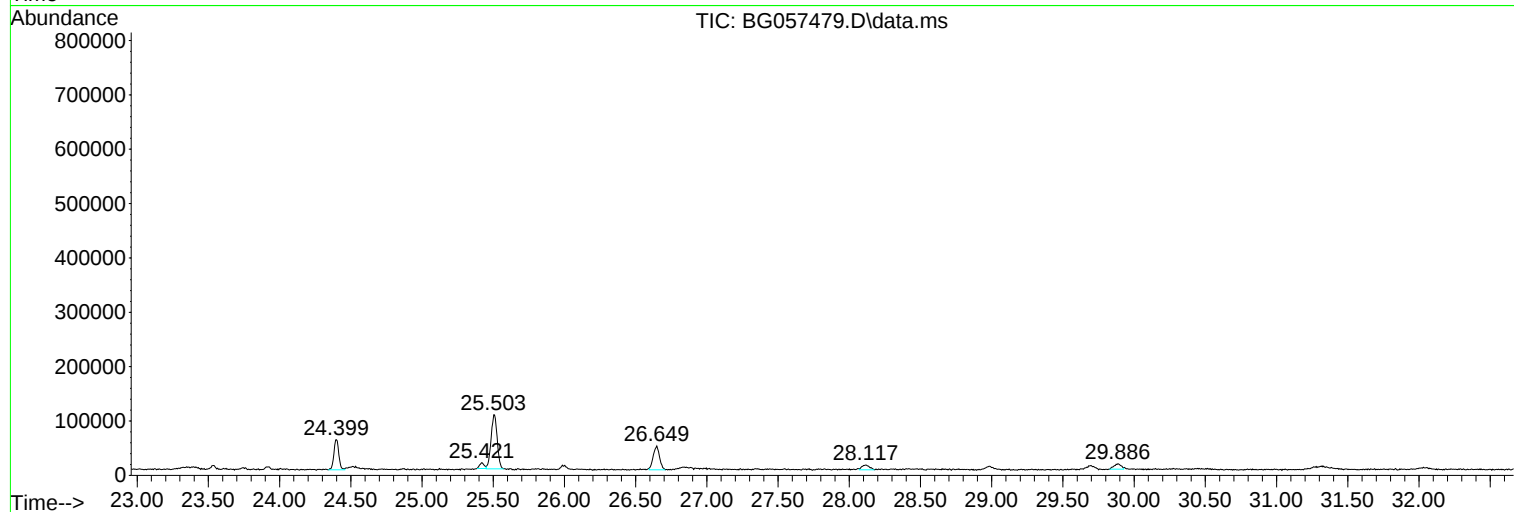
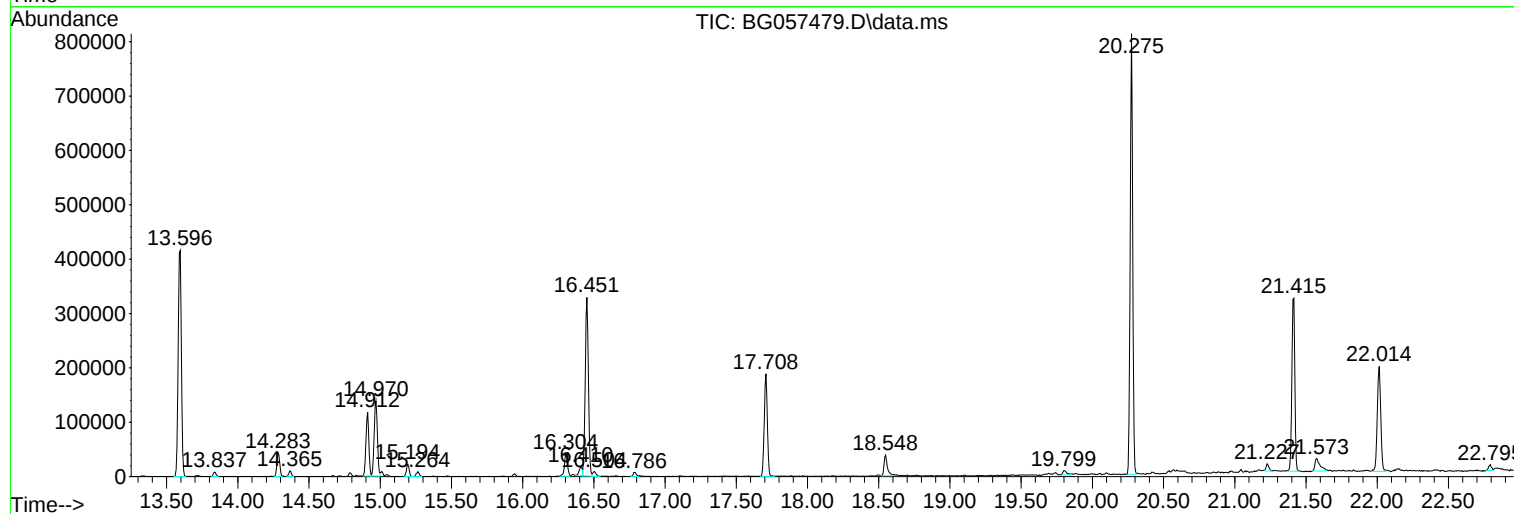
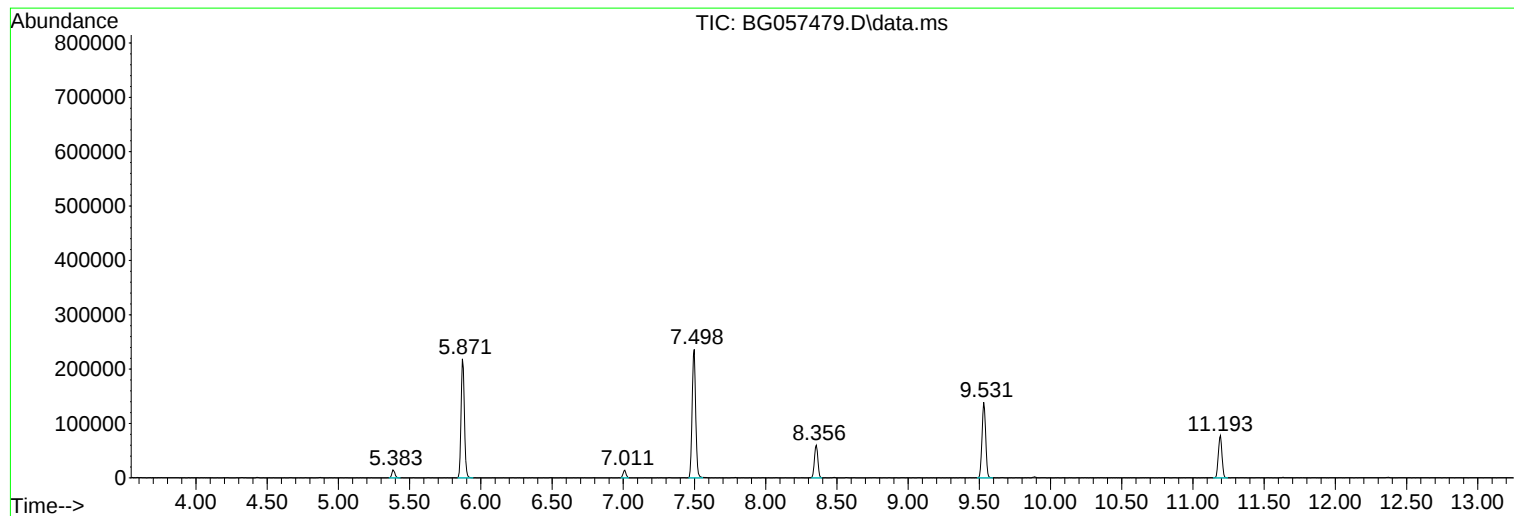
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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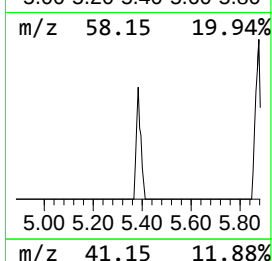
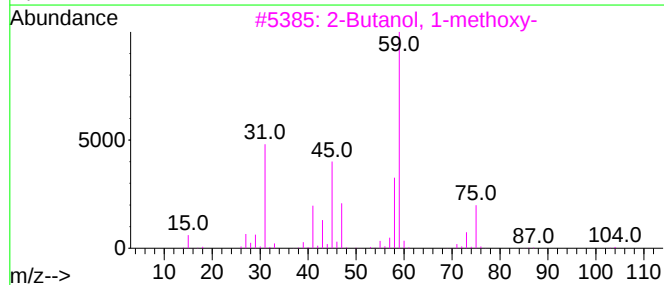
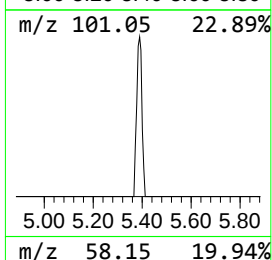
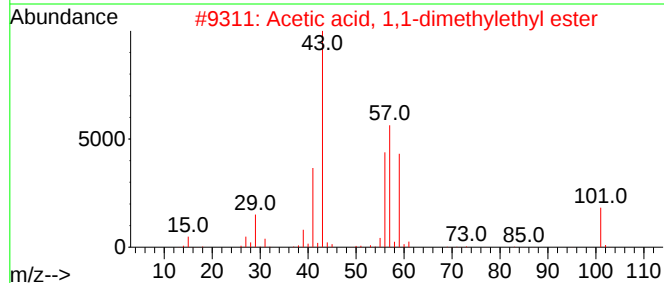
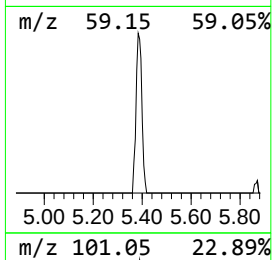
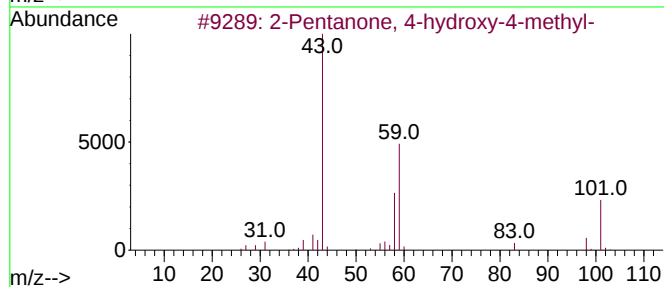
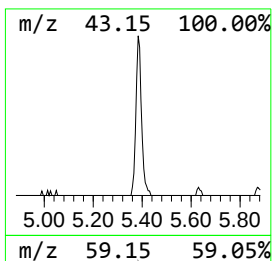
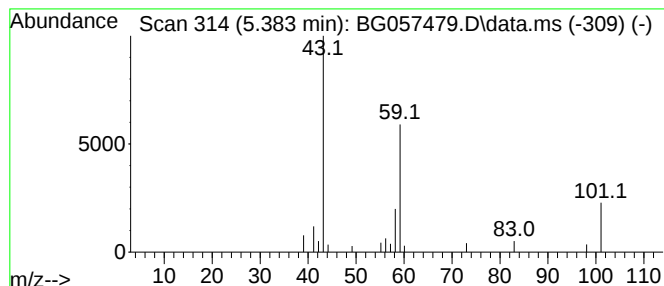
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.383	4.32 ng	21881	1,4-Dichlorobenzene-d4	8.356	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	33
3	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	25
4	2-Butanol, 1-chloro-	108	C4H9ClO	001873-25-2	12
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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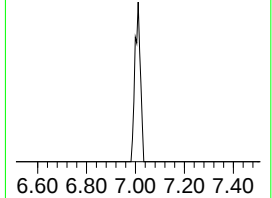
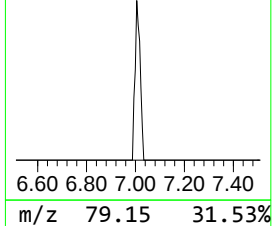
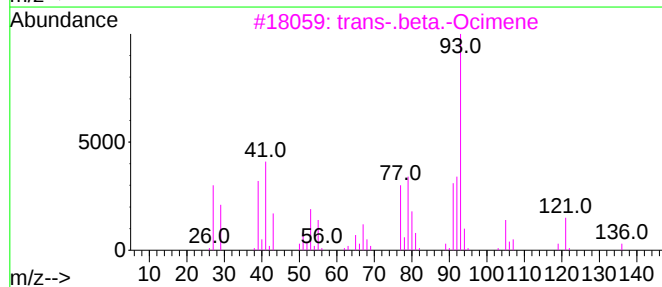
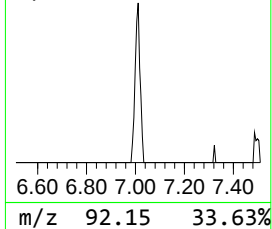
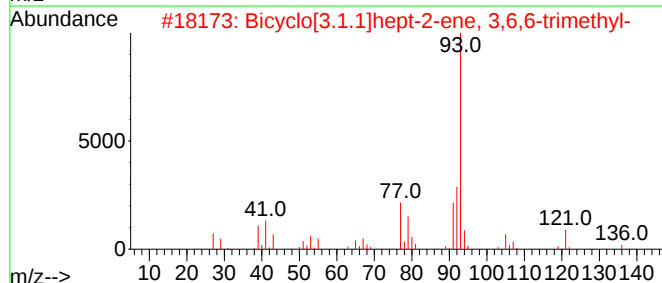
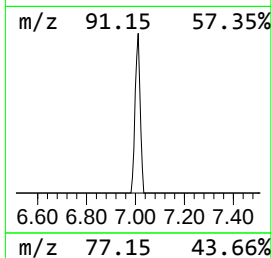
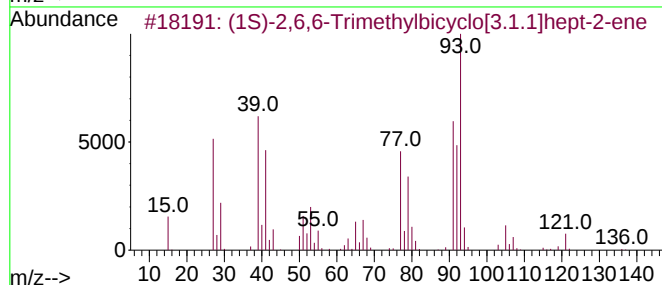
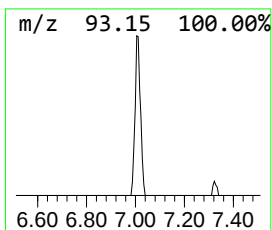
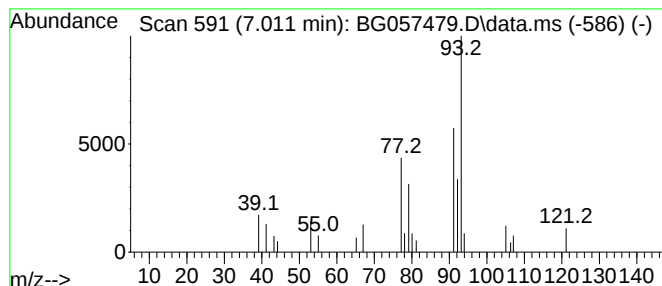
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 (1S)-2,6,6-Trimethylbicyclo... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.011	4.11 ng	20822	1,4-Dichlorobenzene-d4	8.356

