

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
 Data File : BG058629.D
 Acq On : 7 Aug 2023 16:18
 Operator : MA/JU
 Sample : 03862-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EQUIPMENT-BLANK-1

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-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058629.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.583	80	84	89	rVB	43481	57880	1.32%	0.262%
2	4.352	208	215	228	rVB2	57910	115188	2.63%	0.521%
3	5.386	384	391	401	rBV	334074	531949	12.13%	2.405%
4	6.985	658	663	674	rVB	189038	327317	7.46%	1.480%
5	7.813	796	804	809	rBV	133899	222027	5.06%	1.004%
6	7.872	809	814	822	rVB	76370	118303	2.70%	0.535%
7	8.976	994	1002	1014	rBV	504429	925107	21.10%	4.183%
8	9.135	1022	1029	1040	rVB3	28258	58632	1.34%	0.265%
9	10.616	1274	1281	1293	rVB	196158	353735	8.07%	1.600%
10	11.139	1362	1370	1376	rBV	284004	491855	11.22%	2.224%
11	11.203	1376	1381	1393	rVB	327997	592930	13.52%	2.681%
12	11.421	1410	1418	1423	rBV7	27211	69215	1.58%	0.313%
13	11.485	1423	1429	1435	rVV5	23841	73028	1.67%	0.330%
14	11.556	1435	1441	1453	rVB3	119764	232038	5.29%	1.049%
15	12.384	1573	1582	1586	rBV3	27997	69978	1.60%	0.316%
16	12.496	1595	1601	1615	rBV	100014	174067	3.97%	0.787%
17	12.907	1666	1671	1682	rVB3	28079	46051	1.05%	0.208%
18	13.077	1693	1700	1715	rBV	1358780	2238249	51.05%	10.121%
19	13.365	1740	1749	1764	rBV	2352180	4384764	100.00%	19.827%
20	14.458	1929	1935	1944	rBV	353694	554762	12.65%	2.509%
21	15.951	2182	2189	2208	rBV	1241271	1997622	45.56%	9.033%
22	17.208	2396	2403	2413	rBV	510861	794137	18.11%	3.591%
23	17.490	2436	2451	2453	rBV3	26556	88977	2.03%	0.402%
24	18.095	2549	2554	2565	rBV4	52252	105047	2.40%	0.475%
25	19.065	2713	2719	2730	rVB	39432	68152	1.55%	0.308%
26	19.258	2744	2752	2760	rBV6	59875	138661	3.16%	0.627%
27	19.505	2789	2794	2803	rBV2	376334	492714	11.24%	2.228%
28	19.828	2842	2849	2859	rBV	2679586	3650132	83.25%	16.505%
29	20.504	2956	2964	2975	rBV	761892	1161695	26.49%	5.253%
30	21.444	3118	3124	3134	rBV2	536413	897124	20.46%	4.057%
31	21.879	3191	3198	3207	rBV2	91410	183686	4.19%	0.831%
32	22.555	3308	3313	3324	rVB4	55995	100198	2.29%	0.453%
33	24.517	3636	3647	3664	rBV2	270637	799914	18.24%	3.617%

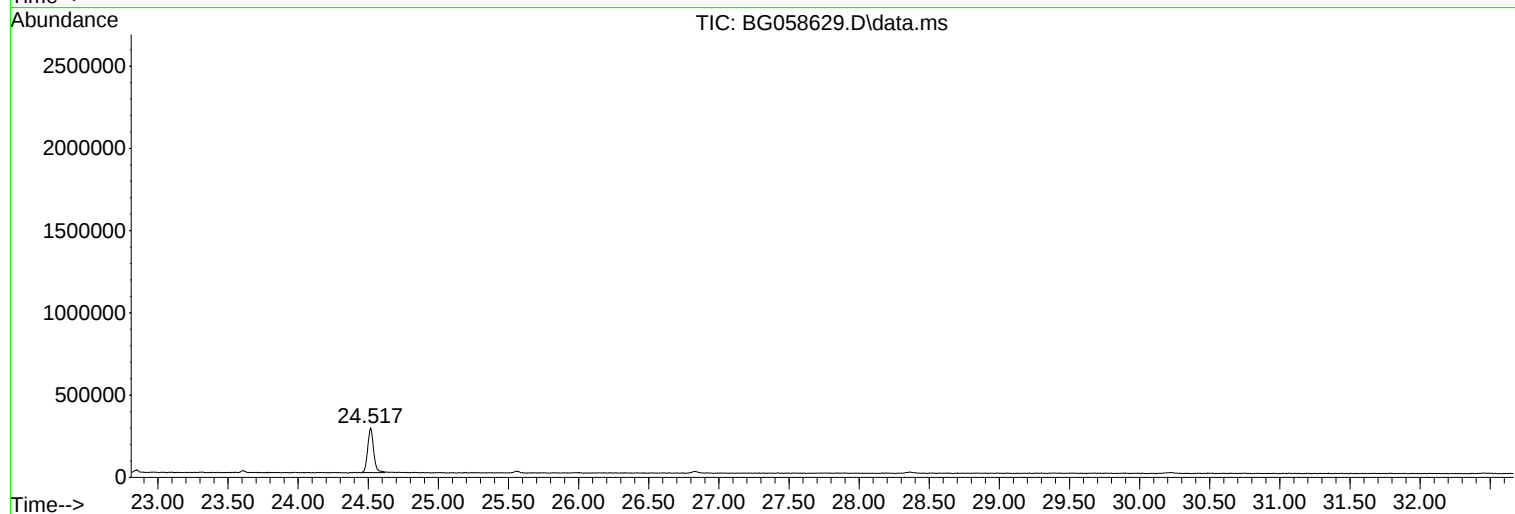
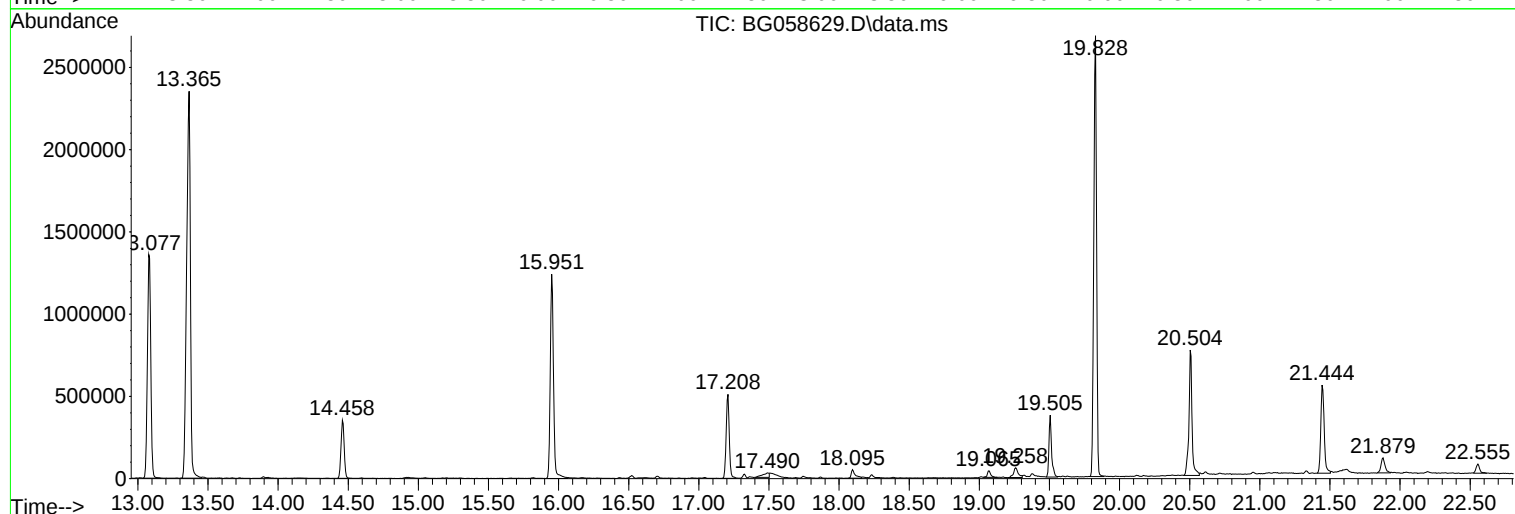
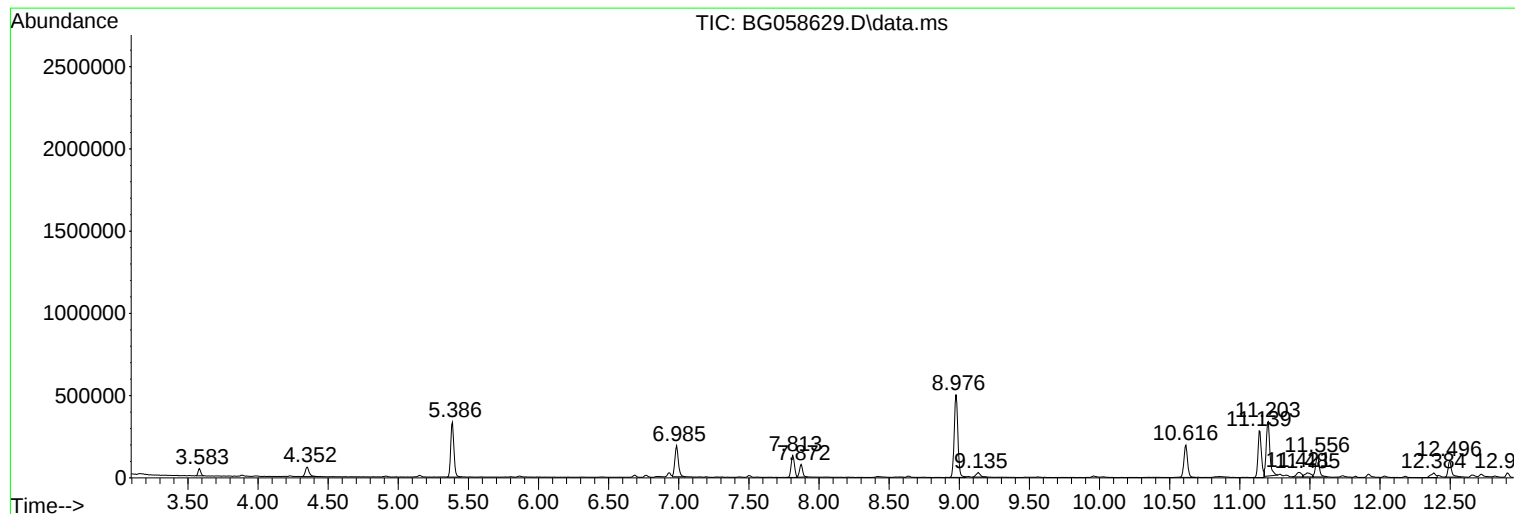
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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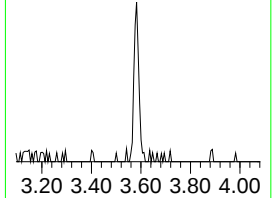
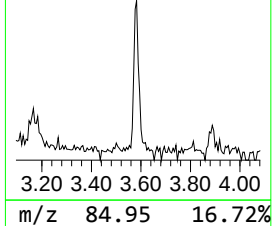
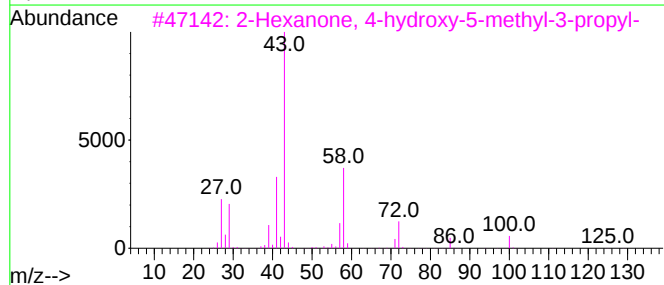
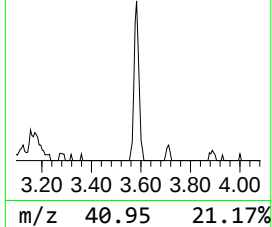
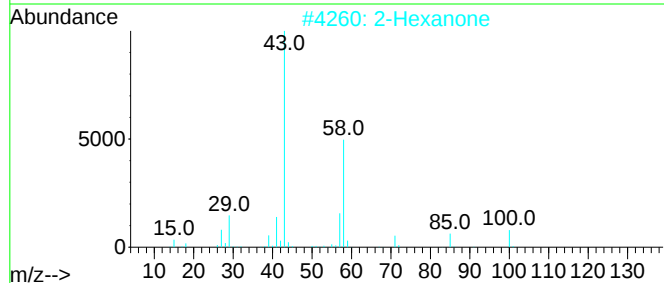
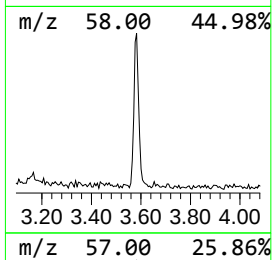
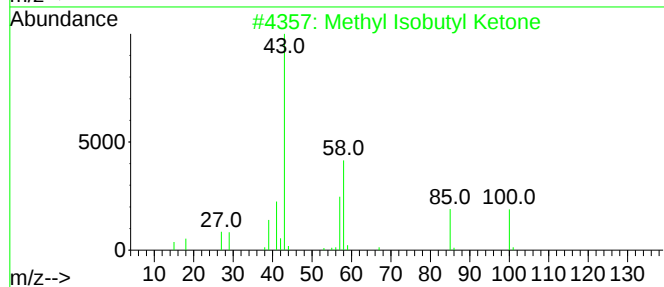
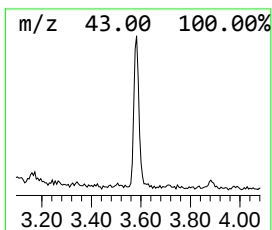
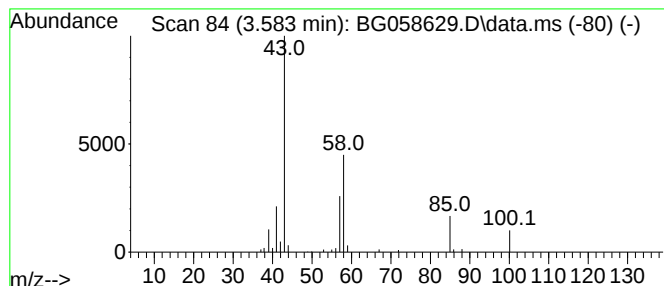
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Methyl Isobutyl Ketone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.583	5.21 ng	57880	1,4-Dichlorobenzene-d4	7.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	90
2			2-Hexanone	100	C6H12O	000591-78-6	78
3			2-Hexanone, 4-hydroxy-5-methyl-3...	172	C10H20O2	061141-74-0	43
4			2-Hexanone, 4-hydroxy-3-propyl-	158	C9H18O2	062338-17-4	43
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	37



