

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
 Data File : BG057538.D
 Acq On : 24 May 2023 17:29
 Operator : CG/JU
 Sample : 02869-11
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP19

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: BG057538.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	309	315	321	rBV	15681	24630	1.77%	0.377%
2	5.879	390	398	411	rBB	277566	462137	33.25%	7.073%
3	7.006	585	590	596	rVB	23734	36516	2.63%	0.559%
4	7.500	667	674	684	rBV	288011	515904	37.11%	7.895%
5	8.358	813	820	827	rBV	64463	109738	7.89%	1.679%
6	9.538	1012	1021	1031	rBV	170241	307231	22.10%	4.702%
7	11.195	1294	1303	1311	rBV	81250	147987	10.65%	2.265%
8	13.592	1704	1711	1720	rBV	479528	729862	52.51%	11.170%
9	14.285	1824	1829	1835	rVB2	73741	99377	7.15%	1.521%
10	14.908	1929	1935	1940	rBV	19951	28016	2.02%	0.429%
11	14.972	1940	1946	1951	rBV	136277	208921	15.03%	3.197%
12	15.947	2105	2112	2117	rVB	58303	87368	6.29%	1.337%
13	16.306	2169	2173	2183	rVB	57103	83803	6.03%	1.283%
14	16.411	2183	2191	2193	rBV2	26551	38746	2.79%	0.593%
15	16.453	2193	2198	2206	rVB	420583	652559	46.94%	9.987%
16	17.710	2406	2412	2422	rVB	183297	280923	20.21%	4.299%
17	18.550	2549	2555	2561	rBV2	31419	60988	4.39%	0.933%
18	19.801	2764	2768	2780	rBV4	29642	60550	4.36%	0.927%
19	20.277	2843	2849	2855	rBV	1082946	1390071	100.00%	21.274%
20	21.411	3037	3042	3048	rVB	113605	161417	11.61%	2.470%
21	21.575	3065	3070	3080	rVB2	44715	77144	5.55%	1.181%
22	22.021	3139	3146	3153	rVB2	200645	348459	25.07%	5.333%
23	22.145	3164	3167	3173	rVB4	10808	16906	1.22%	0.259%
24	22.791	3273	3277	3283	rBV4	20318	31882	2.29%	0.488%
25	23.537	3398	3404	3412	rVB2	32112	65971	4.75%	1.010%
26	24.401	3545	3551	3559	rVB3	36197	77782	5.60%	1.190%
27	25.429	3719	3726	3731	rBV3	23126	54297	3.91%	0.831%
28	25.523	3733	3742	3752	rVB	111457	332274	23.90%	5.085%
29	26.645	3929	3933	3943	rVB7	16149	42804	3.08%	0.655%

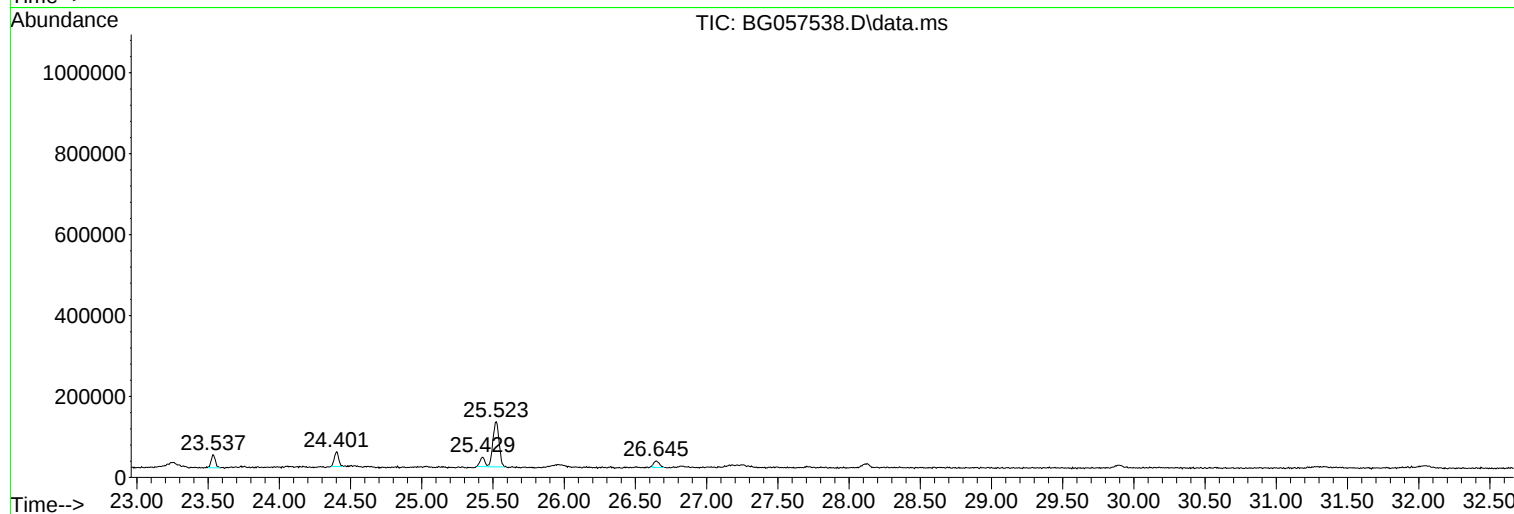
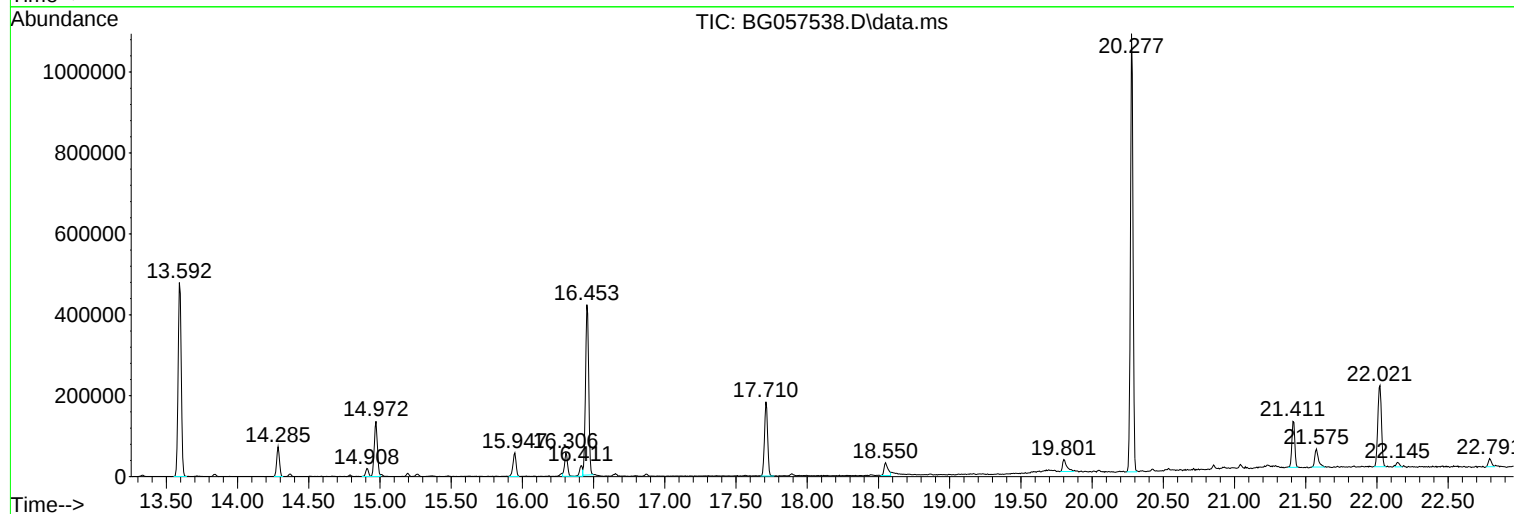
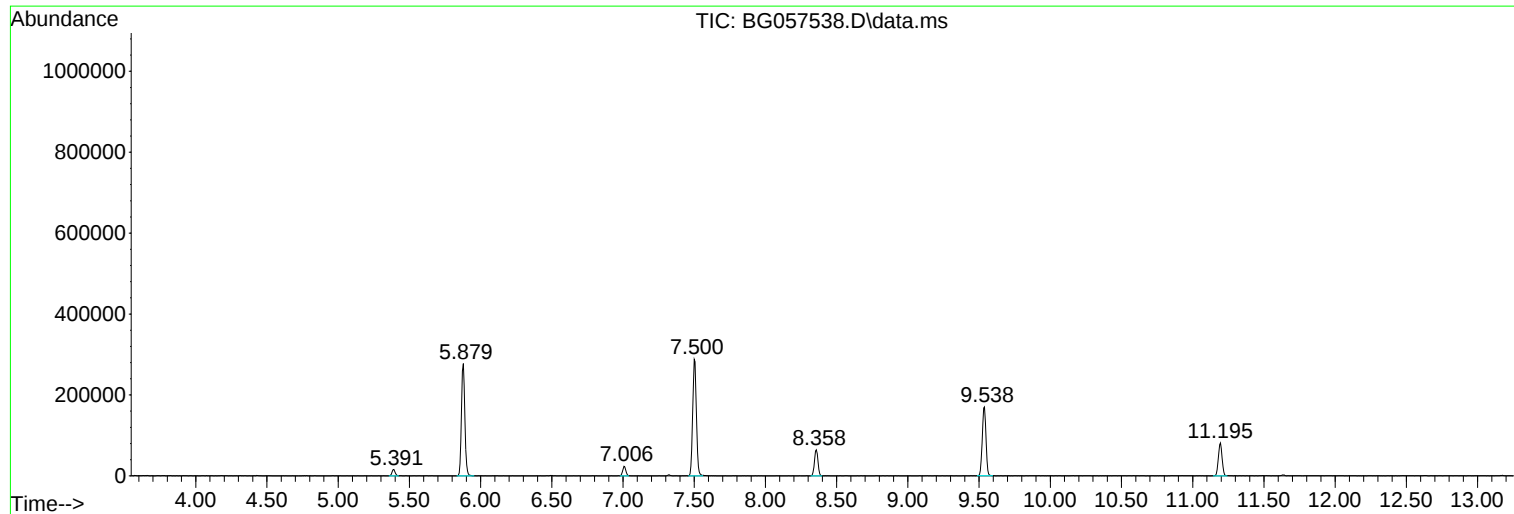
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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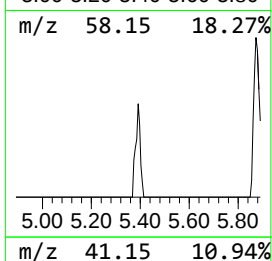
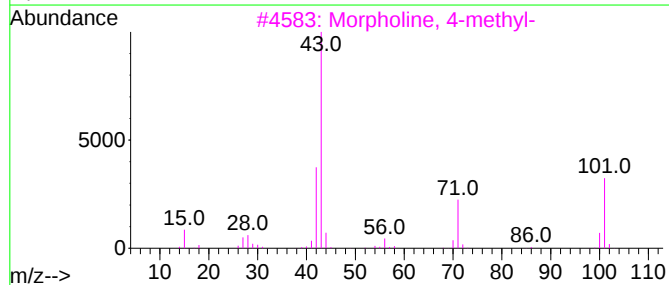
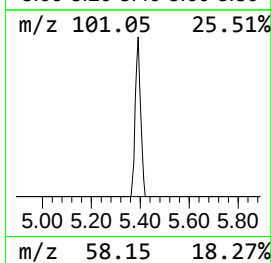
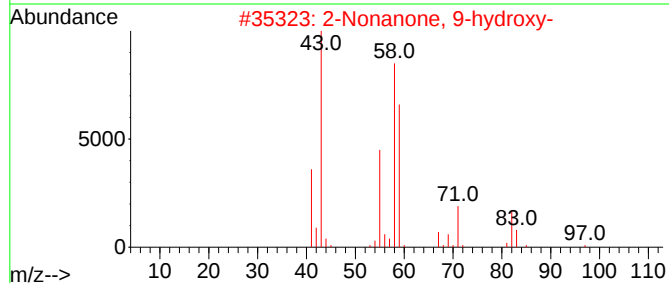
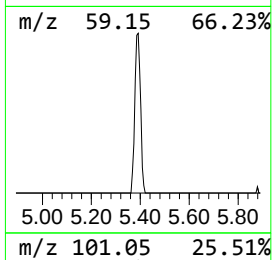
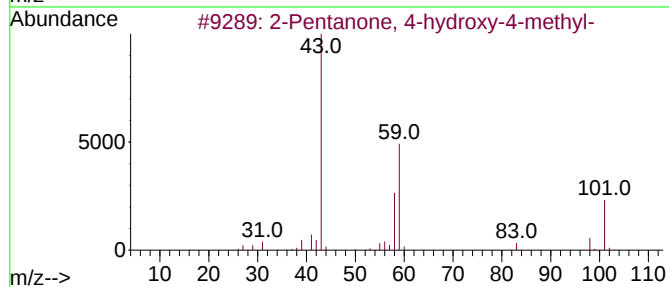
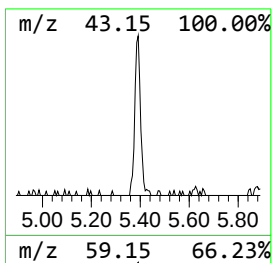
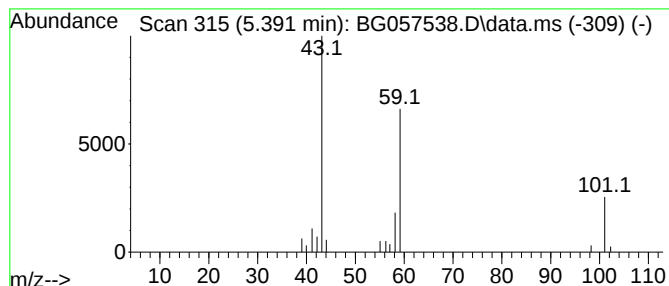
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.391	4.49 ng	24630	1,4-Dichlorobenzene-d4	8.358