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	007785-26-4	90		
2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	78		
3	trans-.beta.-Ocimene	136	C10H16	003779-61-1	72		
4	1,3,6-Heptatriene, 5-methyl-, (E)-	108	C8H12	000818-48-4	50		
5	3,5-Methanocyclopentapyrazole, 3,5-dimethyl-	164	C10H16N2	087143-58-6	42		



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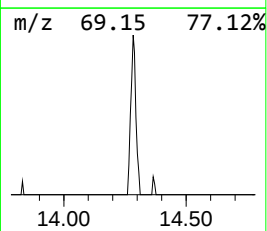
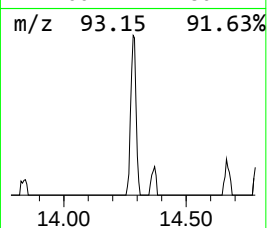
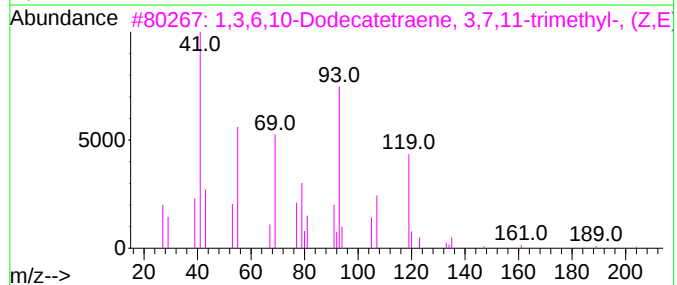
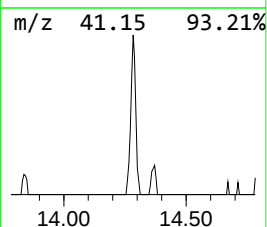
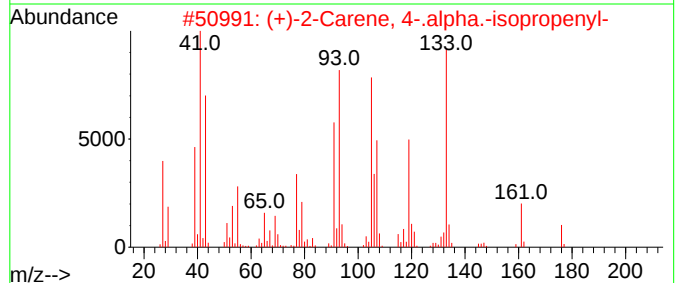
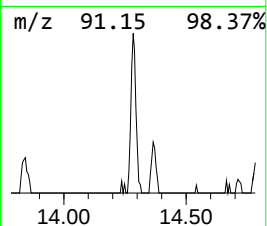
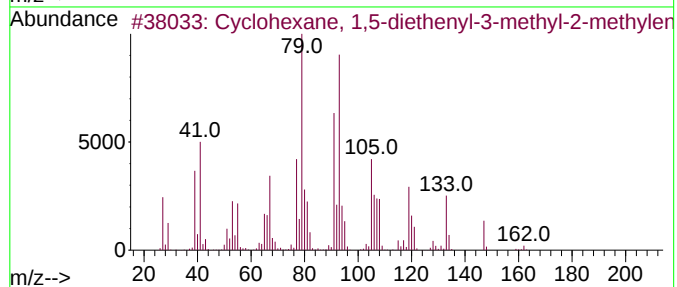
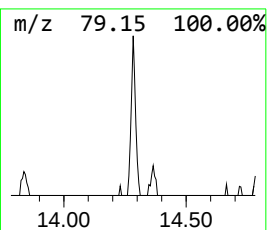
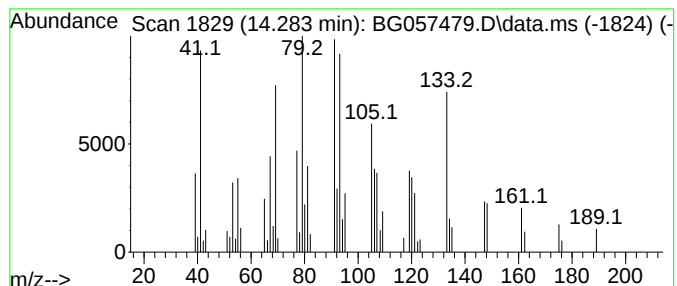
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown14.283 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.283	5.63 ng	61128	Acenaphthene-d10	14.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	49
2			(+)-2-Carene, 4-.alpha.-isopropen...	176	C13H20	1000151-26-0	35
3			1,3,6,10-Dodecatetraene, 3,7,11-...	204	C15H24	026560-14-5	35
4			1,4-Methanophthalazine, 1,4,4a,7...	176	C11H16N2	1000221-84-9	30
5			3-Methylene-1,6-heptadiene	108	C8H12	016626-48-5	30



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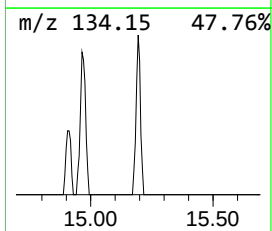