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ALS Vial : 13 Sample Multiplier: 1

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BNA_G
ClientSampleId :
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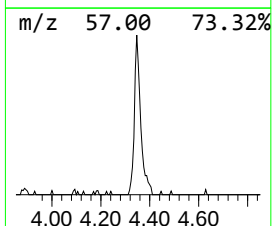
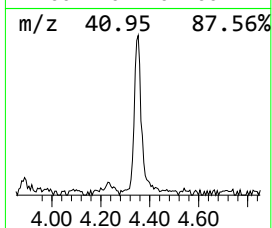
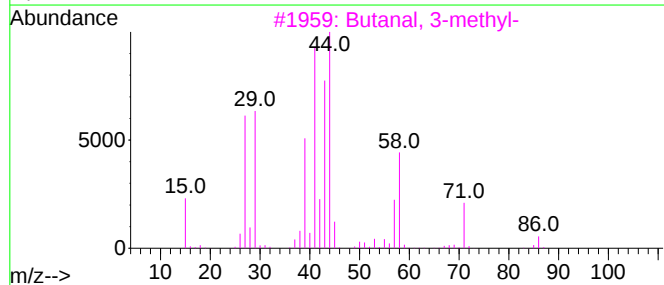
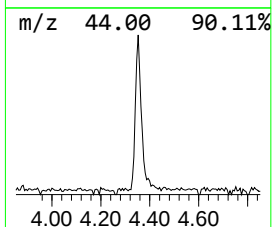
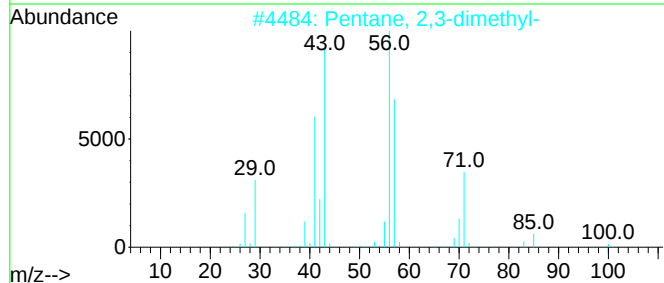
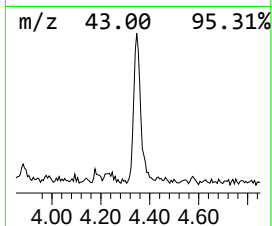
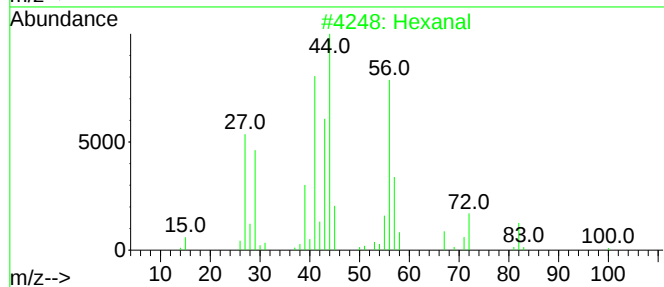
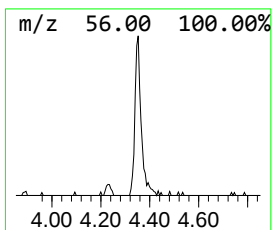
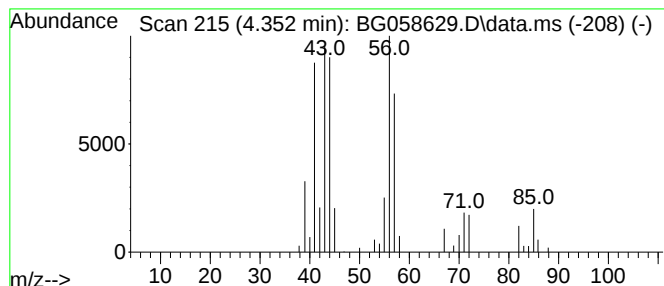
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.352	10.38 ng	115188	1,4-Dichlorobenzene-d4	7.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	64
2			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	35
3			Butanal, 3-methyl-	86	C5H10O	000590-86-3	35
4			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	27
5			Butanal	72	C4H8O	000123-72-8	27



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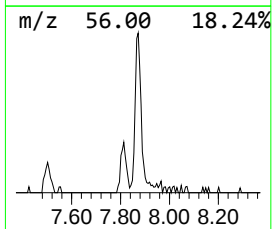
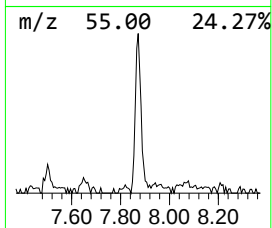
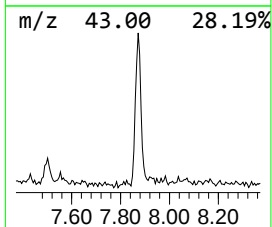
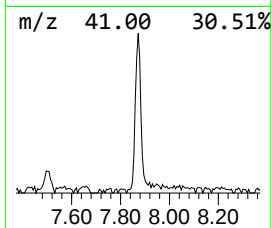
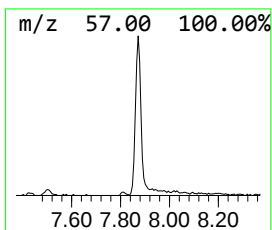
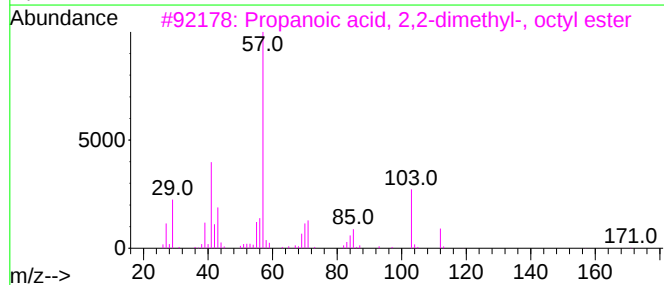
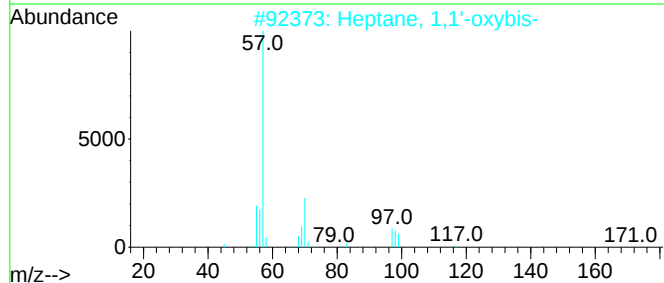
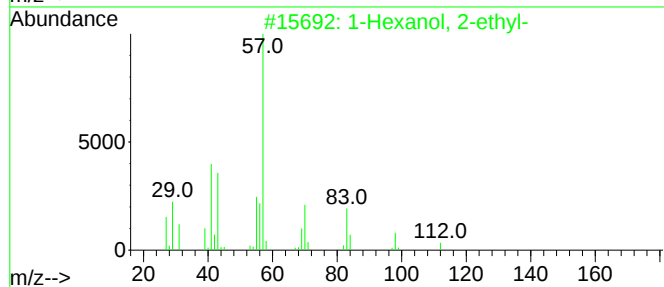
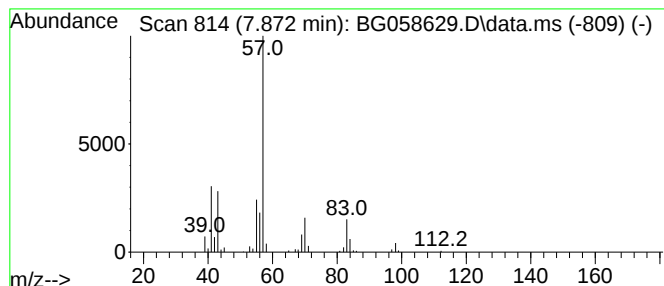
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.872	10.66 ng	118303	1,4-Dichlorobenzene-d4	7.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
3			Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	59
4			Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	53
5			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50