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	12
4			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5			Diacetamide	101	C4H7NO2	000625-77-4	9



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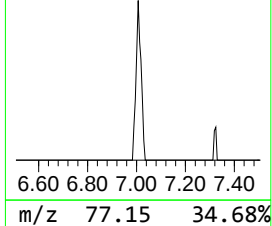
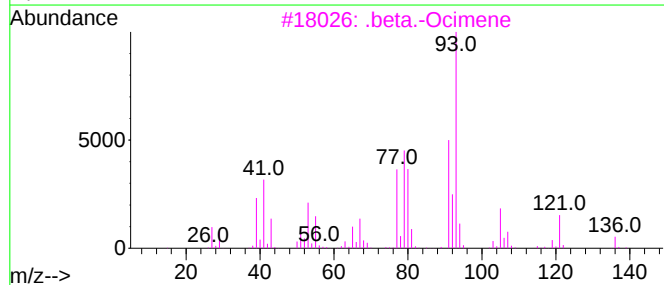
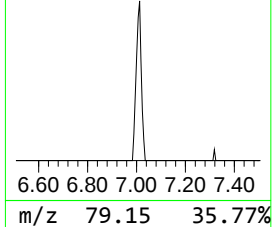
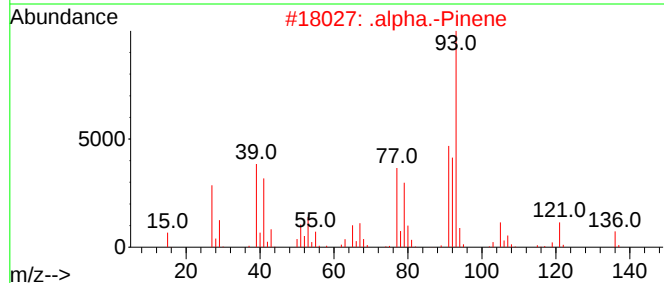
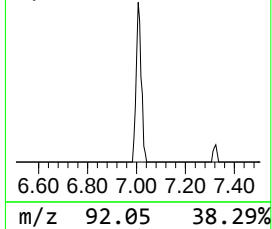
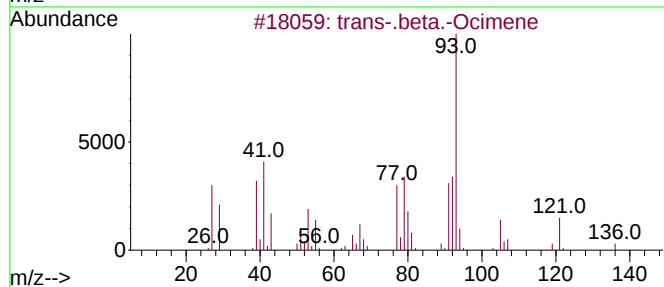
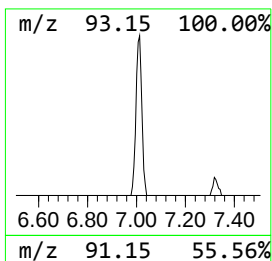
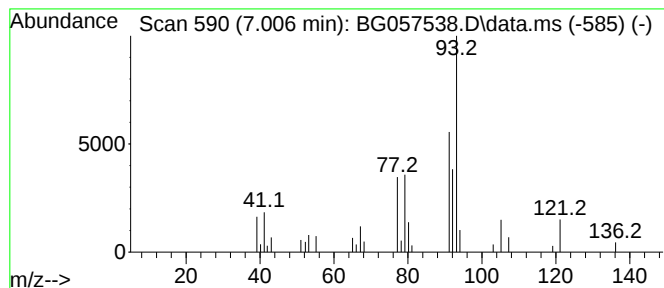
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Peak Number 2 trans-.beta.-Ocimene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.006	6.66 ng	36516	1,4-Dichlorobenzene-d4	8.358