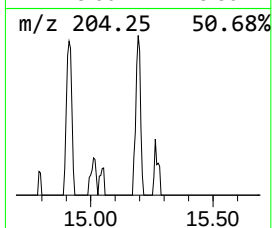
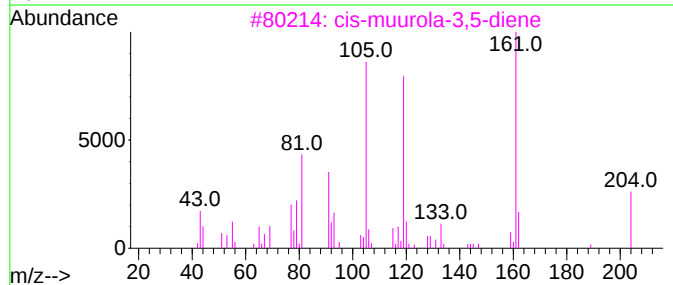
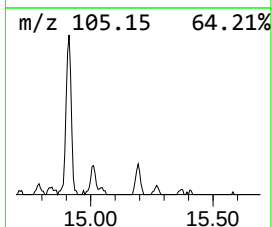
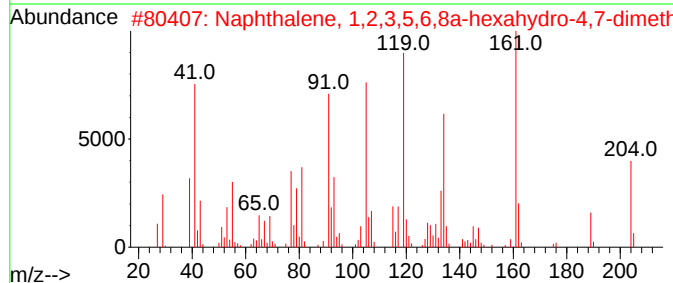
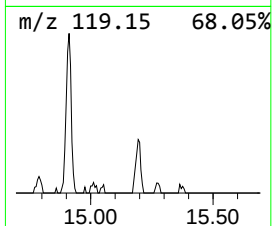
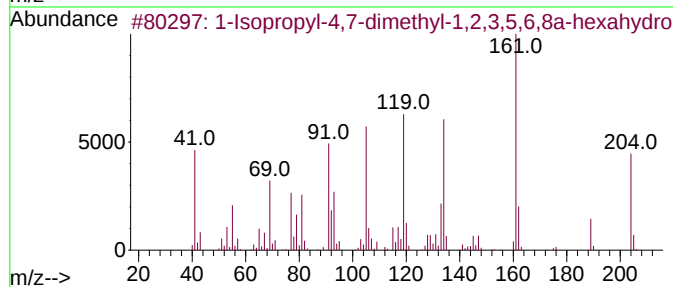
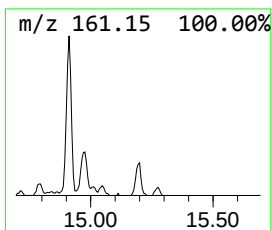
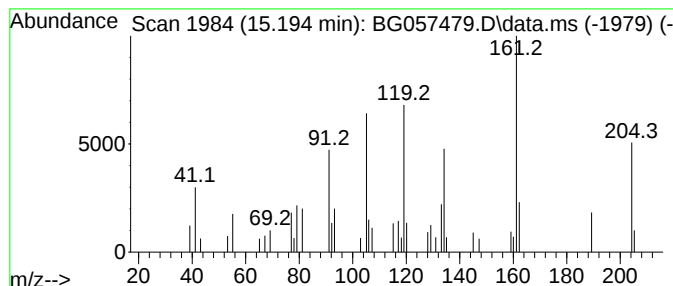
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Isopropyl-4,7-dimethyl-1,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.194	2.76 ng	29967	Acenaphthene-d10	14.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Isopropyl-4,7-dimethyl-1,2,3,5...	204	C15H24	016729-01-4	99
2			Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	98
3			cis-muurolo-3,5-diene	204	C15H24	1000365-95-4	93
4			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	90
5			.alpha.-Muurolene	204	C15H24	010208-80-7	76



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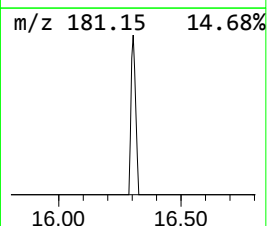
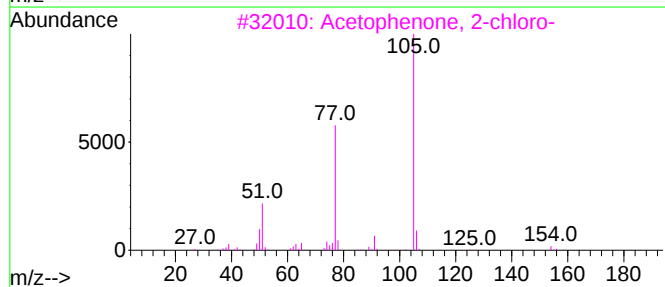
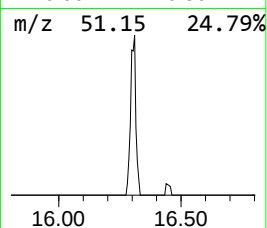
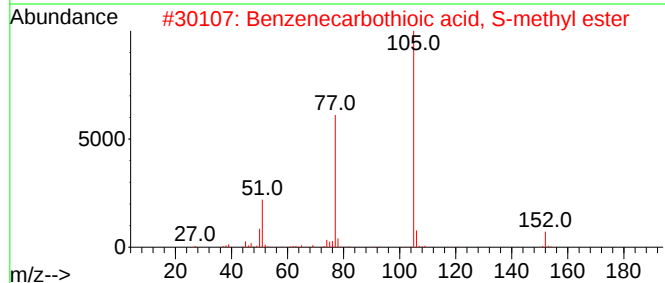
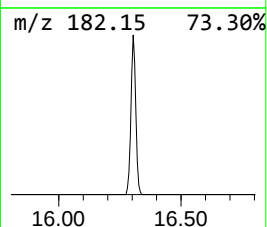
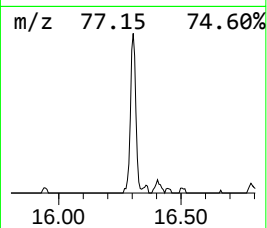
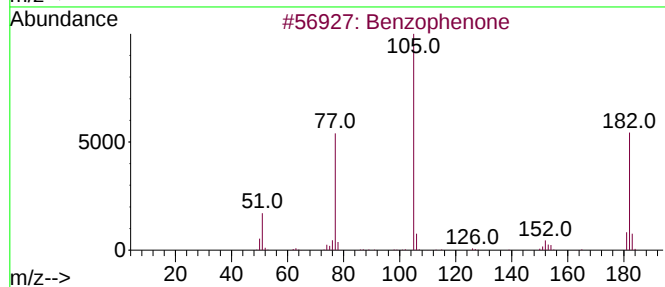
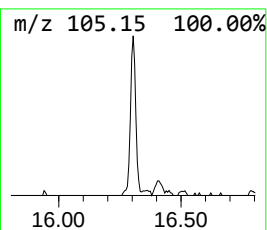
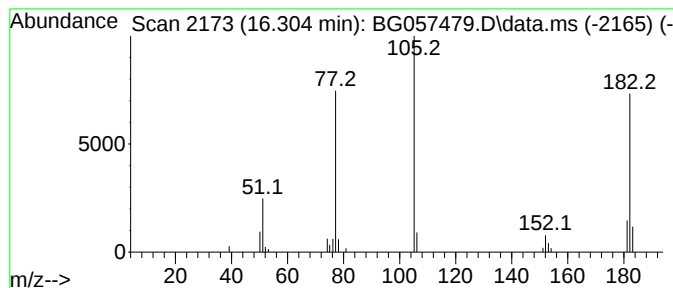
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.304	5.84 ng	63394	Acenaphthene-d10	14.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4			Benzenecarboxylic acid, .alpha.-oxo...	164	C9H8O3	015206-55-0	43