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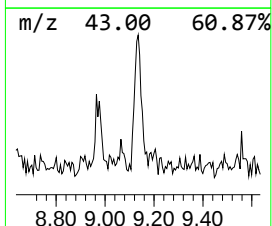
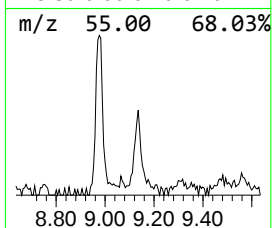
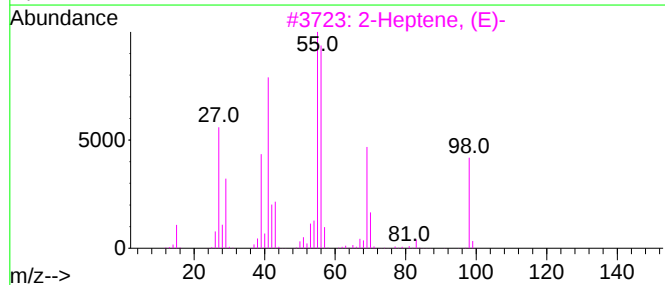
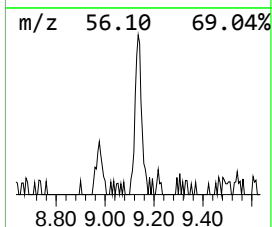
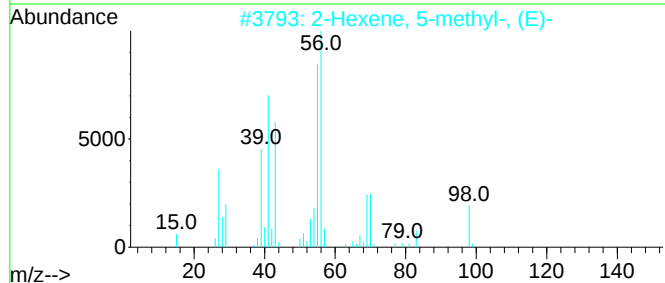
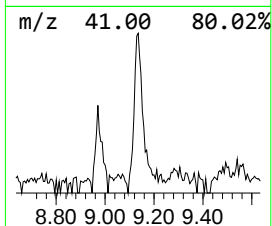
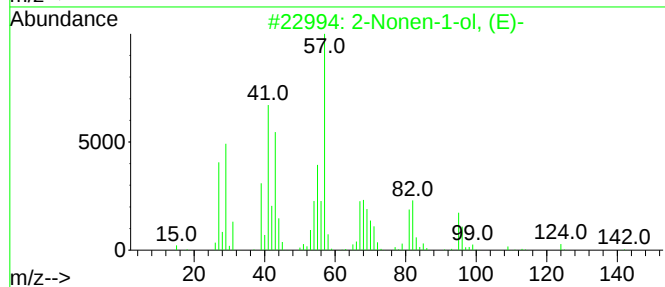
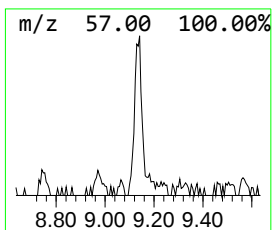
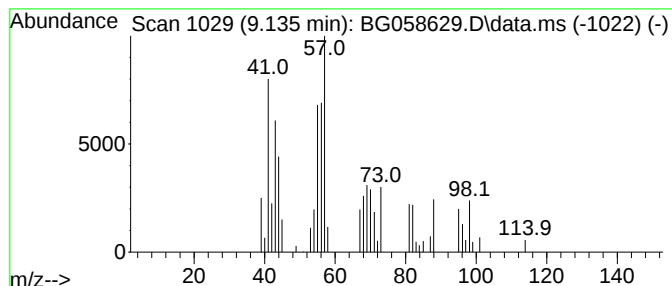
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Peak Number 4 unknown9.135 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.135	5.28 ng	58632	1,4-Dichlorobenzene-d4	7.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonen-1-ol, (E)-			142	C9H18O	031502-14-4	25
2	2-Hexene, 5-methyl-, (E)-			98	C7H14	007385-82-2	22
3	2-Heptene, (E)-			98	C7H14	014686-13-6	18
4	(Z)-2-Heptene			98	C7H14	006443-92-1	18
5	2-Heptene			98	C7H14	000592-77-8	18



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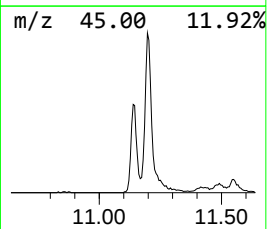
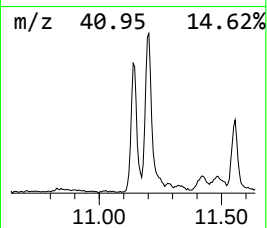
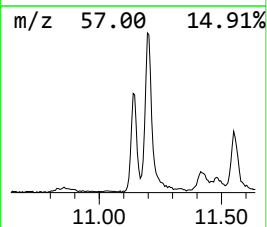
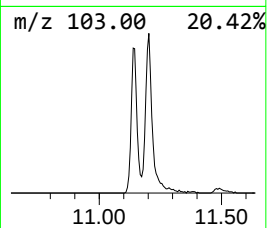
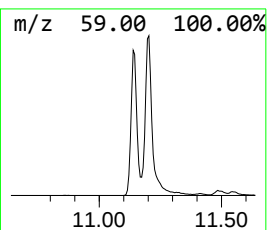
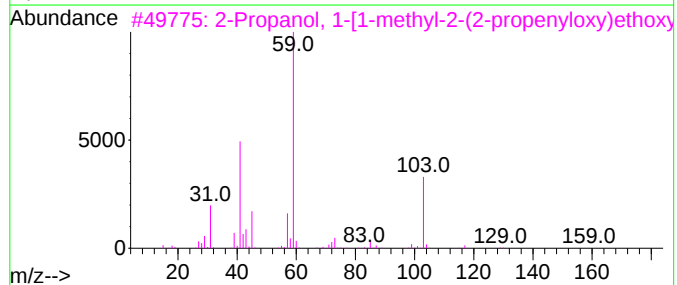
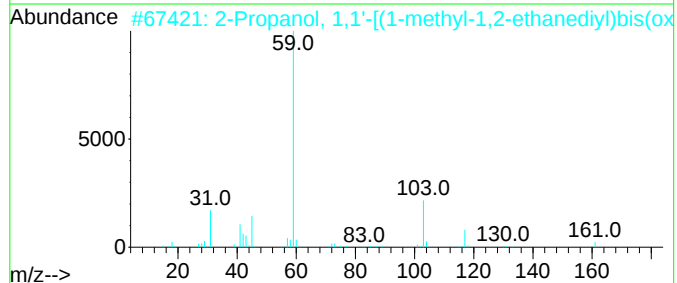
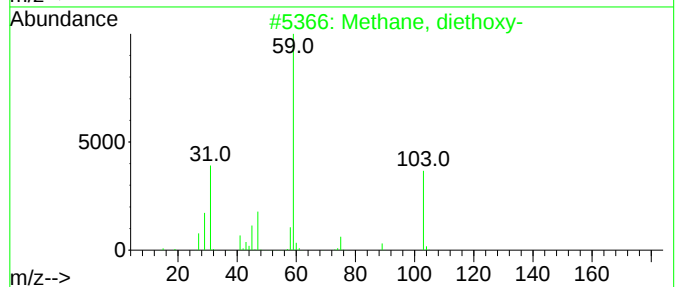
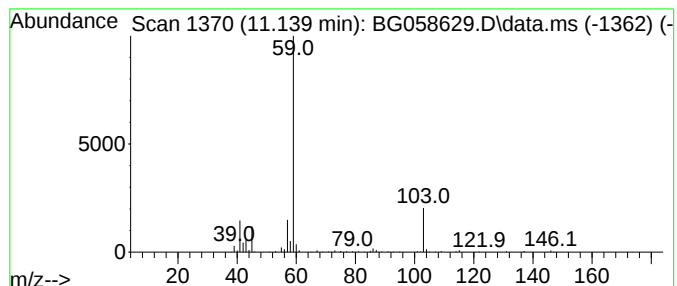
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Methane, diethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.139	27.81 ng	491855	Naphthalene-d8	10.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, diethoxy-	104	C5H12O2	000462-95-3	80
2			2-Propanol, 1,1'-[(1-methyl-1,2-...]	192	C9H20O4	001638-16-0	78
3			2-Propanol, 1-[1-methyl-2-(2-pro...]	174	C9H18O3	055956-25-7	74
4			1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	64
5			Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
Misc :
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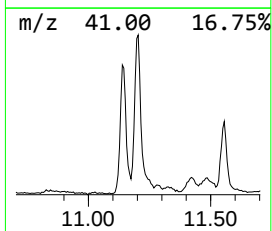
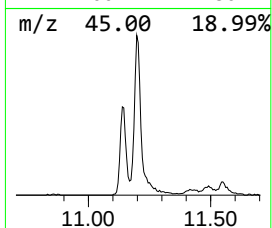
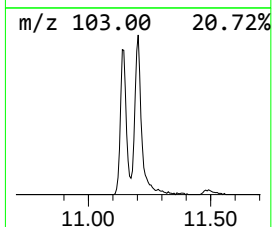
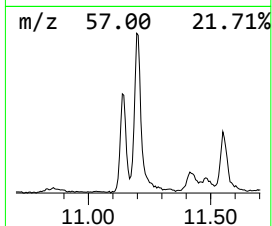
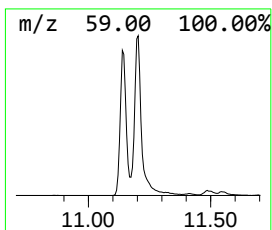
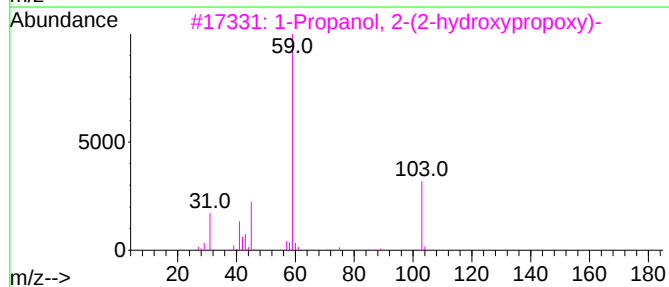
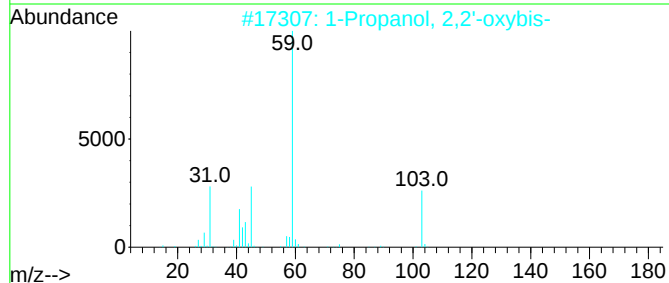
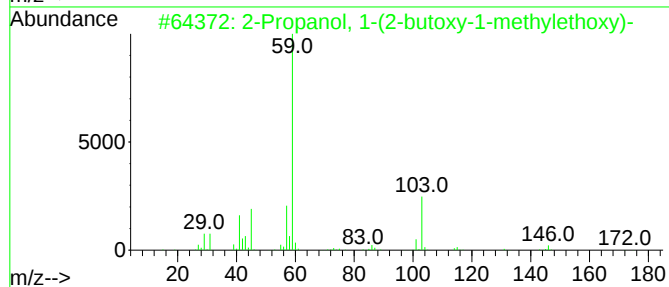
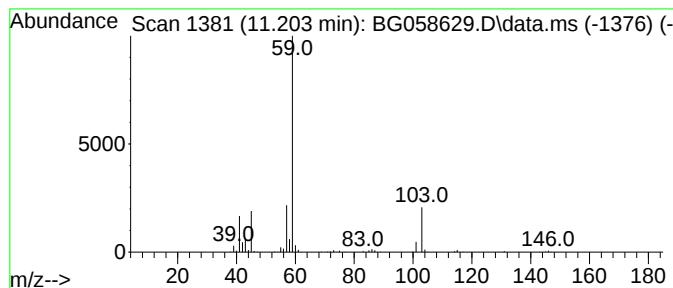
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.203	33.52 ng	592930	Naphthalene-d8	10.616	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	83
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	78
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
4	Tetraglyme	222	C10H22O5	000143-24-8	72
5	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1010367-13-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