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-.beta.-Ocimene	136	C10H16	003779-61-1	94
2			.alpha.-Pinene	136	C10H16	000080-56-8	91
3			.beta.-Ocimene	136	C10H16	013877-91-3	91
4			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	91
5			(+)-4-Carene	136	C10H16	029050-33-7	91



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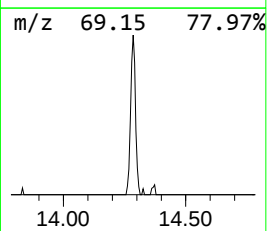
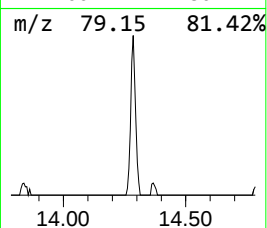
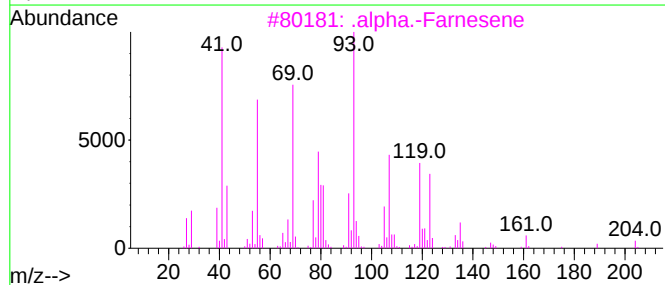
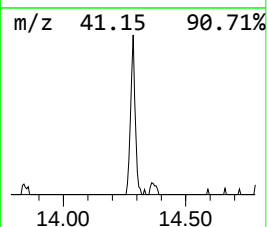
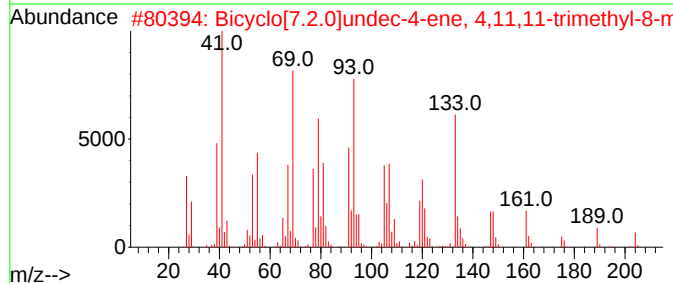
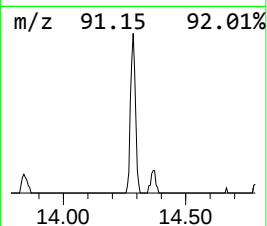
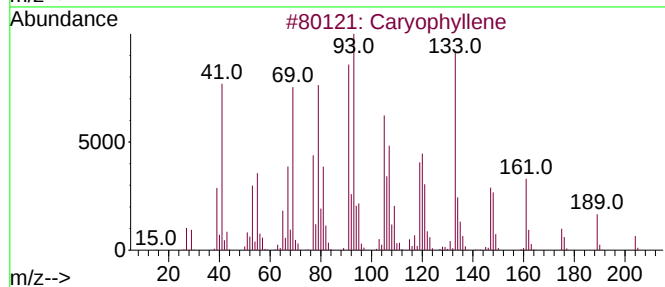
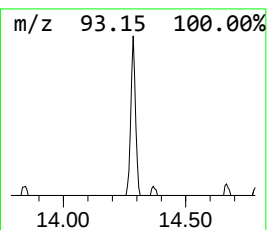
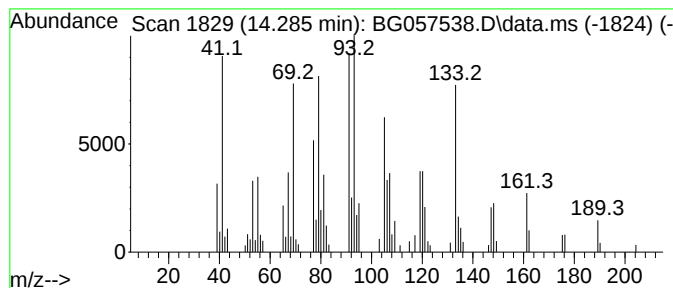
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Peak Number 3 Caryophyllene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.285	9.51 ng	99377	Acenaphthene-d10	14.972

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene	204	C15H24	000087-44-5	99
2			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	83
3			.alpha.-Farnesene	204	C15H24	000502-61-4	43
4			(+)-2-Carene, 4-.alpha.-isopropenyl-	176	C13H20	1000151-26-0	42
5			Bicyclo[5.2.0]nonane, 2-methylen-	204	C15H24	242794-76-9	42



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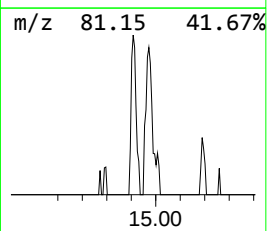
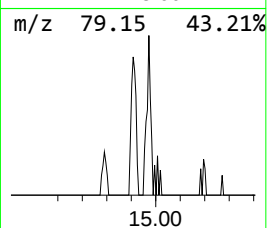
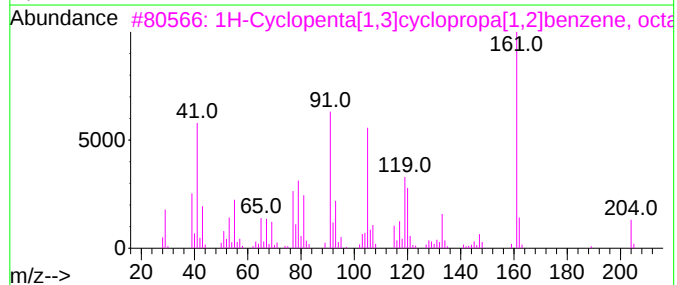
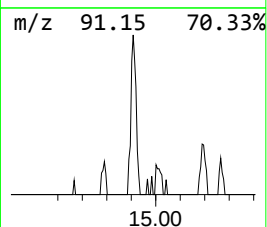
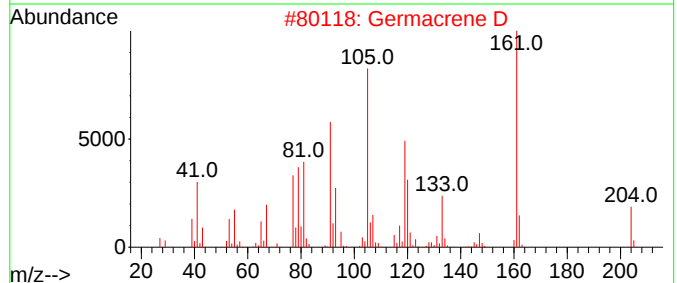
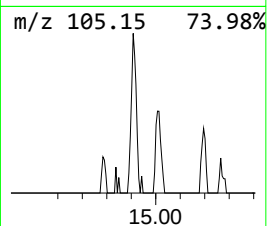
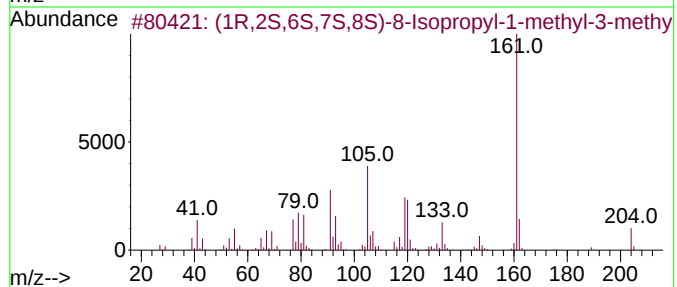
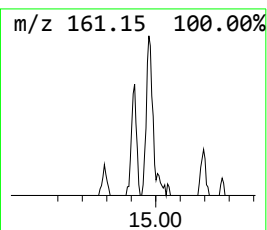
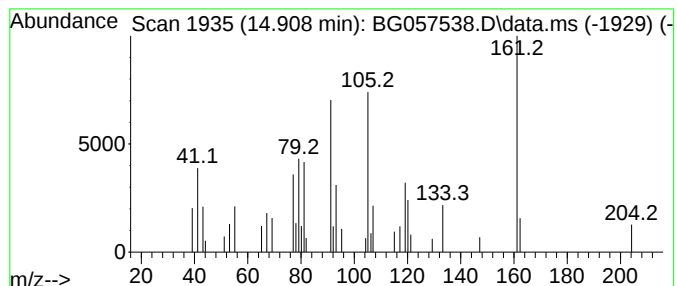
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Peak Number 4 (1R,2S,6S,7S,8S)-8-Isopropy... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.908	2.68 ng	28016	Acenaphthene-d10	14.972