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	43



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Data File : BG057479.D
Acq On : 19 May 2023 23:00
Operator : CG/JU
Sample : 02848-20
Misc :
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Instrument :
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ClientSampleId :
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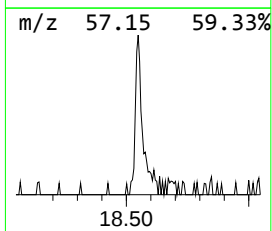
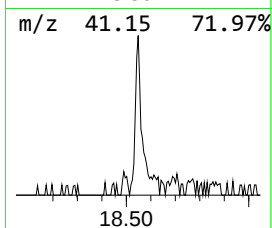
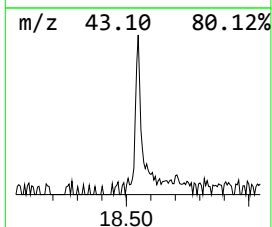
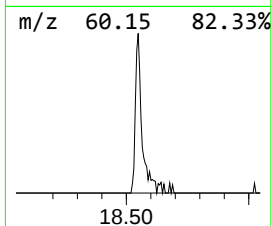
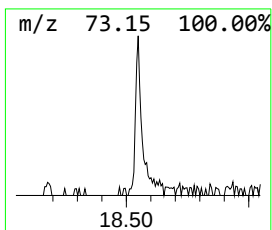
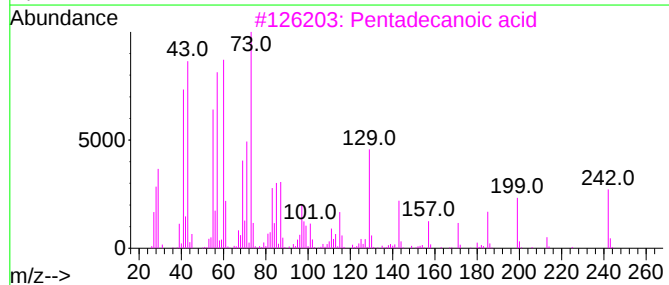
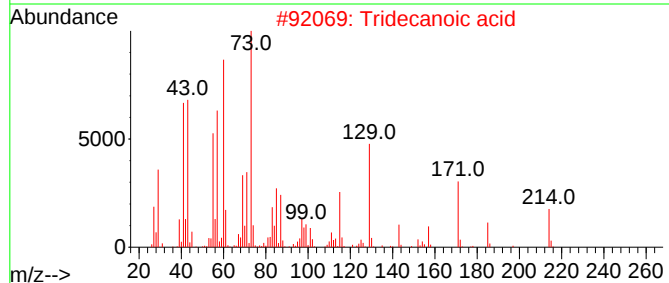
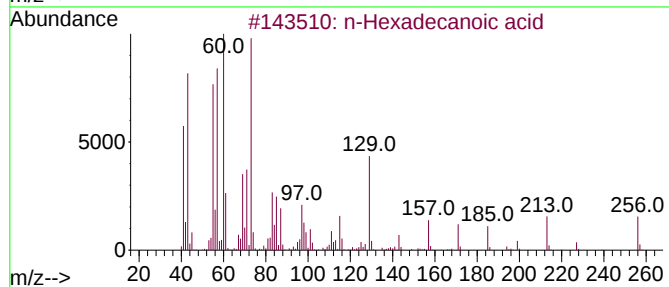
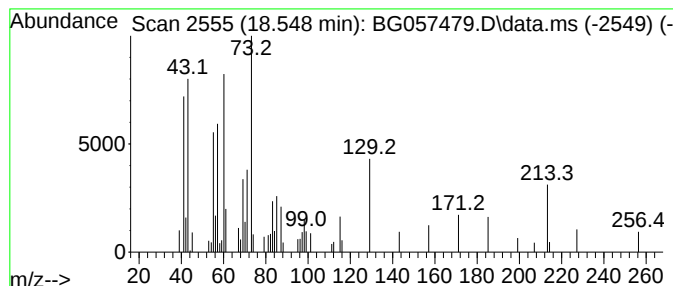
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.548	4.18 ng	59808	Phenanthrene-d10	17.708

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
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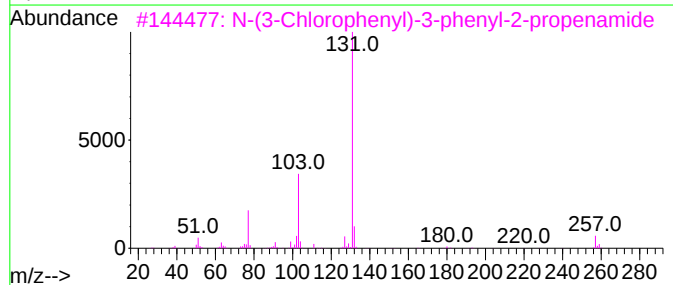
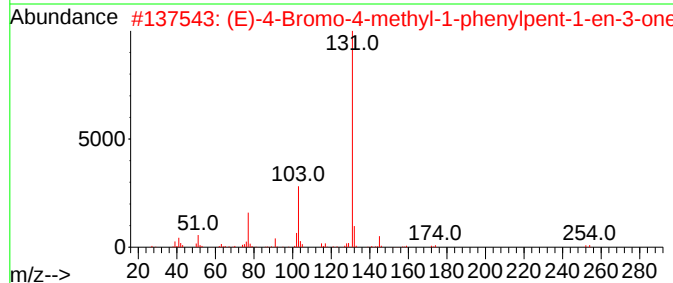
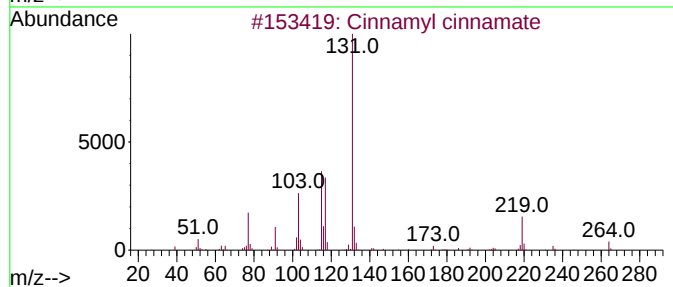
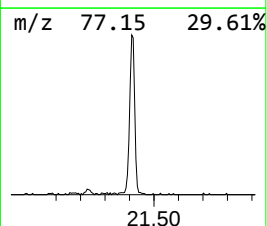
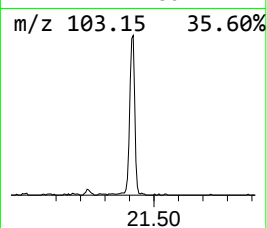
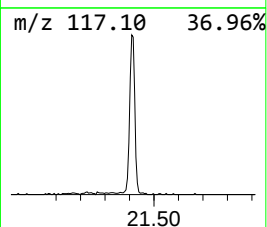
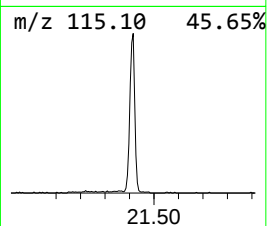
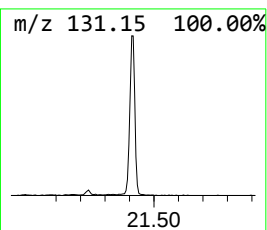