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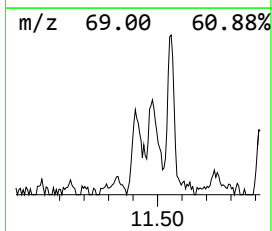
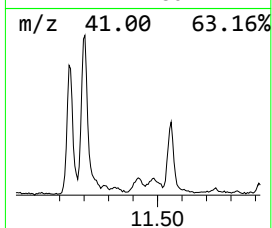
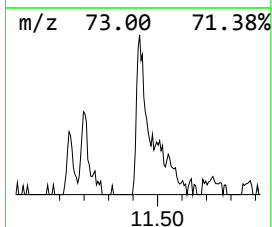
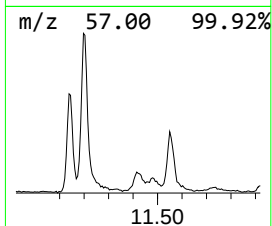
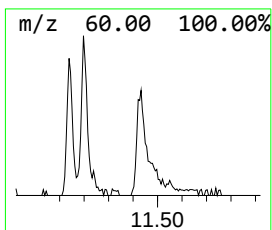
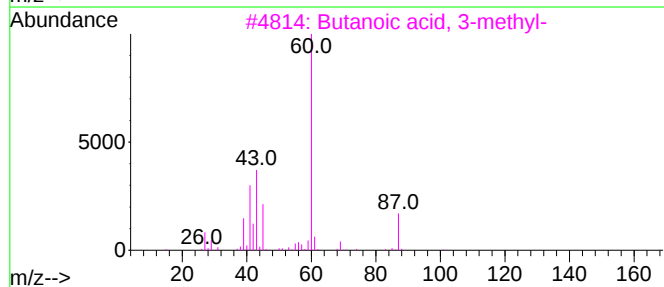
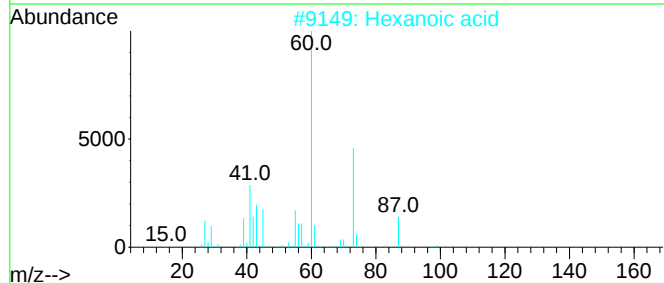
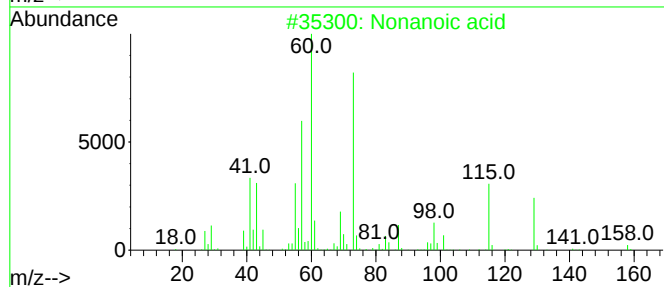
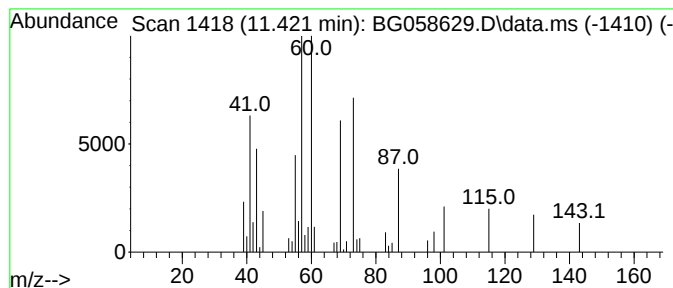
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.421	3.91 ng	69215	Naphthalene-d8	10.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	53
2			Hexanoic acid	116	C6H12O2	000142-62-1	50
3			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	47
4			Heptanoic acid	130	C7H14O2	000111-14-8	45
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
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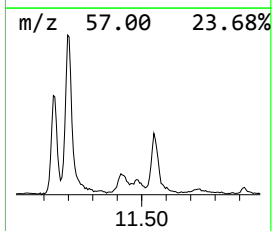
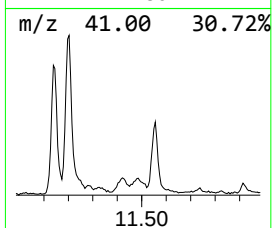
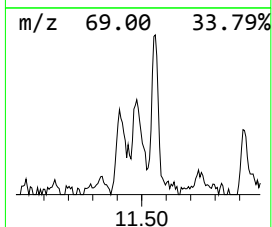
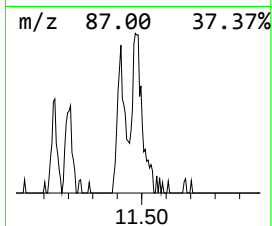
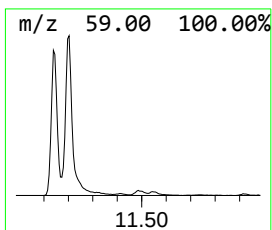
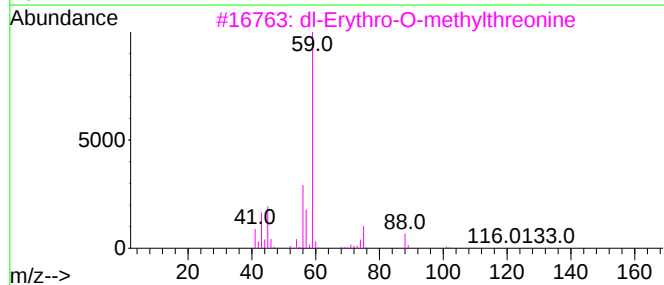
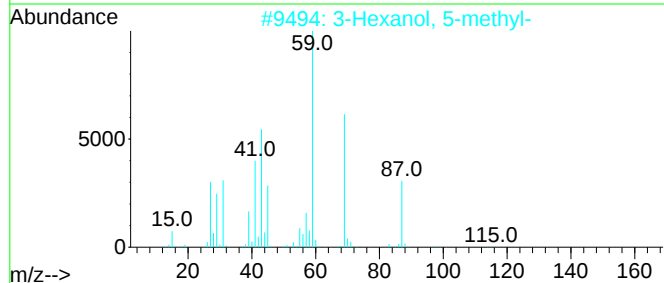
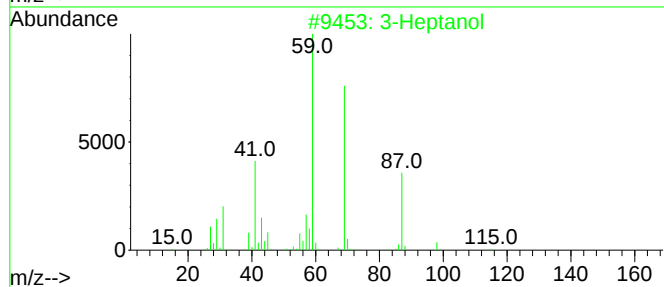
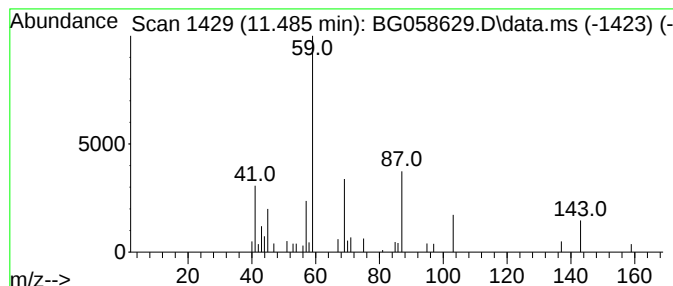
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown11.485 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.485	4.13 ng	73028	Naphthalene-d8		10.616	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Heptanol		116	C7H16O	000589-82-2	38
2	3-Hexanol, 5-methyl-		116	C7H16O	000623-55-2	36
3	dl-Erythro-0-methylthreonine		133	C5H11NO3	1000214-70-7	28
4	Ether, hexyl t-butyl		158	C10H22O	069775-79-7	25
5	2-Hexanol, 2,5-dimethyl-, (S)-		130	C8H18O	003730-60-7	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