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	96		
2	Germacrene D	204	C15H24	023986-74-5	93		
3	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	93		
4	.beta.-GURJUNENE	204	C15H24	1000425-17-9	70		
5	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	70		



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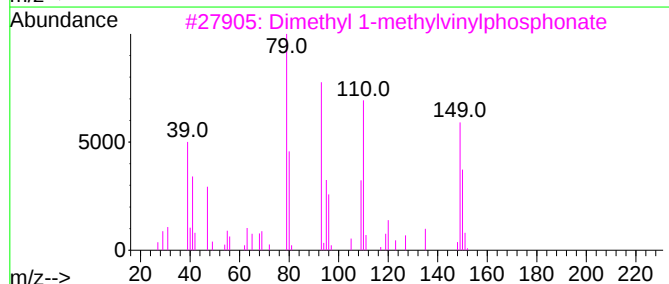
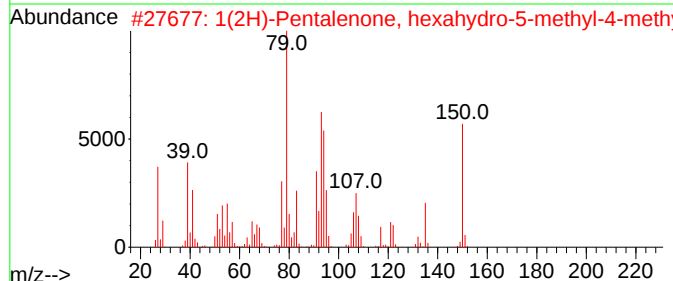
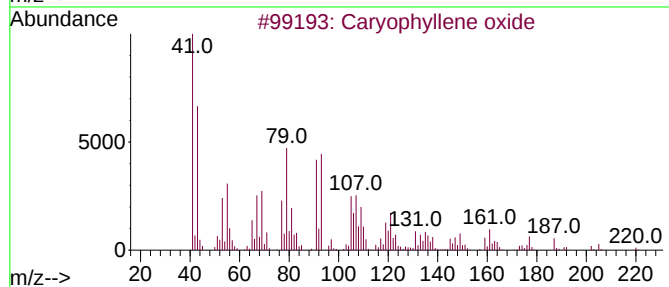
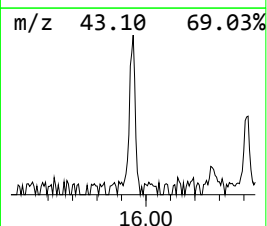
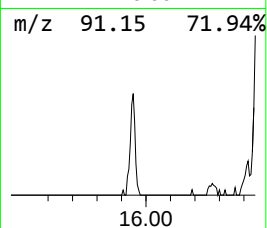
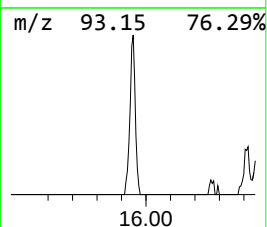
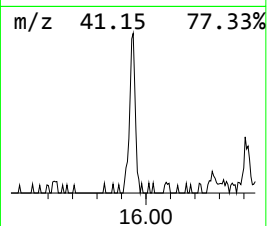
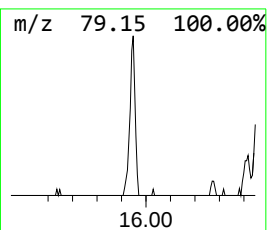
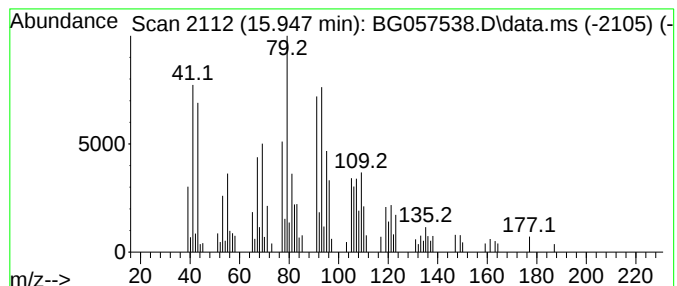
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Peak Number 5 Caryophyllene oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.947	8.36 ng	87368	Acenaphthene-d10	14.972

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene oxide	220	C15H24O	001139-30-6	58
2			1(2H)-Pentalenone, hexahydro-5-m...	150	C10H14O	120587-85-1	58
3			Dimethyl 1-methylvinylphosphonate	150	C5H11O3P	038281-98-0	53
4			Bicyclo[3.1.0]hexan-3-ol, 4-meth...	154	C10H18O	000513-23-5	43
5			3a,6-Methano-3aH-inden-5(4H)-one...	150	C10H14O	016489-26-2	38



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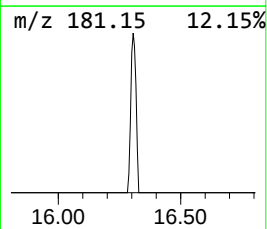
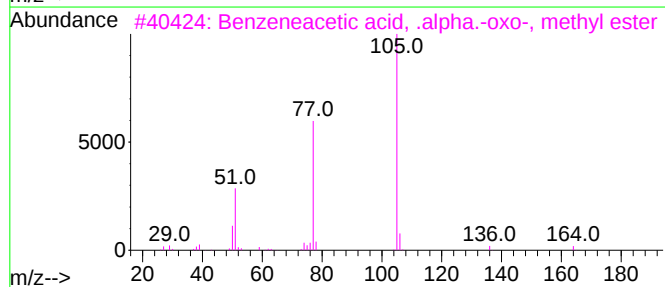
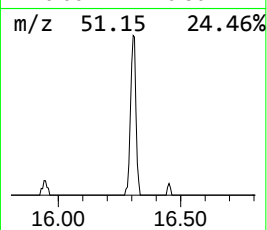
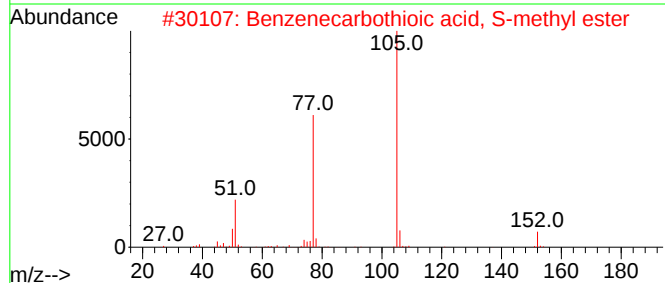
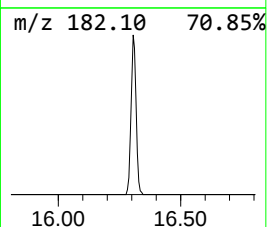
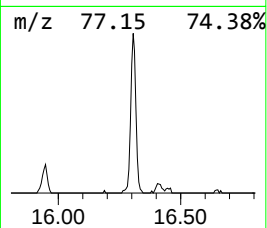
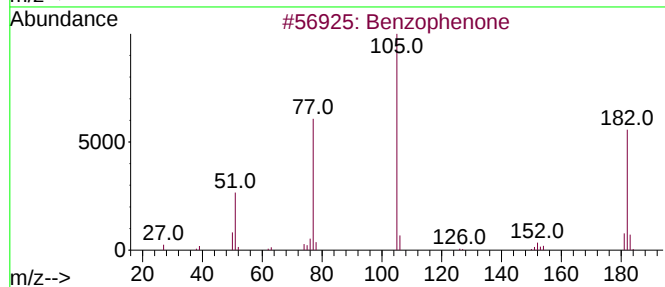
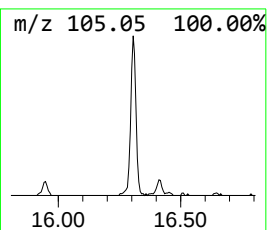
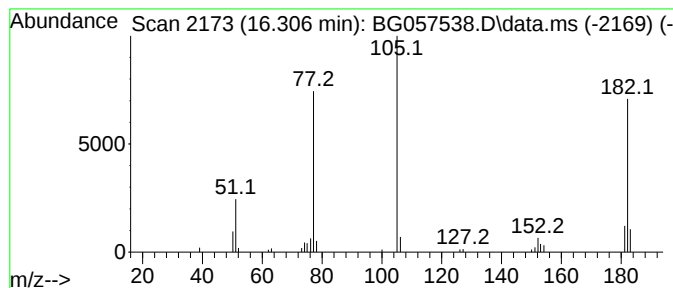
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.306	8.02 ng	83803	Acenaphthene-d10	14.972