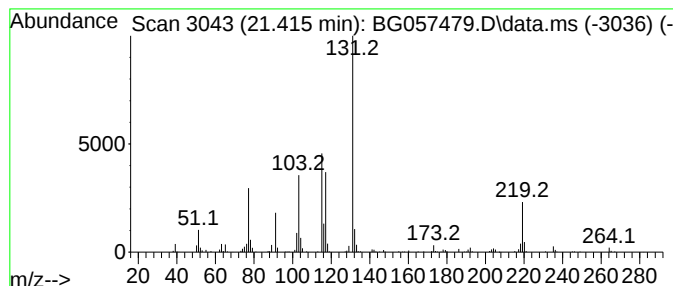
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.415	28.58 ng	456805	Chrysene-d12	22.014

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	47
3			N-(3-Chlorophenyl)-3-phenyl-2-pr...	257	C15H12ClNO	064741-15-7	43
4			Imidazo[1,2-a]pyridine-3-methana...	219	C11H17N3Si	1000497-61-2	43
5			1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
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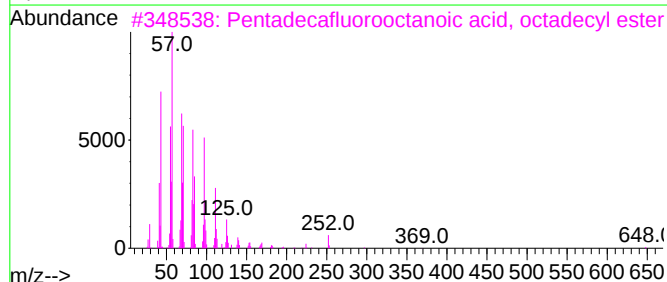
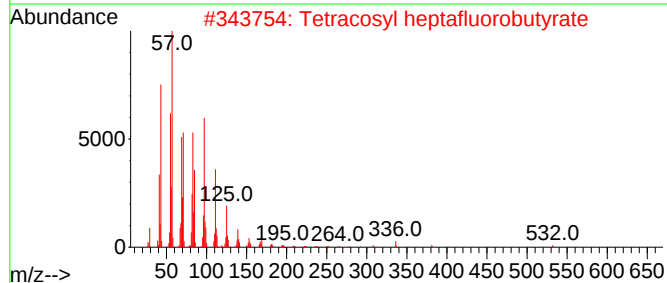
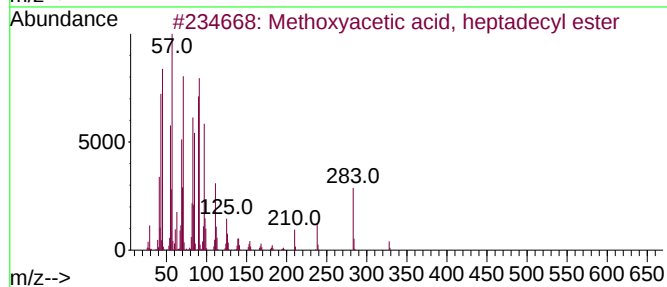
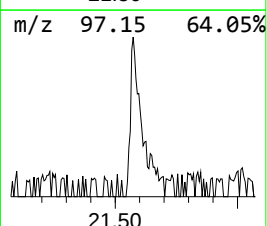
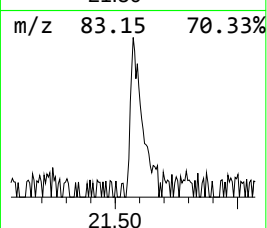
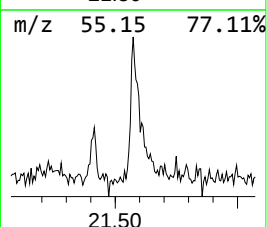
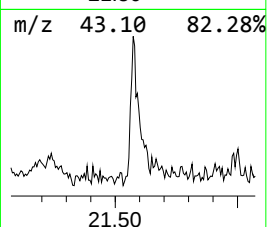
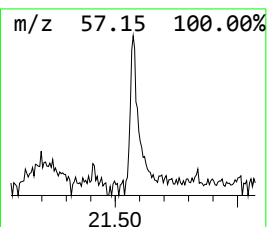
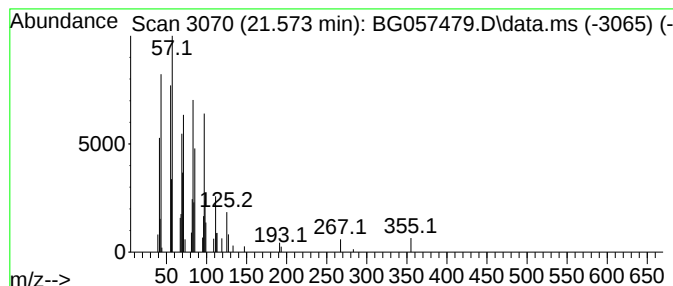
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methoxyacetic acid, heptade... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.573	3.69 ng	59054	Chrysene-d12	22.014

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methoxyacetic acid, heptadecyl e...	328	C20H40O3	1000282-99-1	86
2			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	83
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	83
4			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	83
5			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
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Misc :