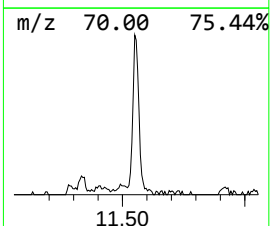
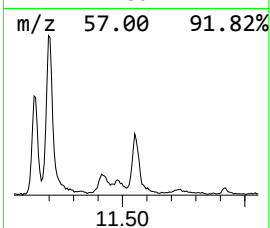
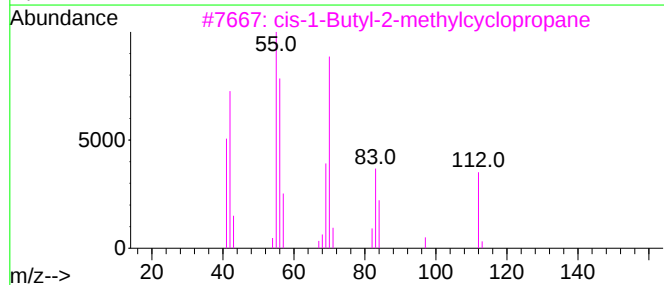
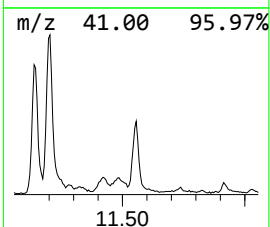
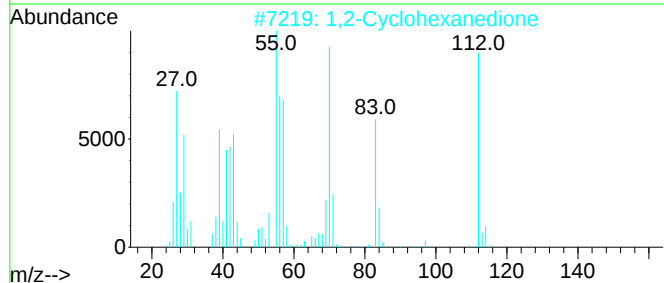
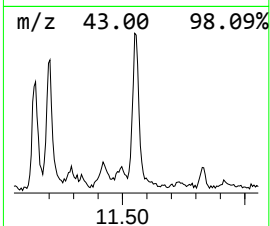
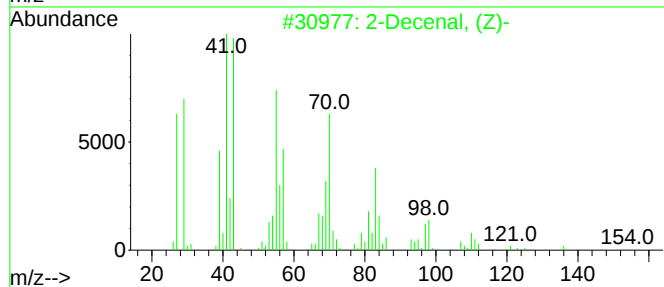
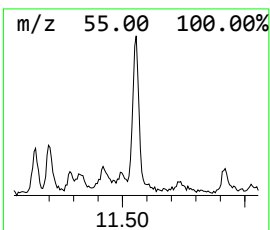
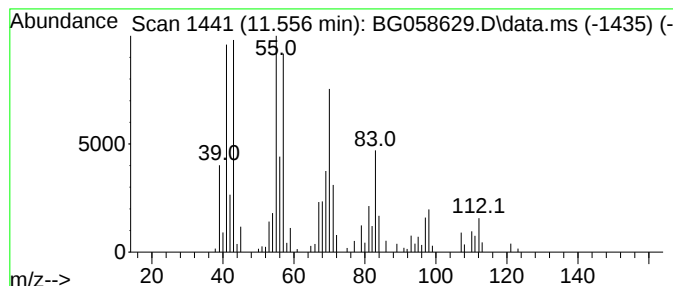
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Decenal, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.556	13.12 ng	232038	Naphthalene-d8	10.616	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decenal, (Z)-	154	C10H18O	002497-25-8	64
2	1,2-Cyclohexanedione	112	C6H8O2	000765-87-7	53
3	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	52
4	1-Fluorooctane	132	C8H17F	000463-11-6	50
5	2-Decenal, (E)-	154	C10H18O	003913-81-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
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ALS Vial : 13 Sample Multiplier: 1

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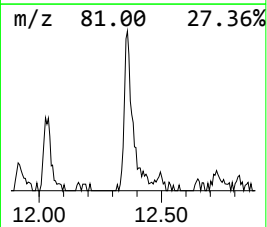
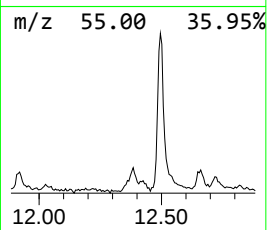
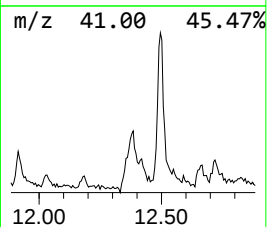
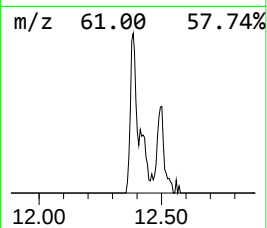
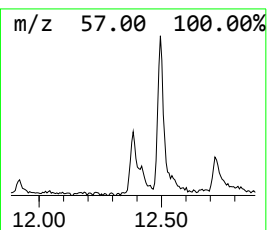
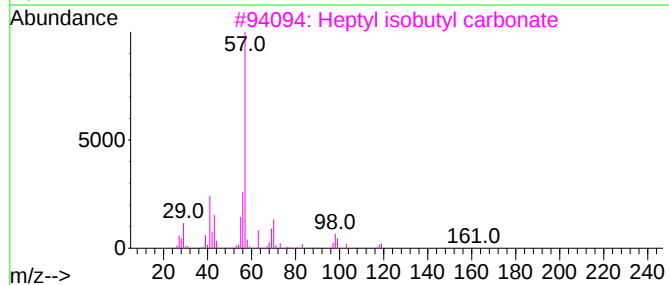
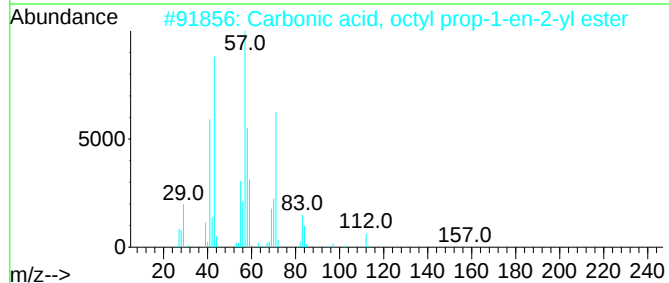
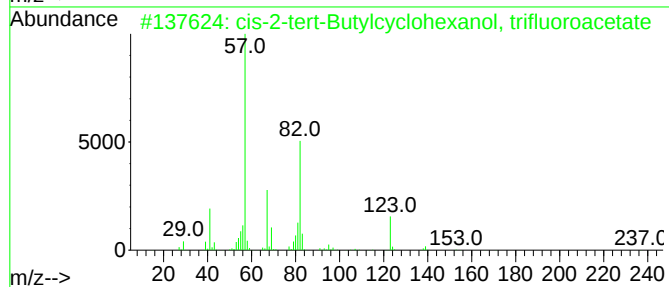
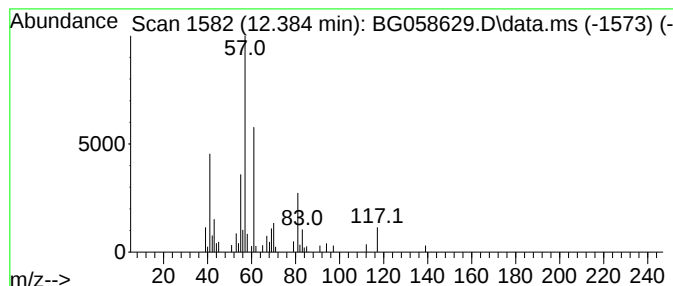
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown12.384 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.384	3.96 ng	69978	Naphthalene-d8	10.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis-2-tert-Butylcyclohexanol, tr...	252	C12H19F3O2	1000467-27-6	16
2		Carbonic acid, octyl prop-1-en-2...	214	C12H22O3	1000382-54-0	13
3		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	12
4		trans-2-tert-Butylcyclohexanol, ...	252	C12H19F3O2	1010467-27-5	12
5		Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
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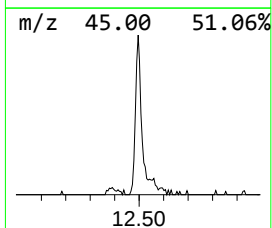
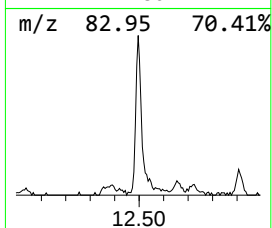
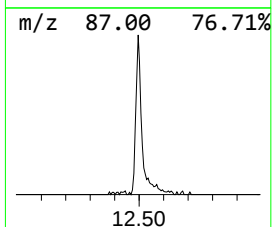
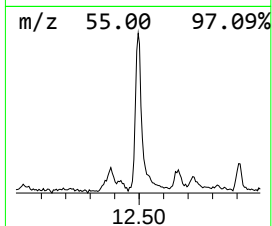
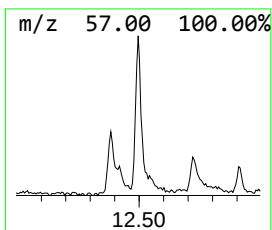
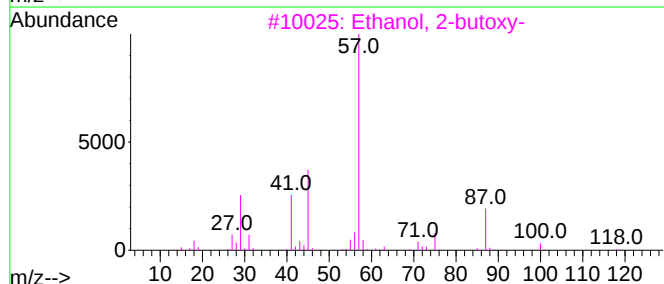
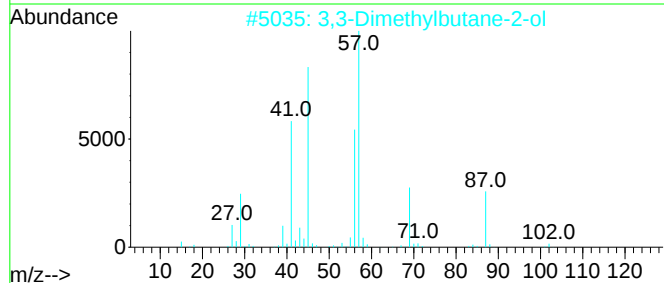
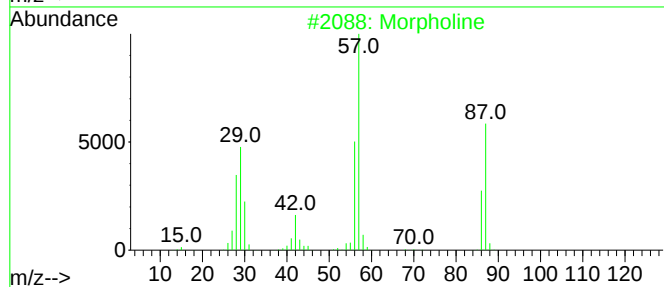
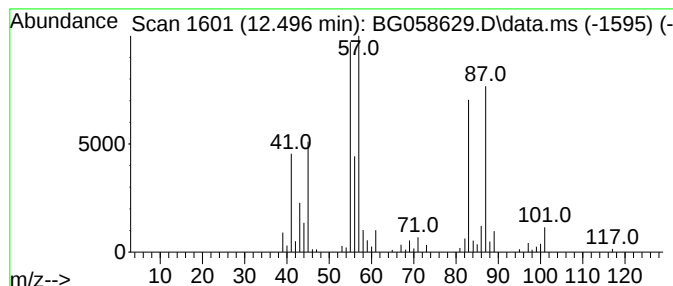
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown12.496 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.496	9.84 ng	174067	Naphthalene-d8	10.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Morpholine	87	C4H9NO	000110-91-8	43
2		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	40
3		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	38
4		1-Pentanamine	87	C5H13N	000110-58-7	38
5		3-Ethyl-5-hexen-3-ol	128	C8H16O	001907-46-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
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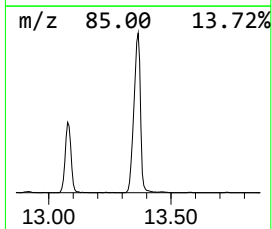
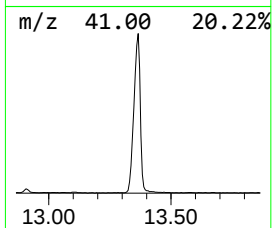
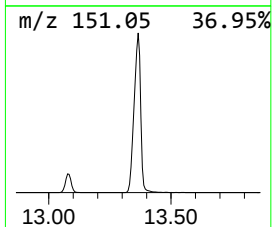
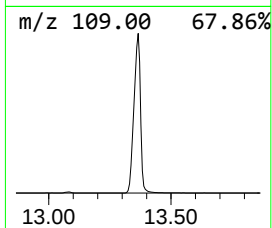
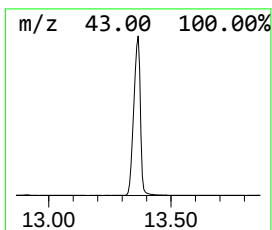
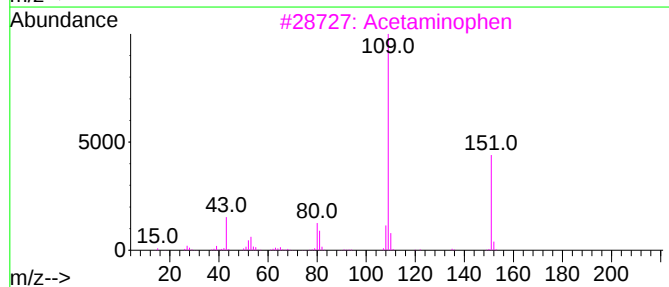
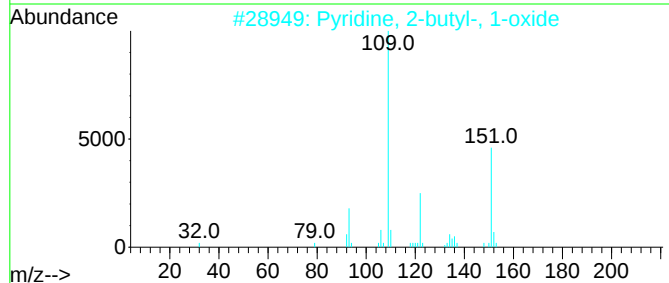
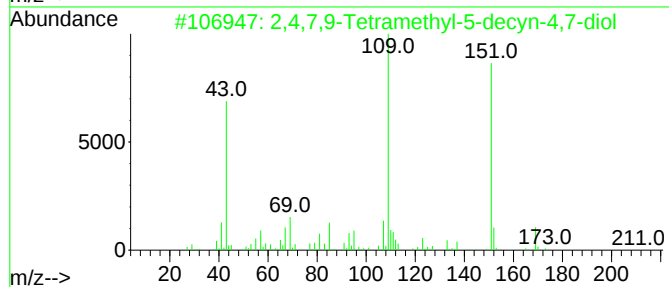
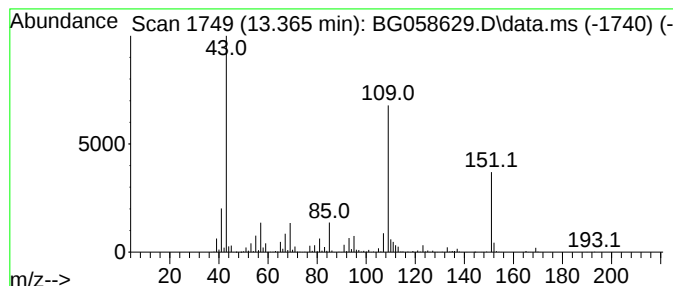
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.365	158.08 ng	4384760	Acenaphthene-d10	14.458