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Benzenecarbothioic acid, S-methy...	164	C9H8O3	015206-55-0	50
4			N-cyanobenzamide	146	C8H6N2O	015150-25-1	50
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
Data File : BG057538.D
Acq On : 24 May 2023 17:29
Operator : CG/JU
Sample : 02869-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

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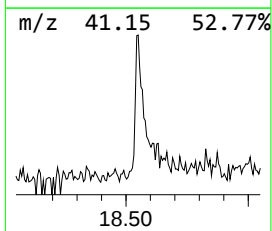
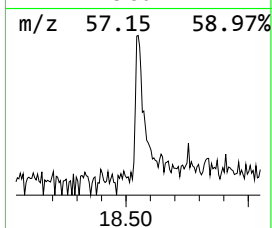
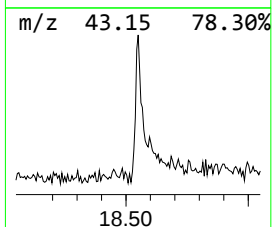
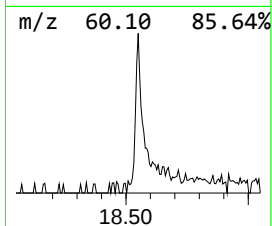
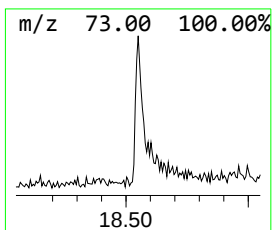
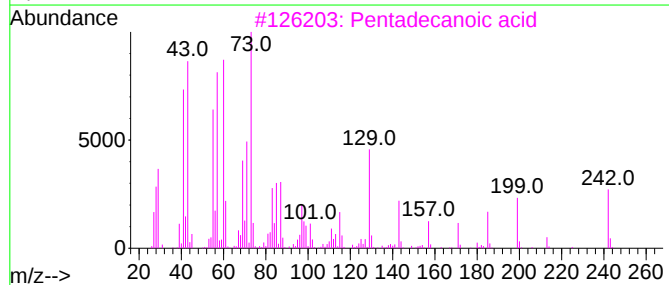
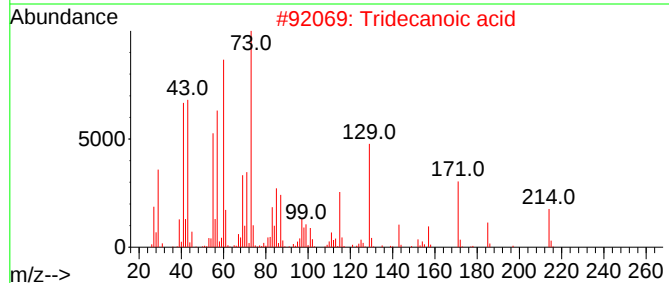
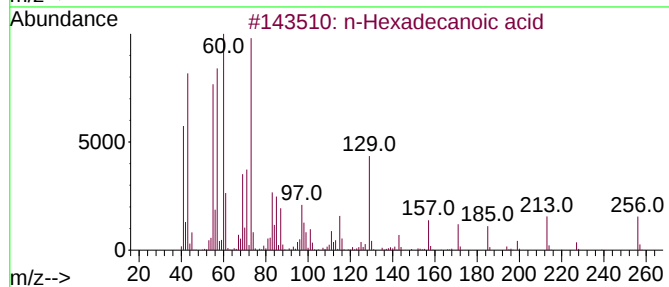
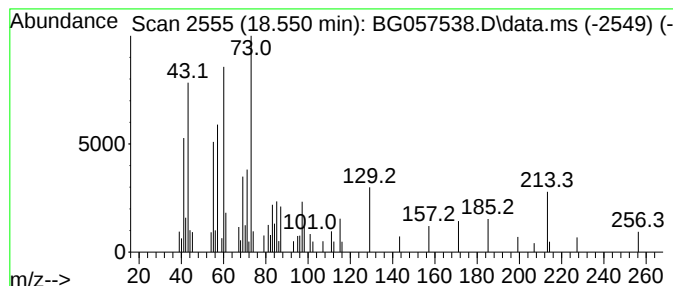
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.550	4.34 ng	60988	Phenanthrene-d10	17.710

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
Data File : BG057538.D
Acq On : 24 May 2023 17:29
Operator : CG/JU
Sample : 02869-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

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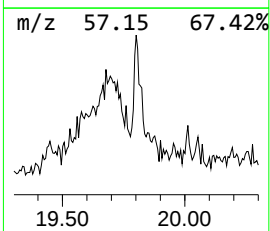
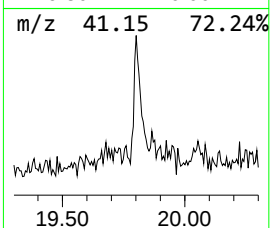
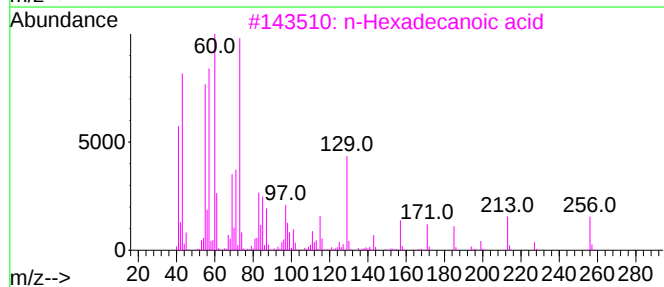
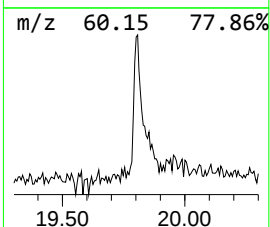
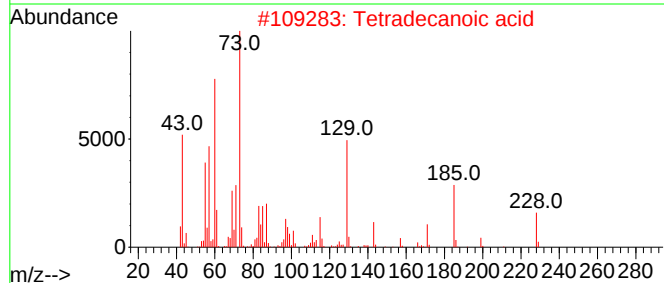
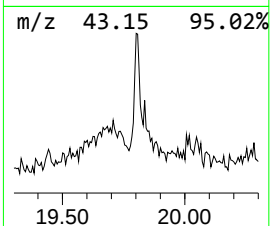
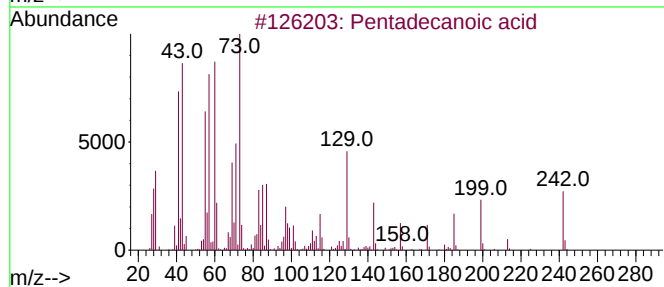
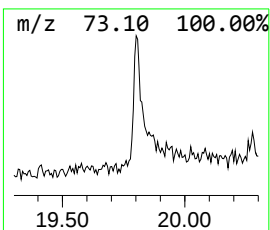
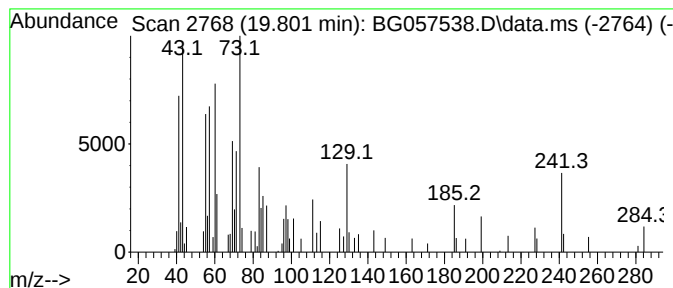
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.801	4.31 ng	60550	Phenanthrene-d10	17.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	52
5			Octadecanoic acid	284	C18H36O2	000057-11-4	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
Data File : BG057538.D
Acq On : 24 May 2023 17:29
Operator : CG/JU
Sample : 02869-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