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ClientSampleId :
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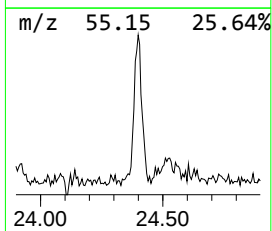
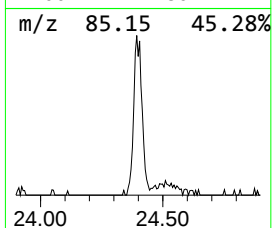
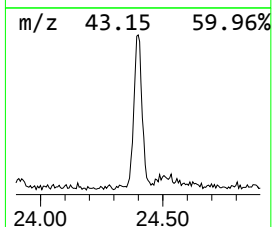
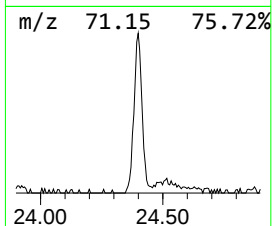
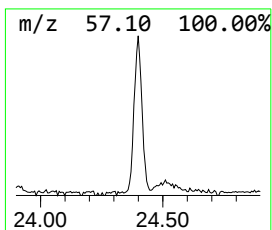
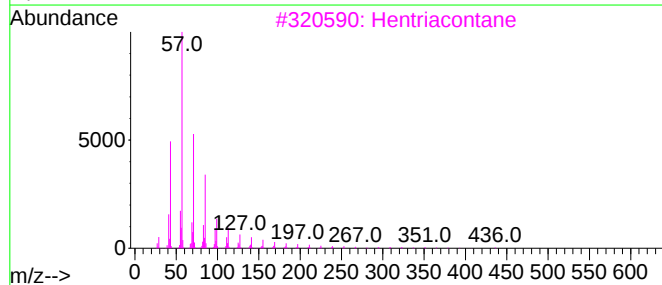
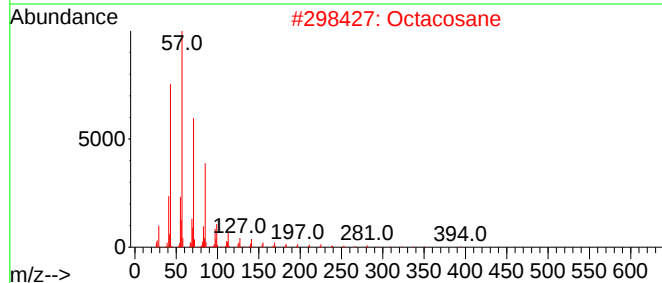
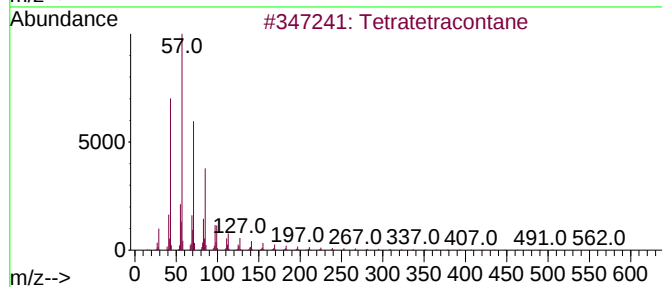
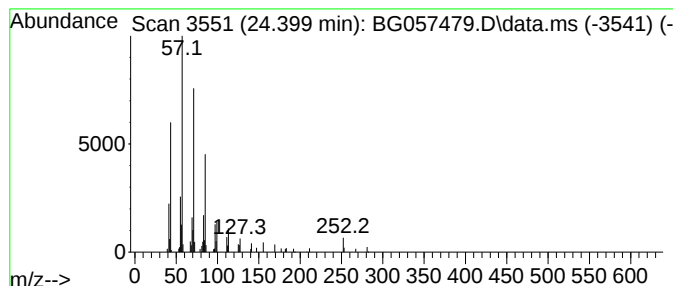
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tetratetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.399	9.07 ng	133586	Perylene-d12	25.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057479.D
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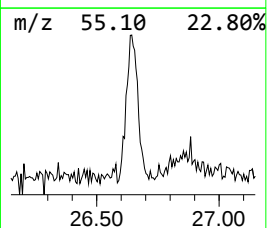
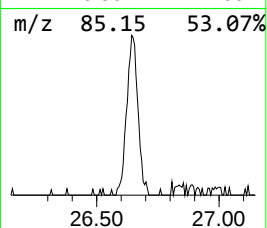
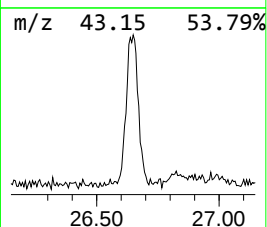
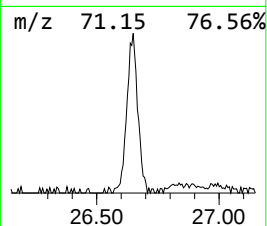
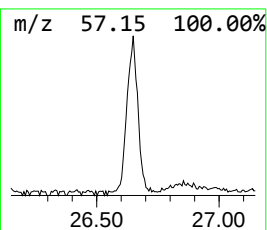
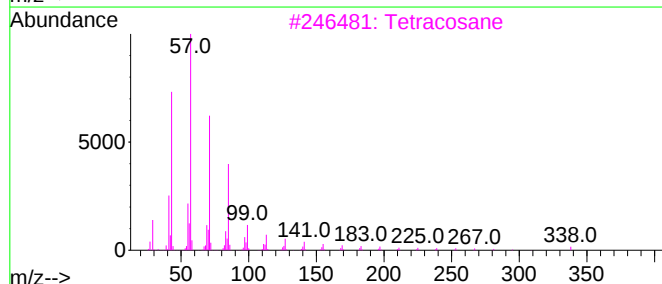
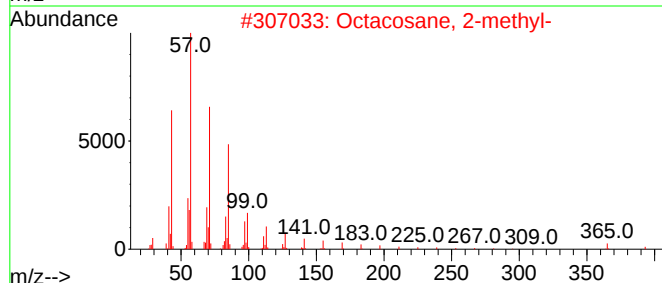
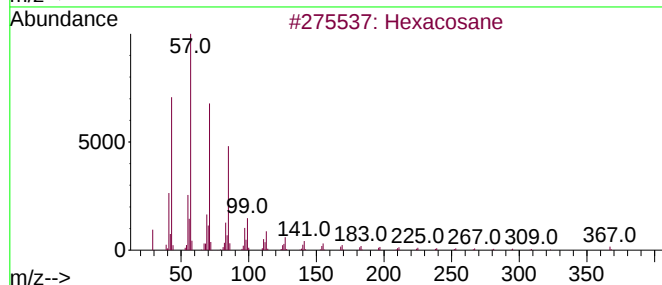
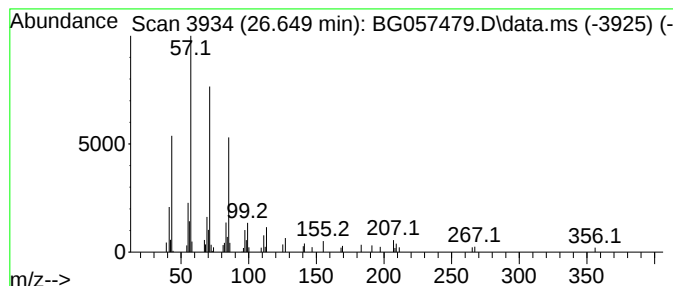
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.649	9.03 ng	132991	Perylene-d12	25.509

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	90
2		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3		Tetracosane	338	C24H50	000646-31-1	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Heptadecane	240	C17H36	000629-78-7	87



