

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072922\
 Data File : BG054446.D
 Acq On : 29 Jul 2022 12:43
 Operator : CG/JU
 Sample : N3895-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RVE-40

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-BG071522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.106	15	20	37	rVB	78925	137725	2.63%	0.972%
2	5.562	432	438	449	rVB	184212	316619	6.04%	2.234%
3	7.178	704	713	726	rBB	193759	356246	6.79%	2.513%
4	7.983	844	850	859	rBB	47446	82654	1.58%	0.583%
5	9.146	1041	1048	1056	rBV	120214	224555	4.28%	1.584%
6	10.797	1321	1329	1336	rBV	65497	119586	2.28%	0.844%
7	13.241	1738	1745	1752	rBV	418965	660823	12.60%	4.662%
8	14.622	1973	1980	1989	rVB	128258	198779	3.79%	1.402%
9	16.114	2228	2234	2245	rBV	433109	669683	12.77%	4.725%
10	17.366	2441	2447	2452	rBV	168370	263399	5.02%	1.858%
11	18.259	2594	2599	2608	rVV3	118987	208703	3.98%	1.472%
12	19.416	2787	2796	2808	rBV2	64326	186407	3.56%	1.315%
13	19.528	2810	2815	2835	rVV	215190	417943	7.97%	2.949%
14	19.781	2855	2858	2866	rVB	34858	57475	1.10%	0.405%
15	19.975	2885	2891	2897	rVV	899773	1219724	23.26%	8.605%
16	21.267	3106	3111	3121	rBV	139257	219378	4.18%	1.548%
17	21.631	3166	3173	3179	rBV	212216	387072	7.38%	2.731%
18	22.436	3301	3310	3318	rBV4	65085	197545	3.77%	1.394%
19	22.906	3384	3390	3398	rVB2	46451	100346	1.91%	0.708%
20	23.447	3476	3482	3489	rVB2	49121	103031	1.97%	0.727%