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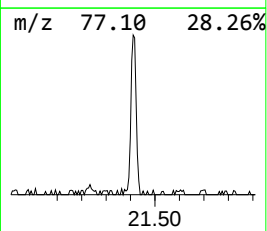
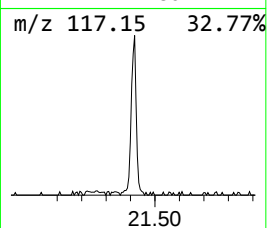
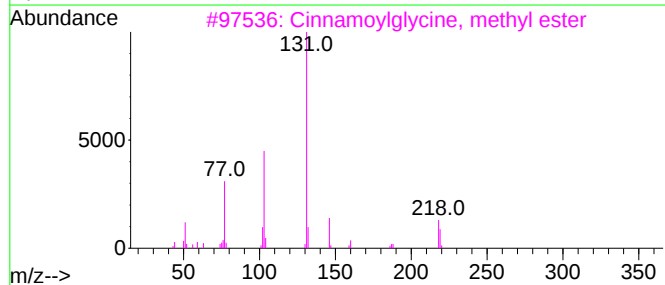
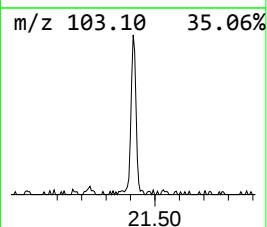
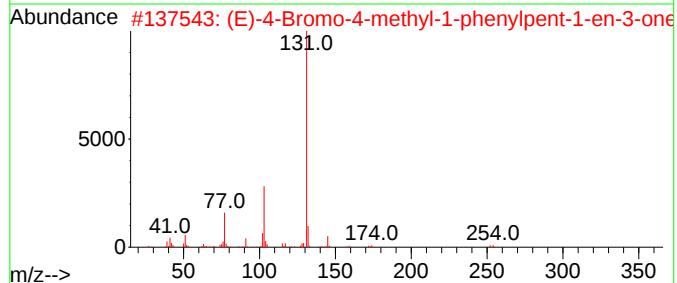
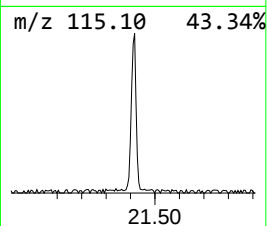
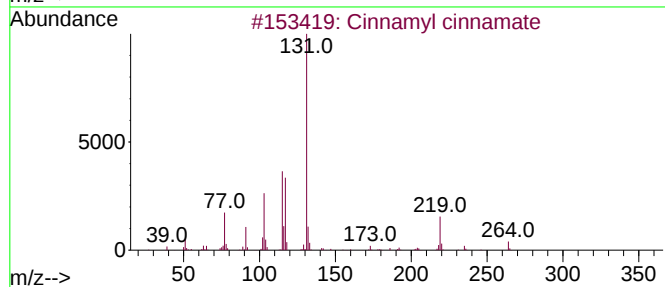
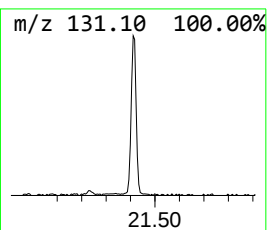
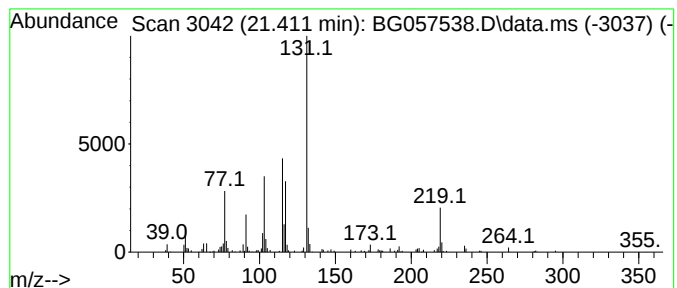
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.410	9.26 ng	161417	Chrysene-d12	22.022

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			Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	47
4			Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	46
5			2-Propenamide, N,N-diethyl-3-phe...	203	C13H17NO	003680-04-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
Data File : BG057538.D
Acq On : 24 May 2023 17:29
Operator : CG/JU
Sample : 02869-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

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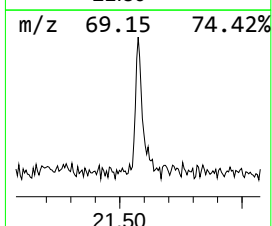
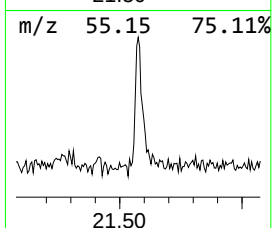
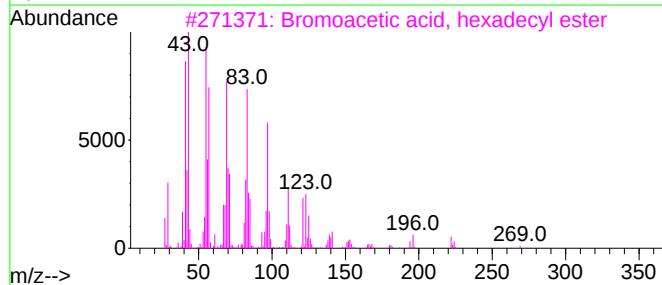
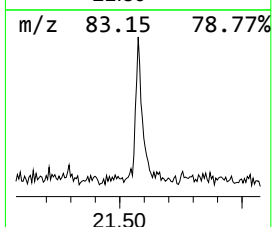
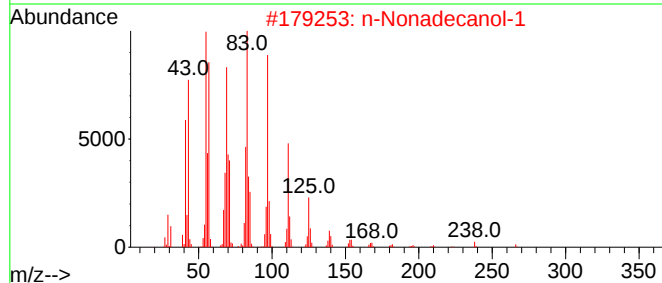
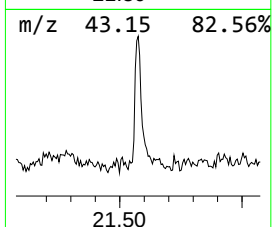
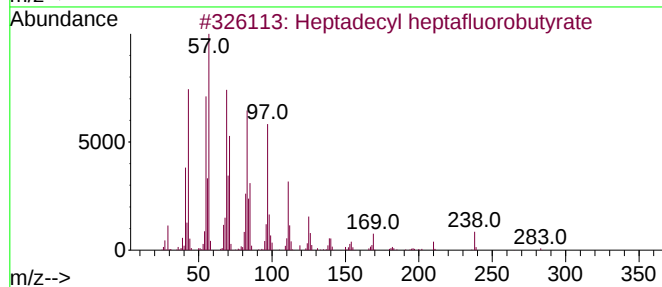
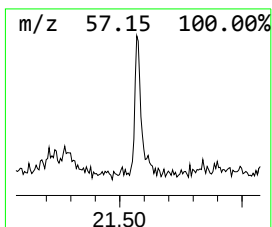
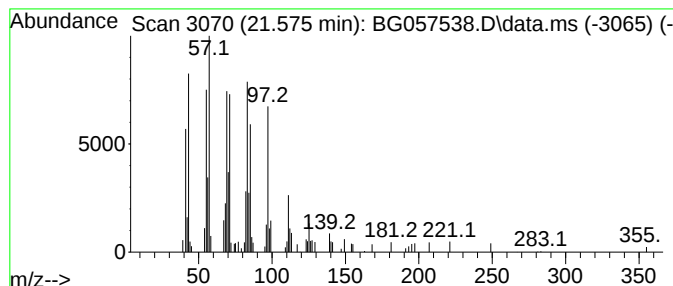
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.575	4.43 ng	77144	Chrysene-d12	22.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	83
3			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	83
4			1-Heptacosanol	396	C27H56O	002004-39-9	83
5			1-Tetracosene	336	C24H48	010192-32-2	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
Data File : BG057538.D
Acq On : 24 May 2023 17:29
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Sample : 02869-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