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53	
3	Acetaminophen	151	C8H9NO2	000103-90-2	49	
4	Metacetamol	151	C8H9NO2	000621-42-1	47	
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	47	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

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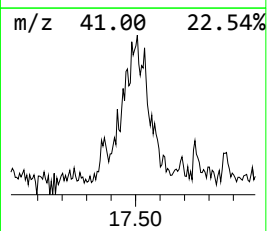
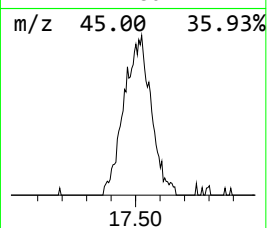
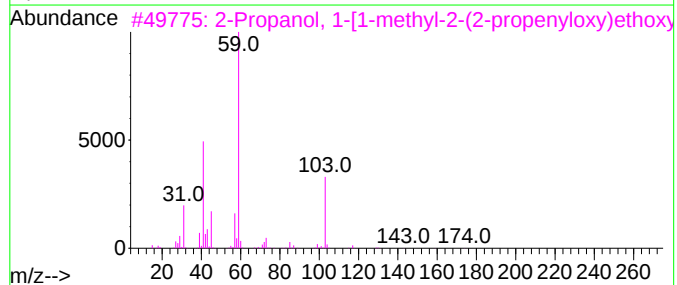
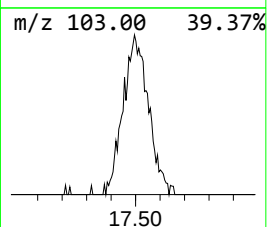
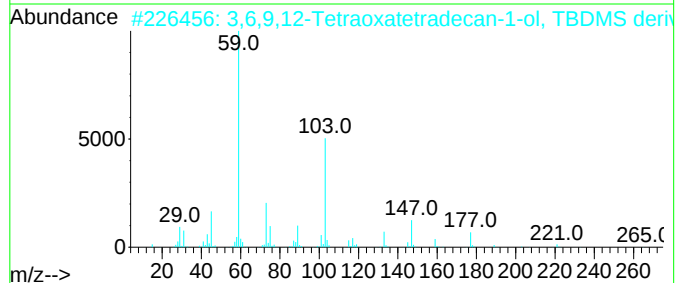
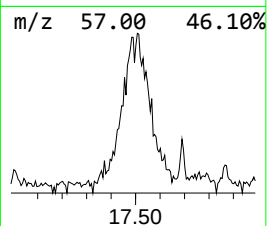
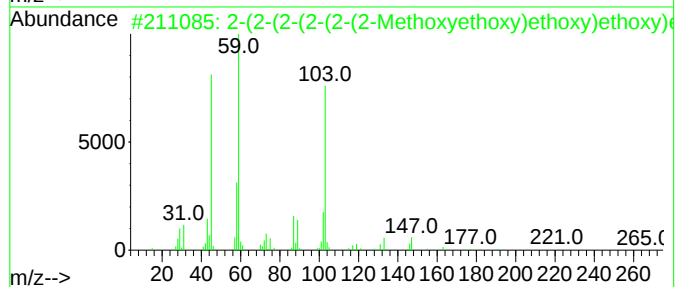
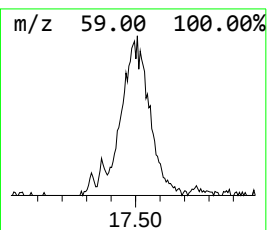
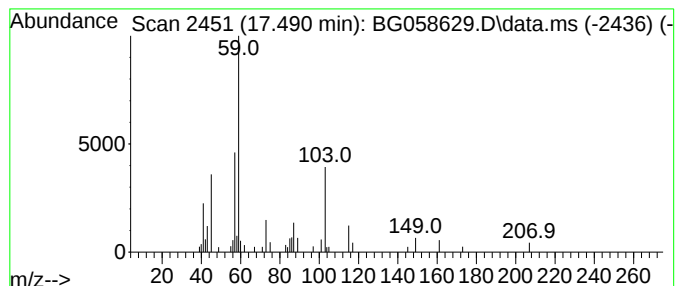
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-(2-(2-(2-(2-(2-Methoxyeth... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.490	2.24 ng	88977	Phenanthrene-d10	17.208

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-(2-(2-(2-(2-Methoxyethoxy)e...	310	C13H26O8	016142-03-3	64		
2	3,6,9,12-Tetraoxatetradecan-1-ol...	322	C15H34O5Si	1000352-09-6	59		
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	53		
4	1-(1-tert-Butoxypropan-2-yloxy)p...	190	C10H22O3	132739-31-2	53		
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

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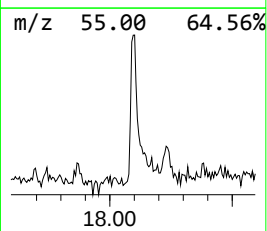
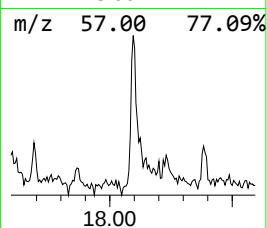
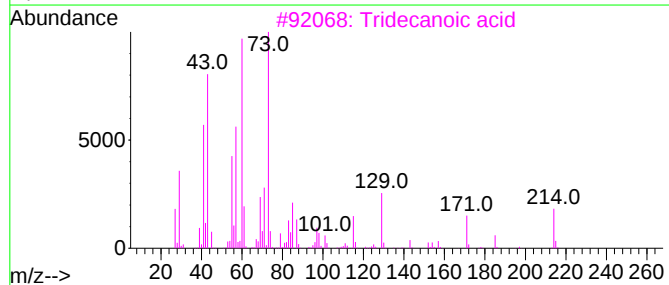
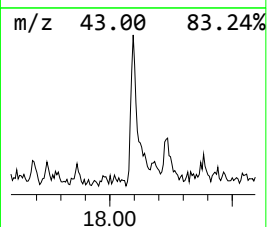
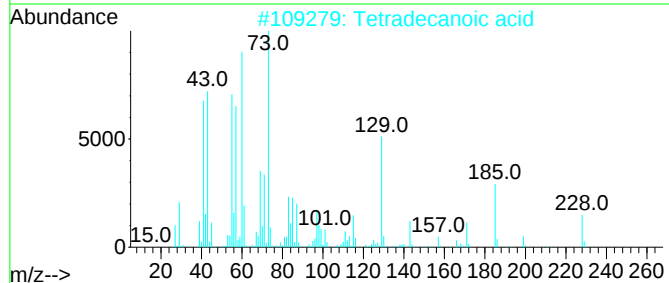
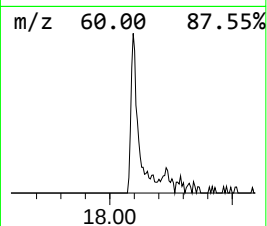
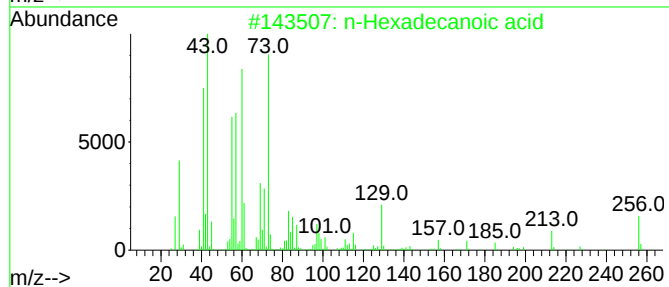
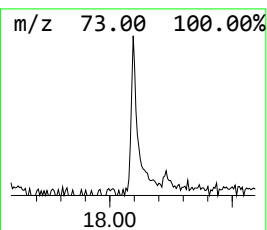
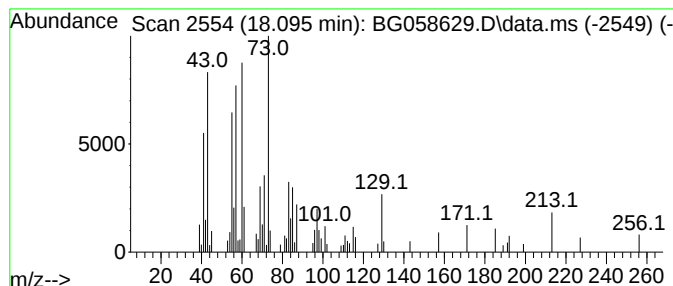
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 n-Hexadecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.095	2.65 ng	105047	Phenanthrene-d10	17.208