21	23.899	3552	3559	3565	rBV3	236424	579186	11.05%	4.086%
22	24.839	3709	3719	3729	rBV2	137522	393036	7.50%	2.773%
23	25.351	3802	3806	3820	rVB6	41472	122737	2.34%	0.866%
24	25.956	3901	3909	3920	rVB2	76995	237431	4.53%	1.675%
25	29.029	4408	4432	4447	rVB3	1061753	5243241	100.00%	36.991%
26	29.875	4562	4576	4597	rVB5	182358	909760	17.35%	6.418%
27	31.185	4789	4799	4818	rVB10	116363	561452	10.71%	3.961%

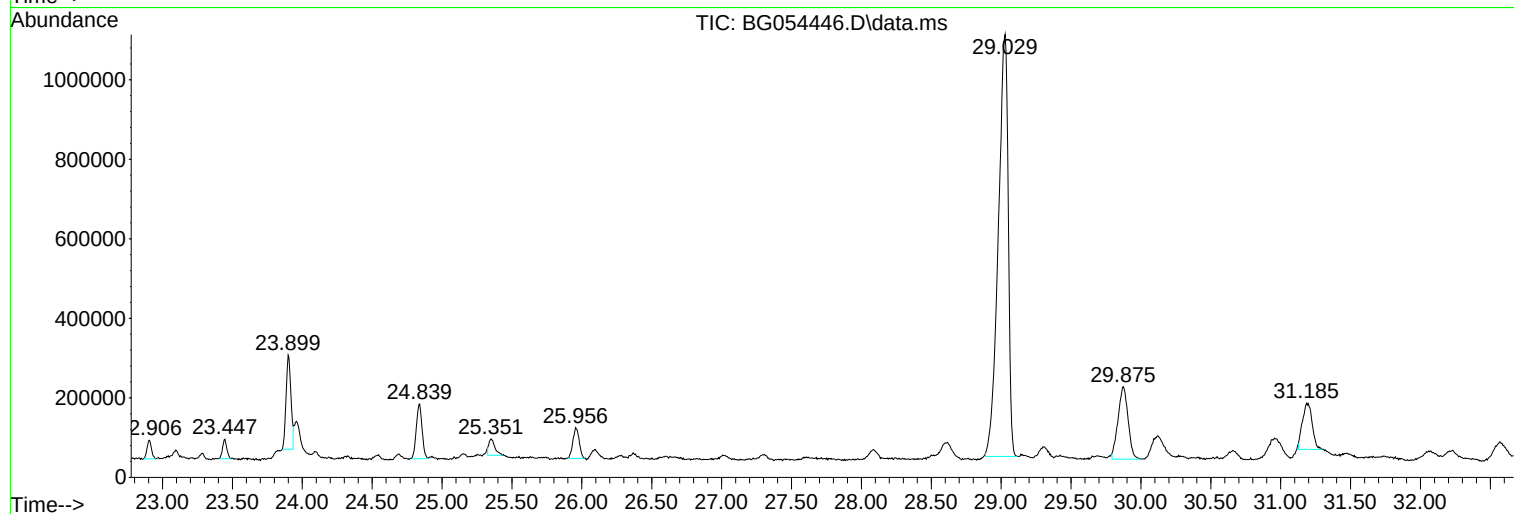
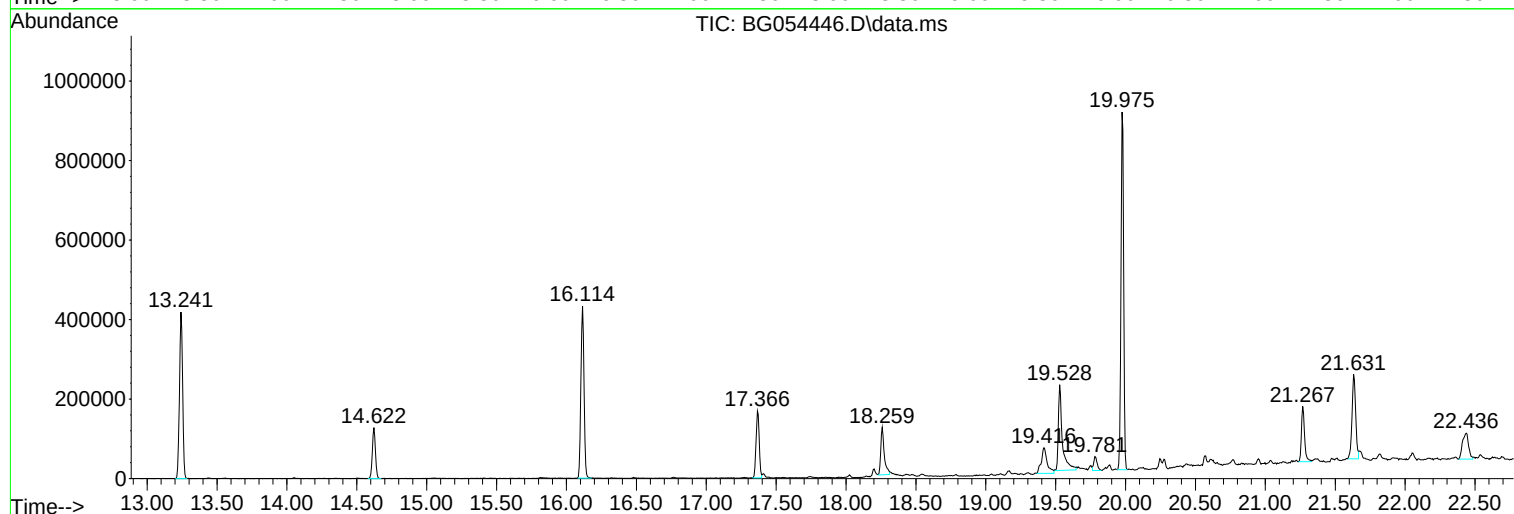
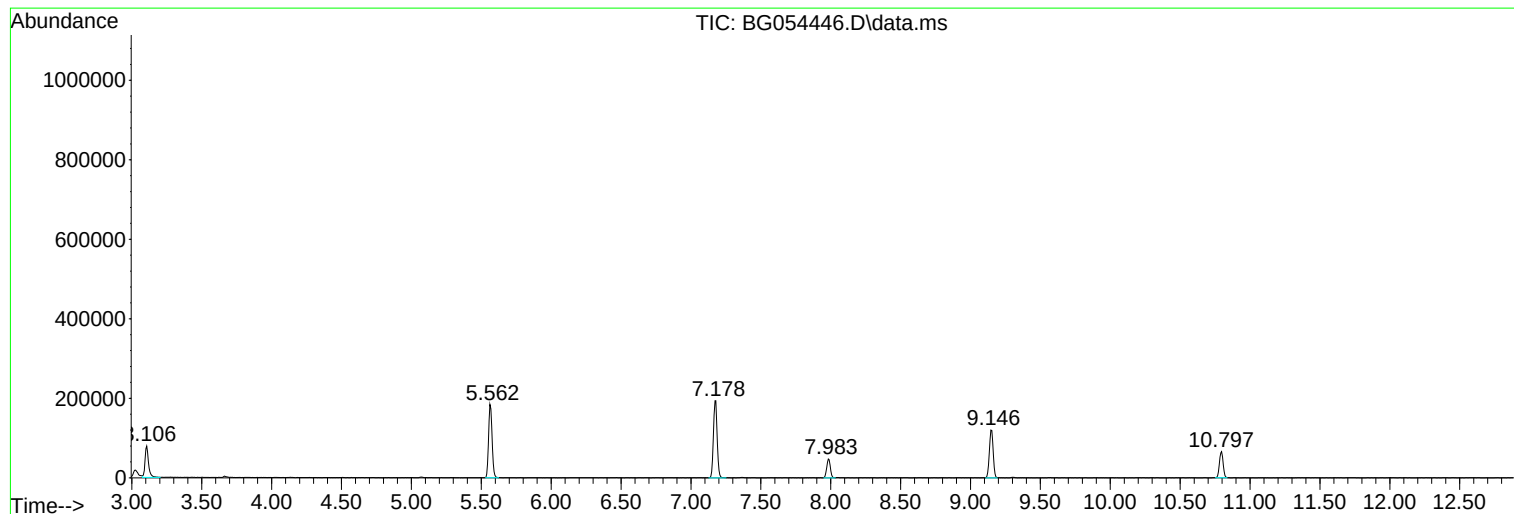
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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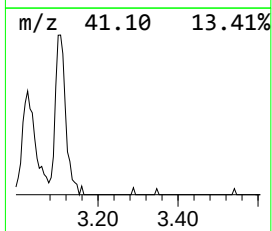