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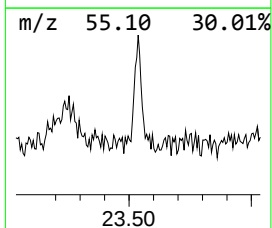
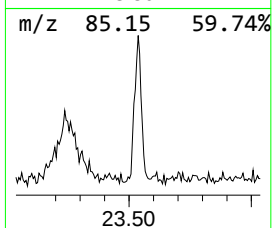
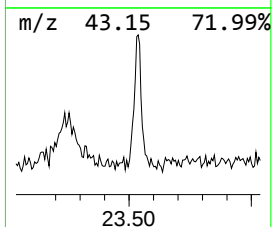
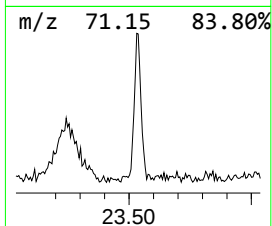
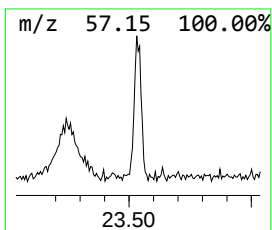
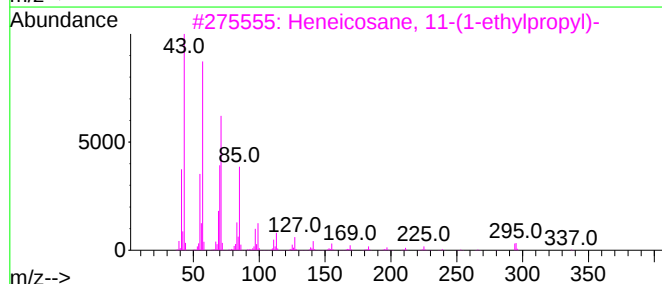
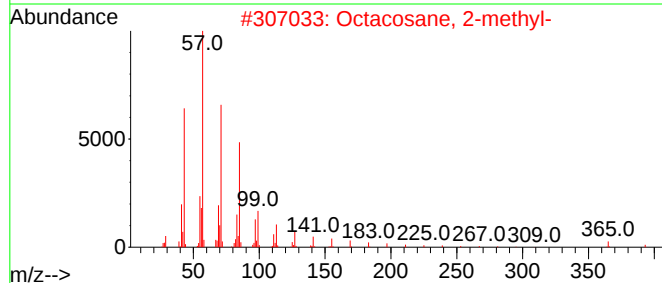
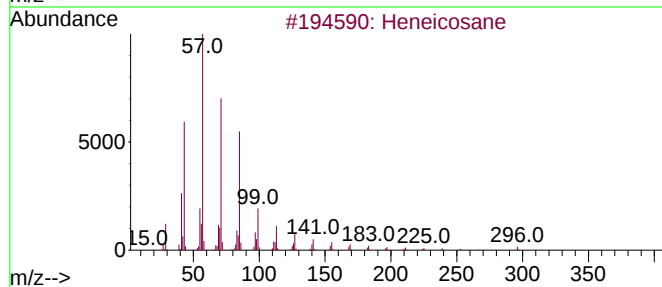
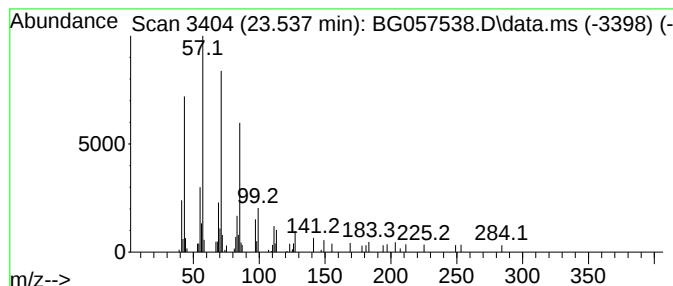
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.537	3.79 ng	65971	Chrysene-d12	22.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4			Eicosane	282	C20H42	000112-95-8	87
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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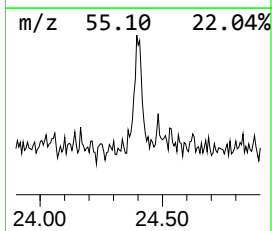
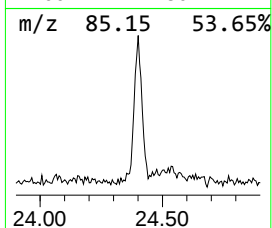
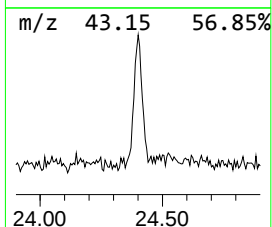
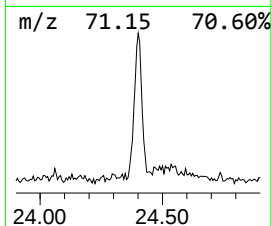
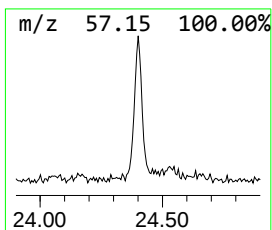
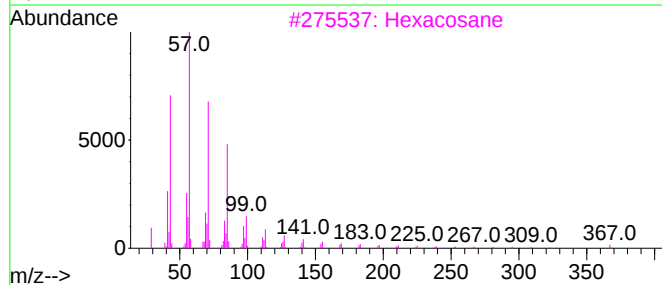
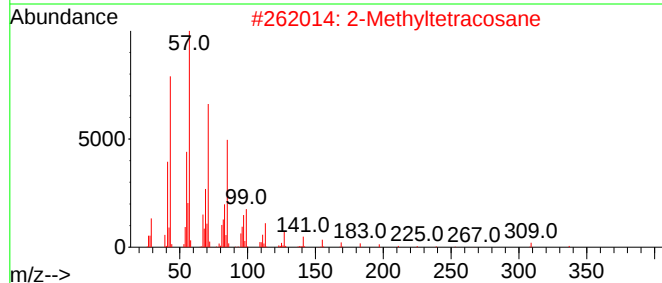
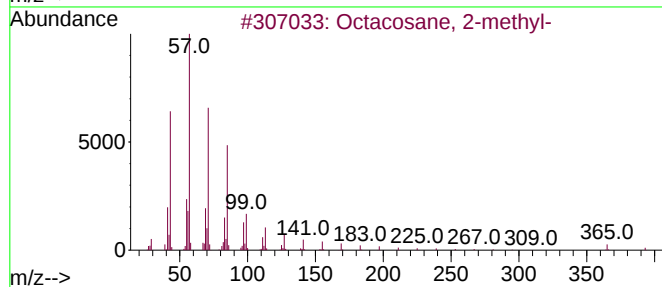
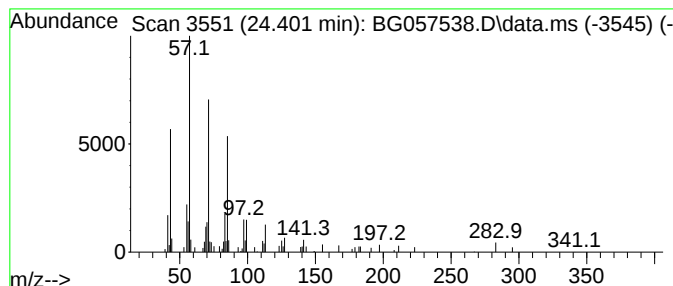
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octacosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.401	4.68 ng	77782	Perylene-d12	25.523

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
2		2-Methyltetracosane	352	C25H52	001560-78-7	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Docosane	310	C22H46	000629-97-0	86
5		Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
Data File : BG057538.D
Acq On : 24 May 2023 17:29
Operator : CG/JU
Sample : 02869-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP19