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3			Tridecanoic acid	214	C13H26O2	000638-53-9	59
4			Dodecanoic acid	200	C12H24O2	000143-07-7	53
5			1-(p-Toluidino)-1-deoxy-.beta.-d...	269	C13H19NO5	1000226-06-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

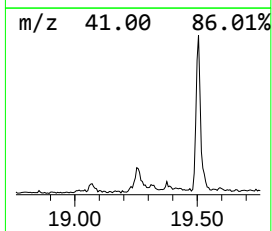
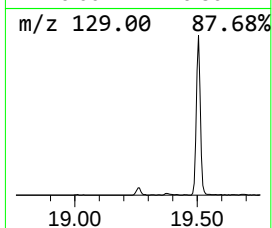
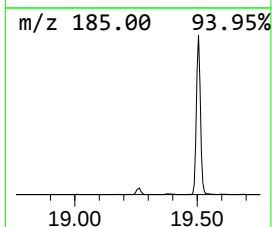
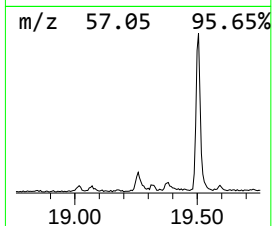
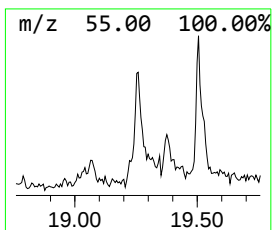
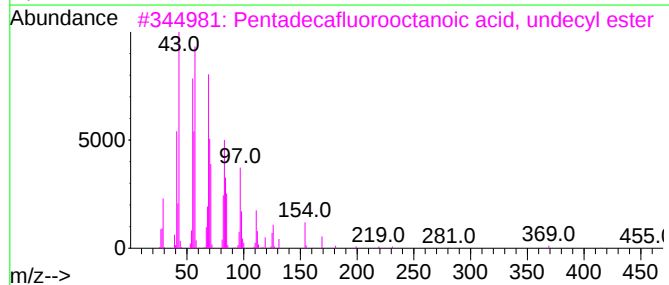
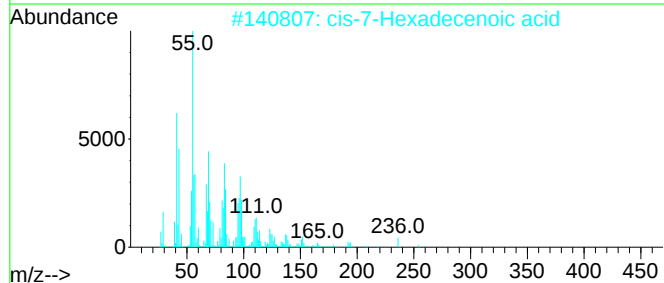
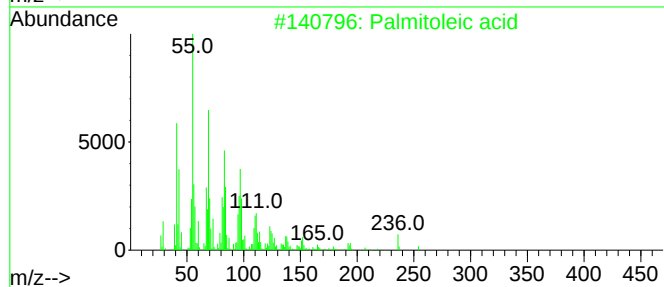
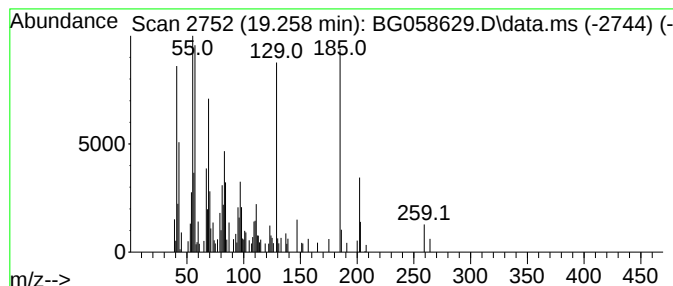
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown19.258 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.258	3.49 ng	138661	Phenanthrene-d10		17.208	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Palmitoleic acid		254	C16H30O2	000373-49-9	38
2	cis-7-Hexadecenoic acid		254	C16H30O2	002416-19-5	30
3	Pentadecafluorooctanoic acid, un...		568	C19H23F15O2	1010406-04-1	30
4	(E)-Hexadec-9-enoic acid		254	C16H30O2	010030-73-6	25
5	4-Methyl-5,6-tetramethylenetetra...		185	C9H15NOS	082947-02-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

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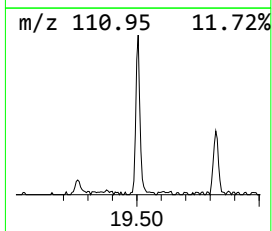
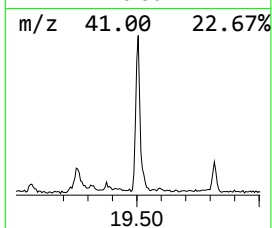
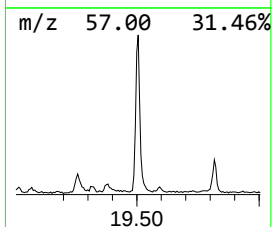
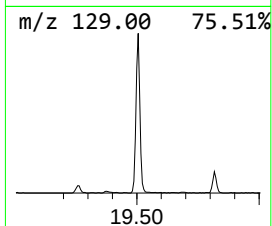
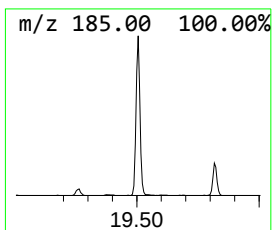
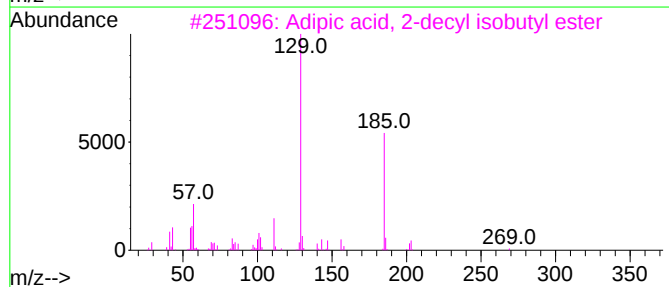
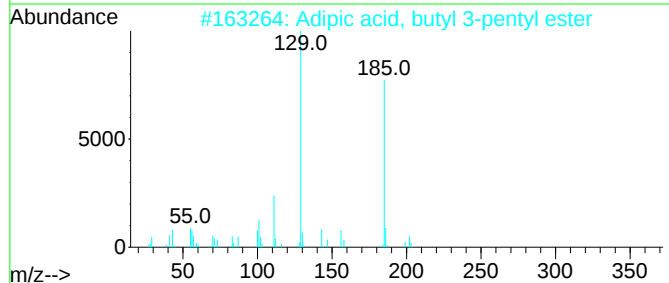
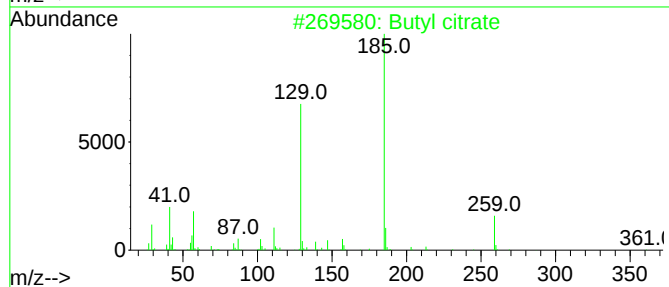
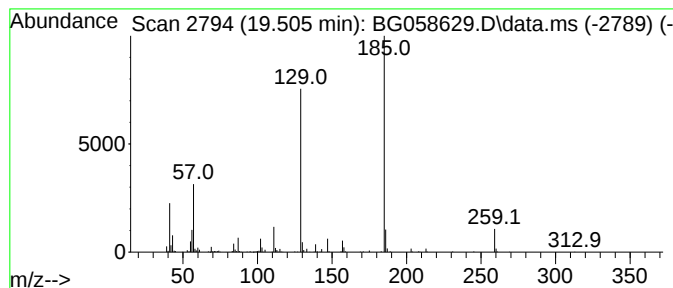
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.505	10.98 ng	492714	Chrysene-d12	21.444

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	91
2			Adipic acid, butyl 3-pentyl ester	272	C15H28O4	1000324-60-5	78
3			Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	78
4			Adipic acid, 2-ethylcyclohexyl i...	312	C18H32O4	1000324-22-5	72
5			Adipic acid, isobutyl 4-methylpe...	286	C16H30O4	1000353-50-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

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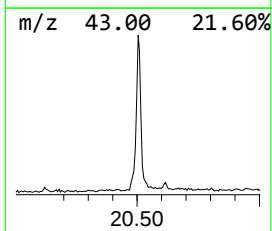
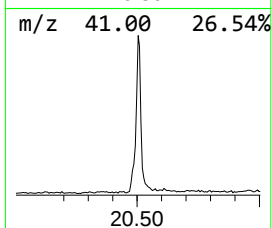
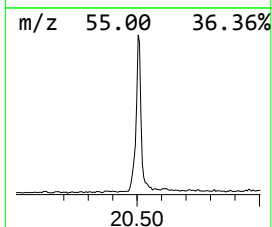
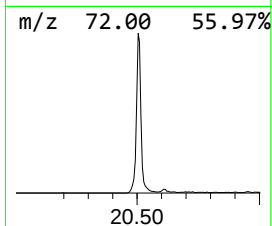
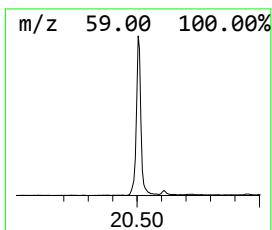
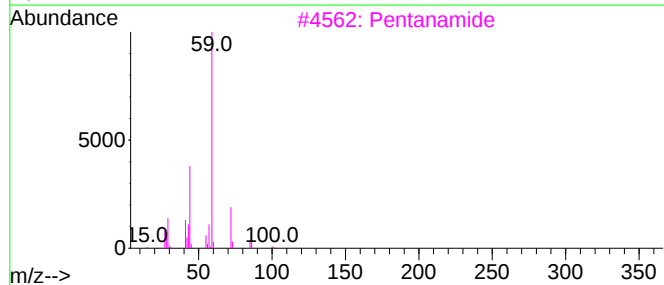
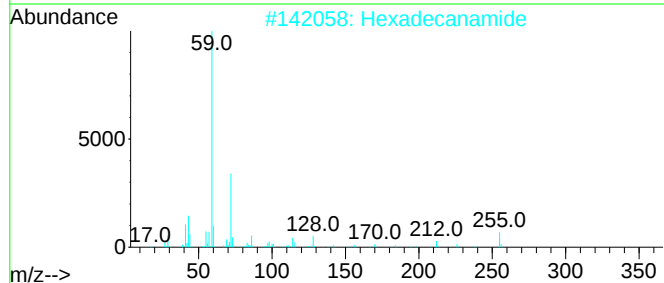
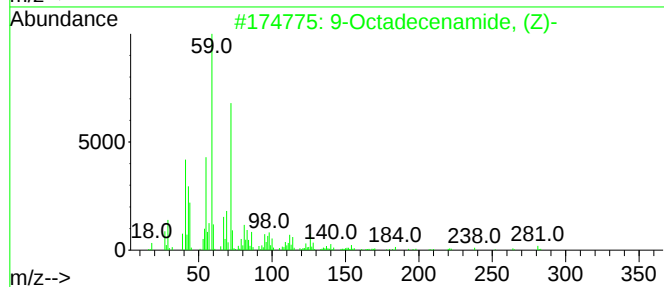
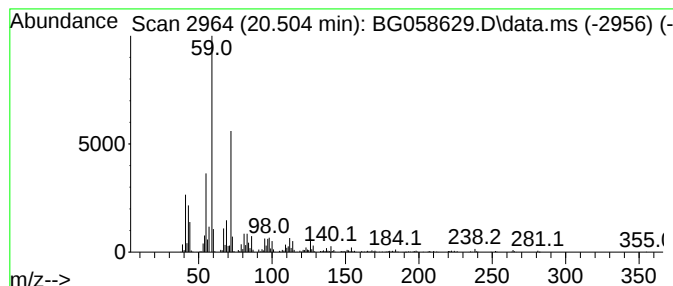
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.504	25.90 ng	1161700	Chrysene-d12	21.444