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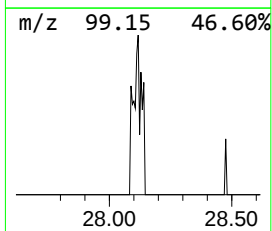
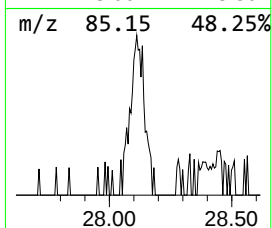
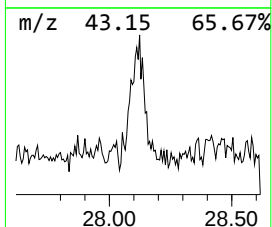
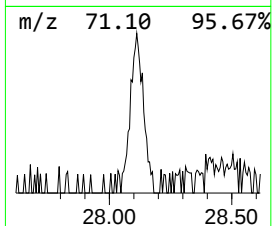
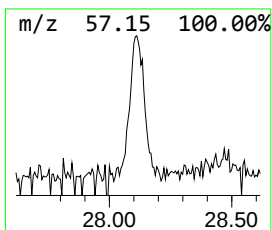
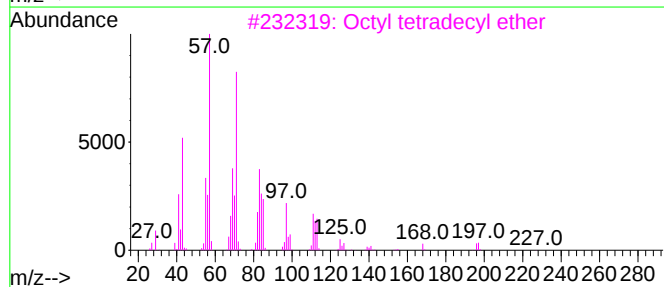
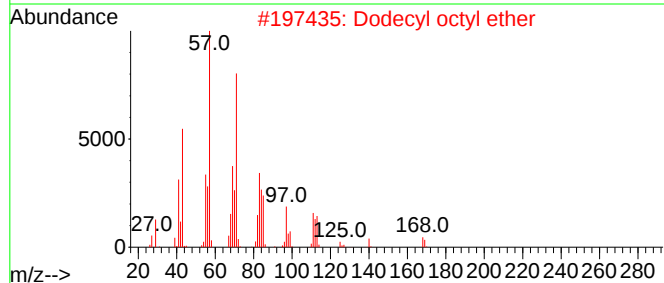
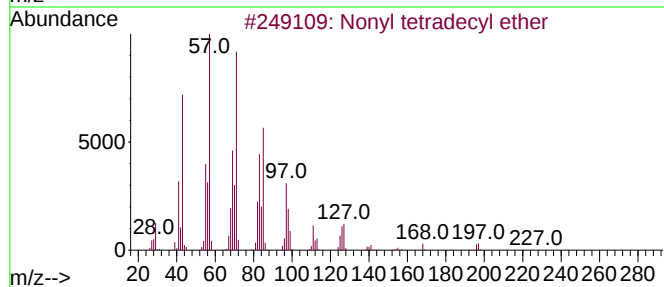
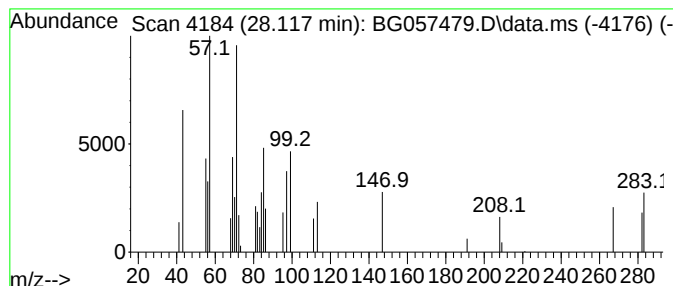
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown28.117 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.117	2.19 ng	32330	Perylene-d12	25.509

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonyl tetradecyl ether	340	C23H48O	1000406-37-6	38
2		Dodecyl octyl ether	298	C20H42O	1000406-38-4	35
3		Octyl tetradecyl ether	326	C22H46O	1000406-38-5	35
4		Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	35
5		Hexadecyl octyl ether	354	C24H50O	1000406-38-6	35



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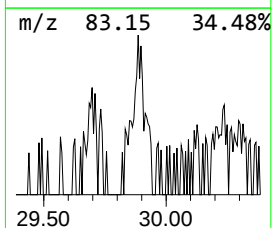
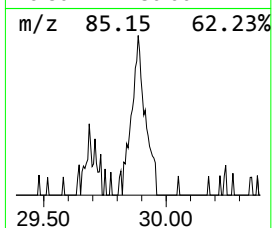
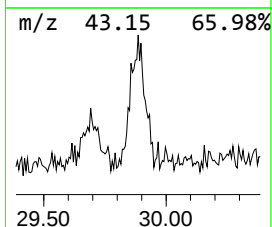
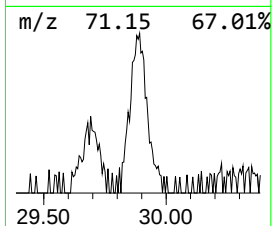
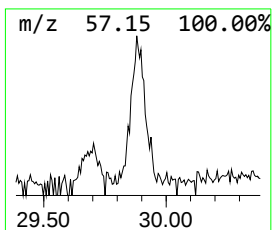
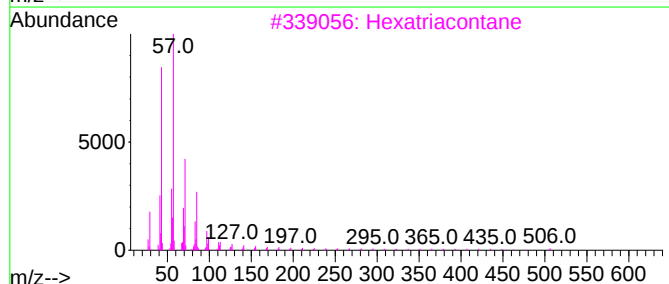
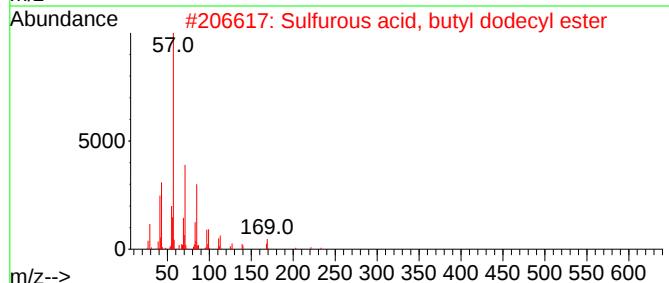
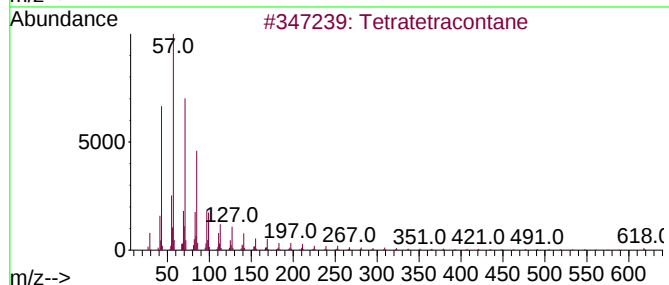
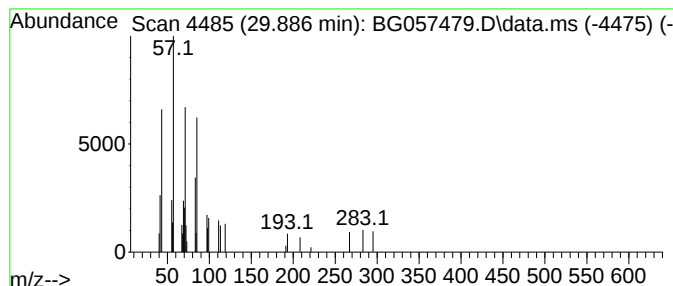