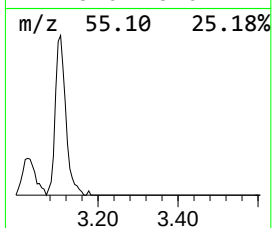
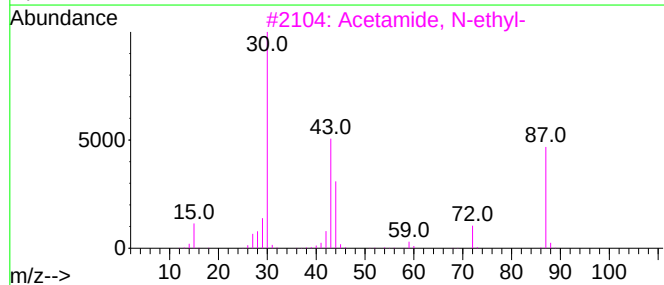
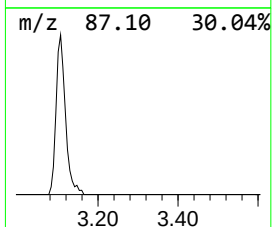
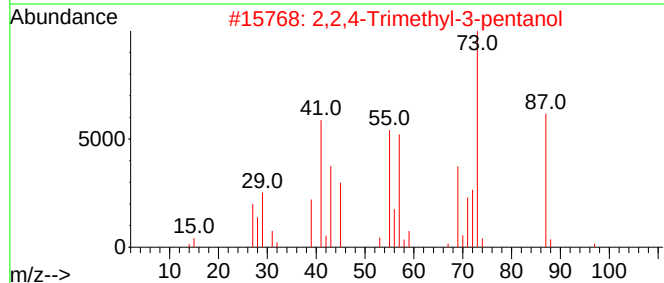
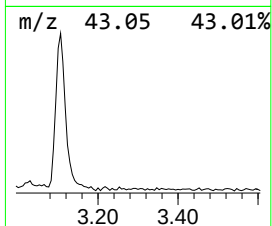
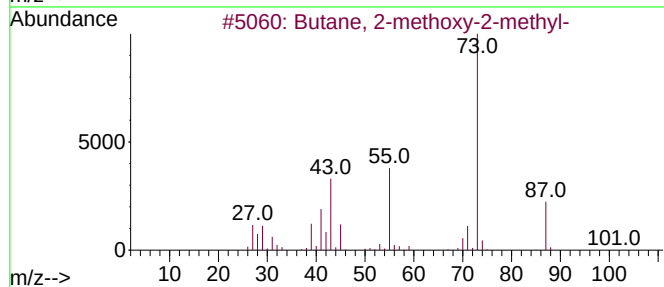
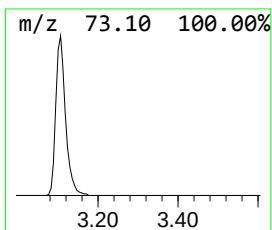
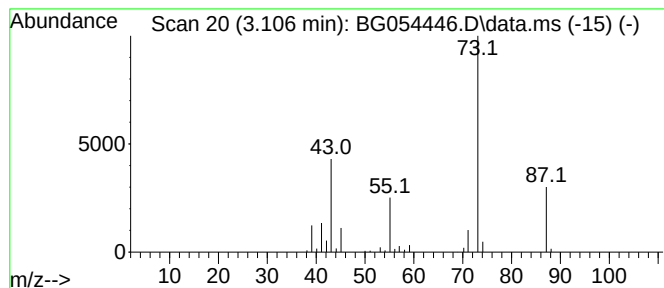
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.106	33.33 ng	137725	1,4-Dichlorobenzene-d4	7.989

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	25
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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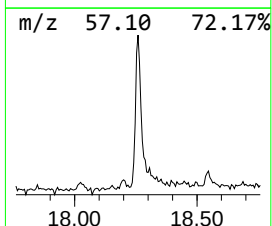
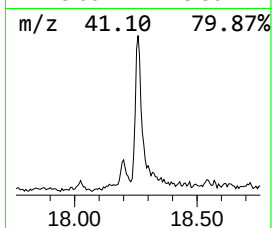