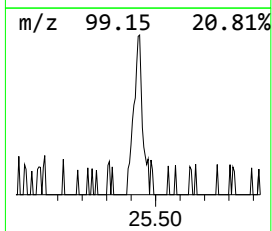
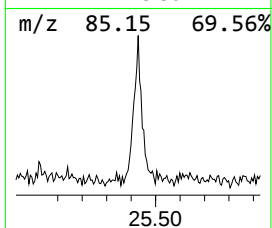
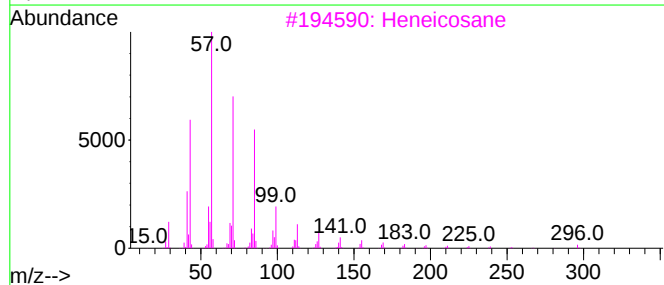
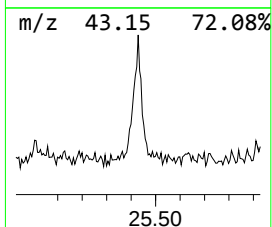
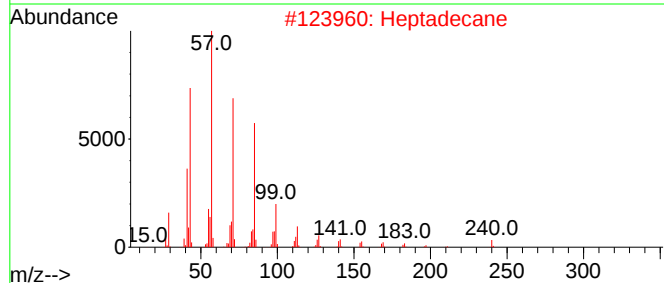
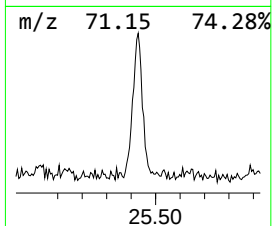
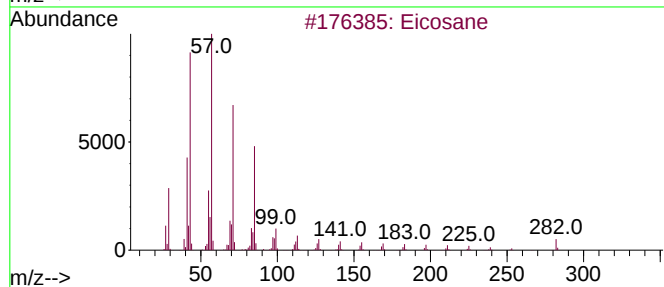
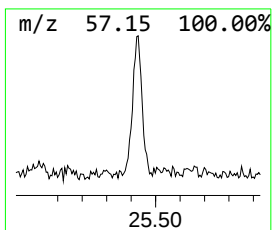
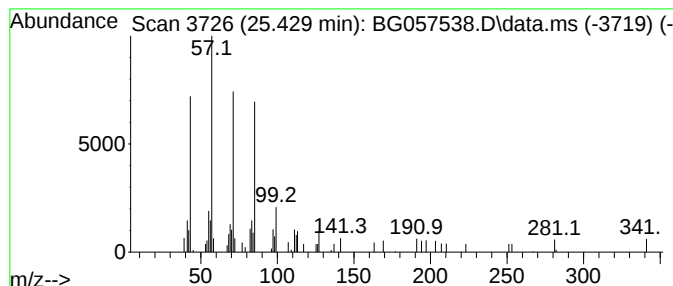
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.429	3.27 ng	54297	Perylene-d12	25.523

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	97
2			Heptadecane	240	C17H36	000629-78-7	87
3			Heneicosane	296	C21H44	000629-94-7	83
4			4-Methylheneicosane	310	C22H46	025117-29-7	83
5			Hexacosane	366	C26H54	000630-01-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
Data File : BG057538.D
Acq On : 24 May 2023 17:29
Operator : CG/JU
Sample : 02869-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

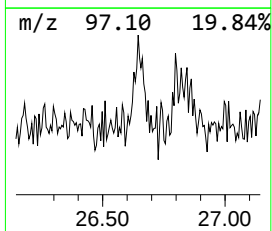
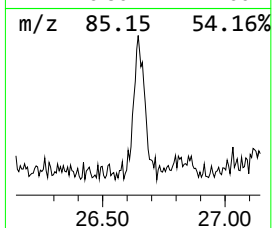
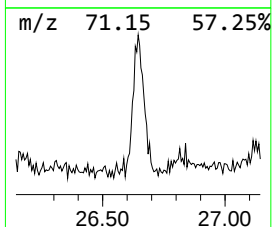
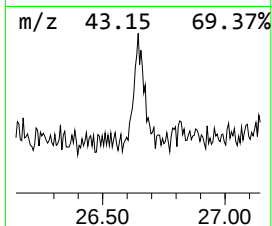
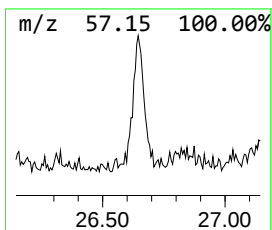
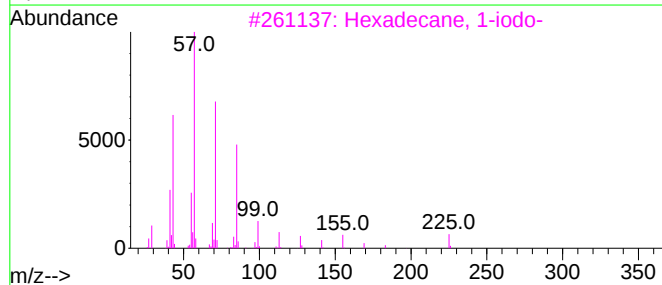
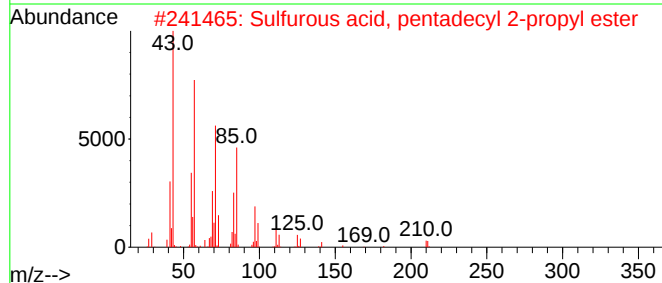
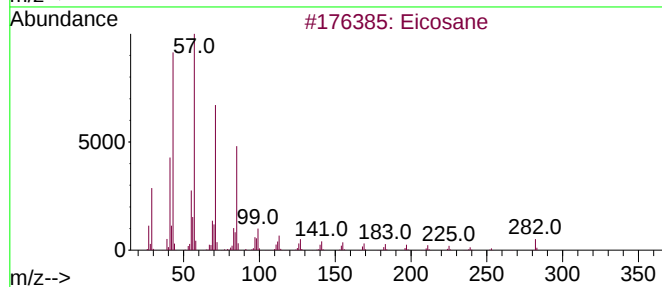
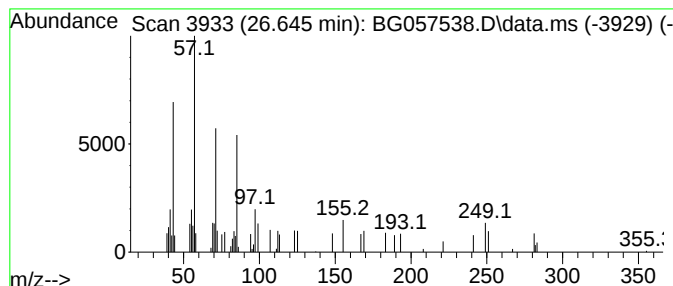
Instrument :
BNA_G
ClientSampleId :
TP19

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 14 Sulfurous acid, pentadecyl ... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
26.645	2.58 ng	42804	Perylene-d12		25.523	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	89
2	Sulfurous acid, pentadecyl 2-pro...		334	C18H38O3S	1000309-12-6	50
3	Hexadecane, 1-iodo-		352	C16H33I	000544-77-4	43
4	Octadecane		254	C18H38	000593-45-3	43
5	Hexadecane, 7,9-dimethyl-		254	C18H38	021164-95-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
Data File : BG057538.D
Acq On : 24 May 2023 17:29
Operator : CG/JU
Sample : 02869-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP19

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-...	5.391	4.5	ng	24630	1	8.358	109738	20.0
trans-.beta.-Oc...	7.006	6.7	ng	36516	1	8.358	109738	20.0
Caryophyllene	14.285	9.5	ng	99377	3	14.972	208921	20.0
(1R,2S,6S,7S,8S...	14.908	2.7	ng	28016	3	14.972	208921	20.0
Caryophyllene o...	15.947	8.4	ng	87368	3	14.972	208921	20.0
Benzophenone	16.306	8.0	ng	83803	3	14.972	208921	20.0
n-Hexadecanoic ...	18.550	4.3	ng	60988	4	17.710	280923	20.0
Pentadecanoic acid	19.801	4.3	ng	60550	4	17.710	280923	20.0
Cinnamyl cinnamate	21.410	9.3	ng	161417	5	22.022	348459	20.0
Heptadecyl hept...	21.575	4.4	ng	77144	5	22.022	348459	20.0
Heneicosane	23.537	3.8	ng	65971	5	22.022	348459	20.0
Octacosane, 2-m...	24.401	4.7	ng	77782	6	25.523	332274	20.0
Eicosane	25.429	3.3	ng	54297	6	25.523	332274	20.0
Sulfurous acid,...	26.645	2.6	ng	42804	6	25.523	332274	20.0