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Sulfurous acid, butyl dodec... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.886	2.39 ng	35207	Perylene-d12	25.509

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	53
2		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	53
3		Hexatriacontane	507	C36H74	000630-06-8	53
4		Docosane	310	C22H46	000629-97-0	50
5		Hentriacontane	437	C31H64	000630-04-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057479.D
Acq On : 19 May 2023 23:00
Operator : CG/JU
Sample : 02848-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP6

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
2-Pentanone, 4-...	5.383	4.3	ng	21881	1	8.356	101281	20.0
(1S)-2,6,6-Trim...	7.011	4.1	ng	20822	1	8.356	101281	20.0
unknown14.283	14.283	5.6	ng	61128	3	14.970	217020	20.0
Germacrene D	14.912	15.0	ng	162424	3	14.970	217020	20.0
1-Isopropyl-4,7...	15.194	2.8	ng	29967	3	14.970	217020	20.0
Benzophenone	16.304	5.8	ng	63394	3	14.970	217020	20.0
n-Hexadecanoic ...	18.548	4.2	ng	59808	4	17.708	285881	20.0
Cinnamyl cinnamate	21.415	28.6	ng	456805	5	22.014	319692	20.0
Methoxyacetic a...	21.573	3.7	ng	59054	5	22.014	319692	20.0
Tetratetracontane	24.399	9.1	ng	133586	6	25.509	294636	20.0
Hexacosane	26.649	9.0	ng	132991	6	25.509	294636	20.0
unknown28.117	28.117	2.2	ng	32330	6	25.509	294636	20.0
Sulfurous acid,...	29.886	2.4	ng	35207	6	25.509	294636	20.0