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2		Hexadecanamide	255	C16H33NO	000629-54-9	72
3		Pentanamide	101	C5H11NO	000626-97-1	64
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	56
5		Nonanamide	157	C9H19NO	001120-07-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
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ALS Vial : 13 Sample Multiplier: 1

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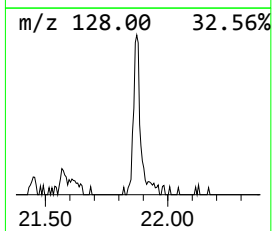
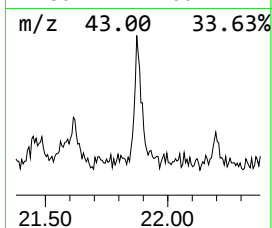
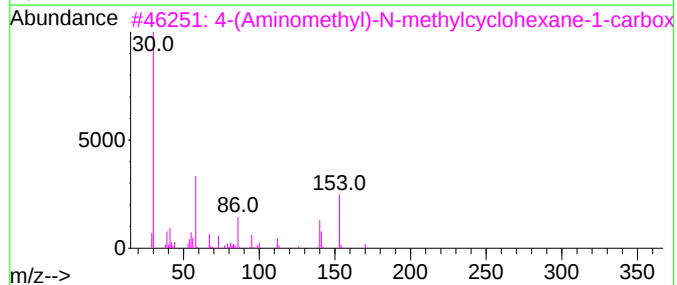
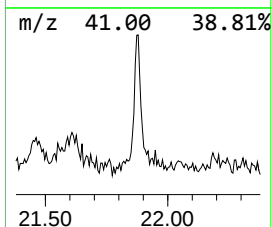
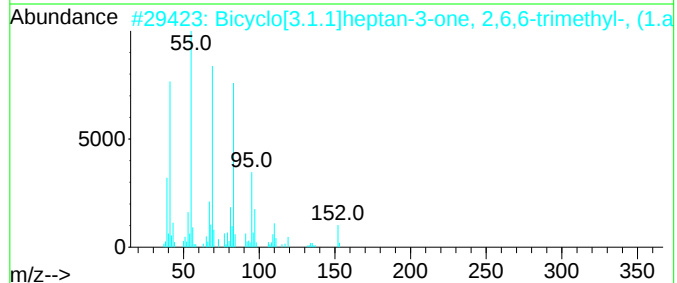
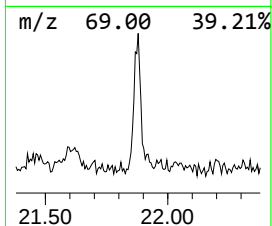
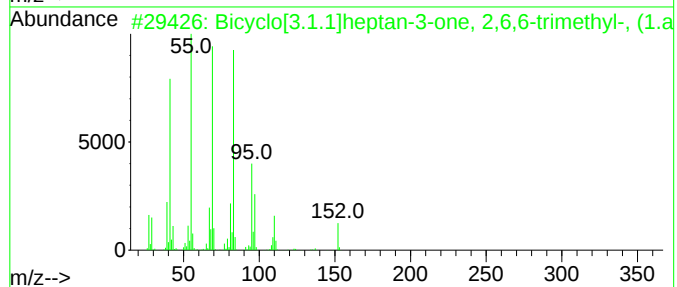
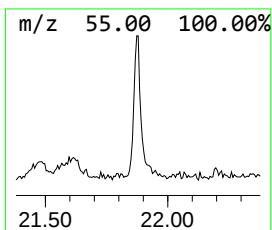
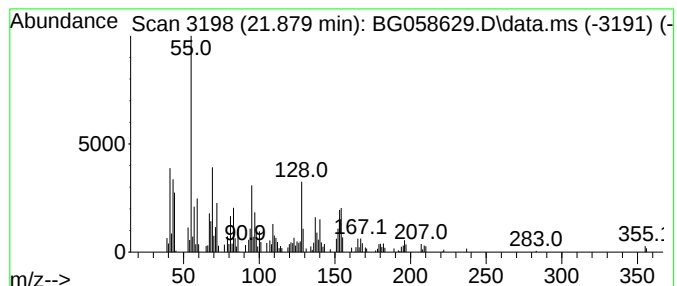
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown21.879 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.879	4.09 ng	183686	Chrysene-d12	21.444

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	15
2			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	11
3			4-(Aminomethyl)-N-methylcyclohex...	170	C9H18N2O	1000459-82-8	11
4			Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	10
5			10-Aminodecanoic acid, O-methyl ...	201	C11H23NO2	1010497-26-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EQUIPMENT-BLANK-1

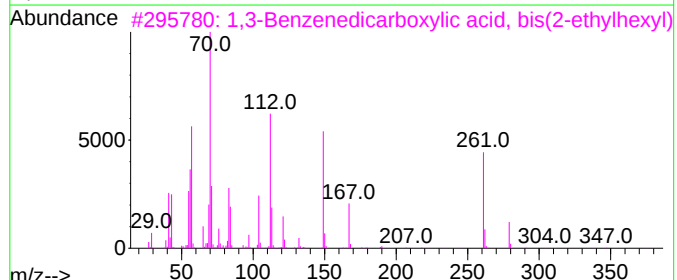
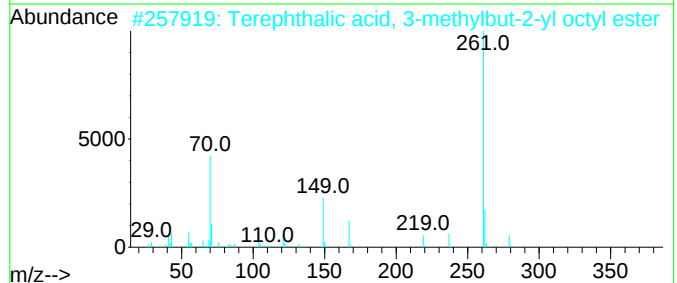
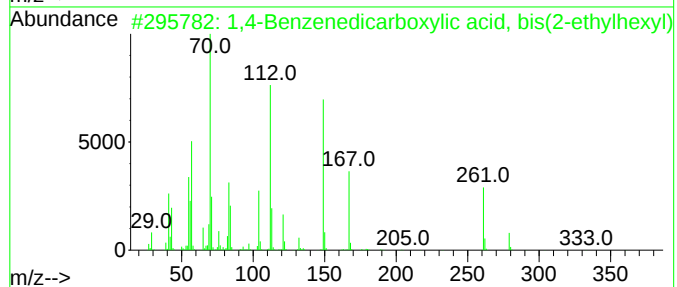
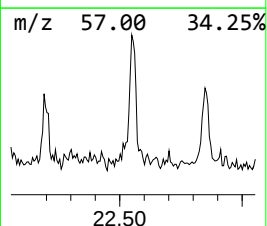
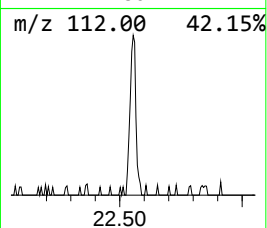
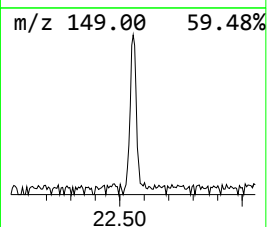
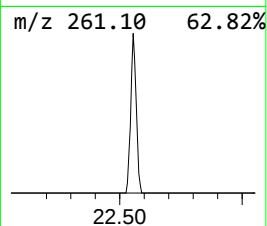
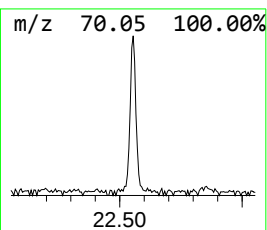
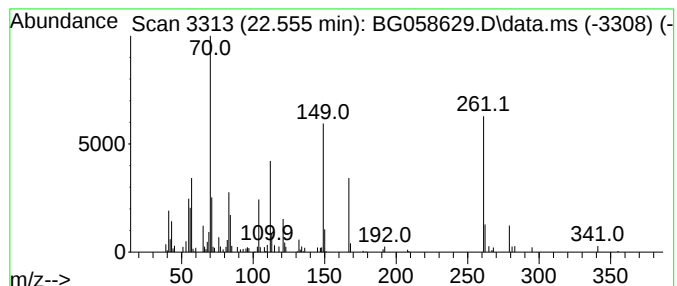
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 1,4-Benzenedicarboxylic aci... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.555	2.23 ng	100198	Chrysene-d12	21.444

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	59
4			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	35
5			1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080723\
Data File : BG058629.D
Acq On : 7 Aug 2023 16:18
Operator : MA/JU
Sample : 03862-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EQUIPMENT-BLANK-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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
Methyl Isobutyl...	3.583	5.2	ng	57880	1	7.813	222027	20.0
Hexanal	4.352	10.4	ng	115188	1	7.813	222027	20.0
1-Hexanol, 2-et...	7.872	10.7	ng	118303	1	7.813	222027	20.0
unknown9.135	9.135	5.3	ng	58632	1	7.813	222027	20.0
Methane, diethoxy-	11.139	27.8	ng	491855	2	10.616	353735	20.0
2-Propanol, 1-(...	11.203	33.5	ng	592930	2	10.616	353735	20.0
Nonanoic acid	11.421	3.9	ng	69215	2	10.616	353735	20.0
unknown11.485	11.485	4.1	ng	73028	2	10.616	353735	20.0
2-Decenal, (Z)-	11.556	13.1	ng	232038	2	10.616	353735	20.0
unknown12.384	12.384	4.0	ng	69978	2	10.616	353735	20.0
unknown12.496	12.496	9.8	ng	174067	2	10.616	353735	20.0
2,4,7,9-Tetrame...	13.365	158.1	ng	4384760	3	14.458	554762	20.0
2-(2-(2-(2-(2-(...	17.490	2.2	ng	88977	4	17.208	794137	20.0
n-Hexadecanoic ...	18.095	2.6	ng	105047	4	17.208	794137	20.0
unknown19.258	19.258	3.5	ng	138661	4	17.208	794137	20.0
Butyl citrate	19.505	11.0	ng	492714	5	21.444	897124	20.0
9-Octadecenamid...	20.504	25.9	ng	1161700	5	21.444	897124	20.0
unknown21.879	21.879	4.1	ng	183686	5	21.444	897124	20.0
1,4-Benzenedica...	22.555	2.2	ng	100198	5	21.444	897124	20.0