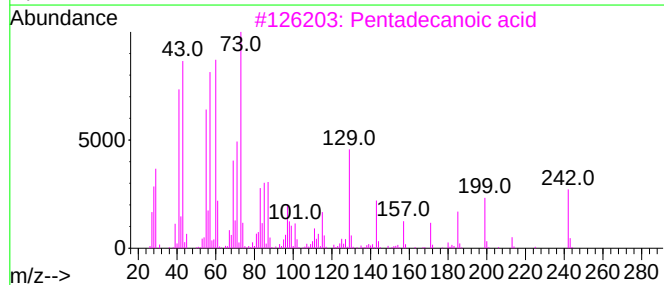
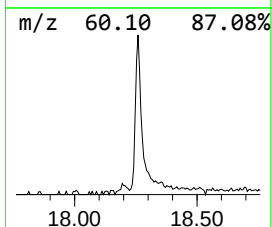
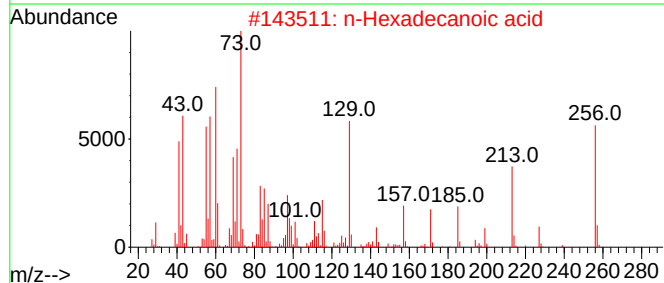
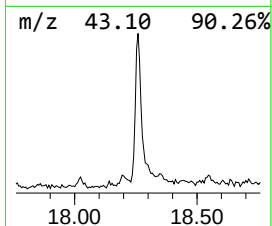
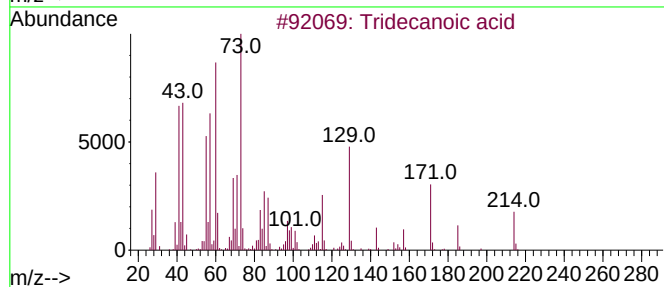
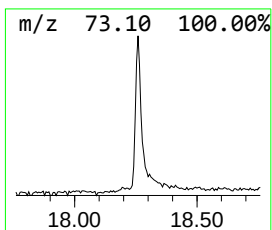
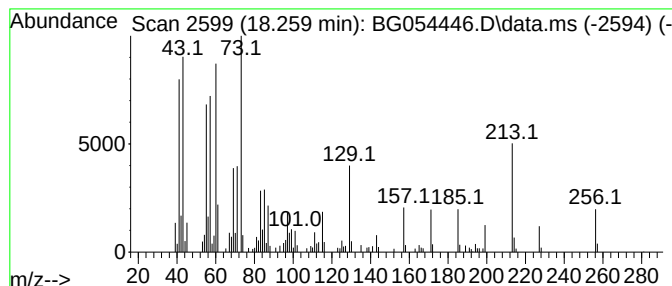
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.259	15.85 ng	208703	Phenanthrene-d10	17.366

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	97
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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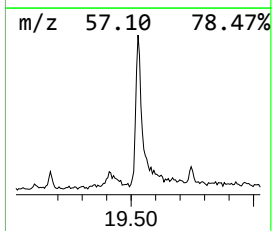
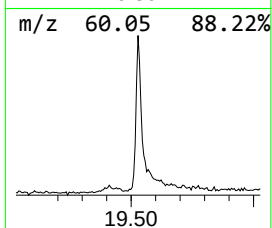
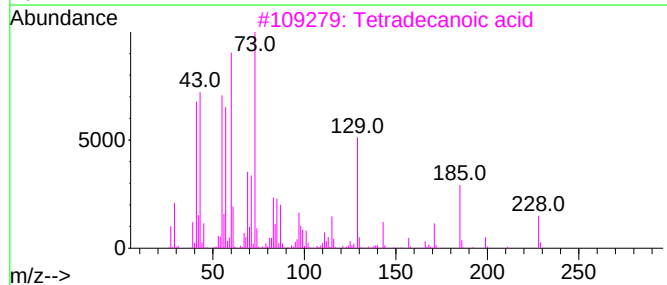
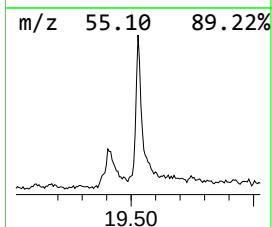
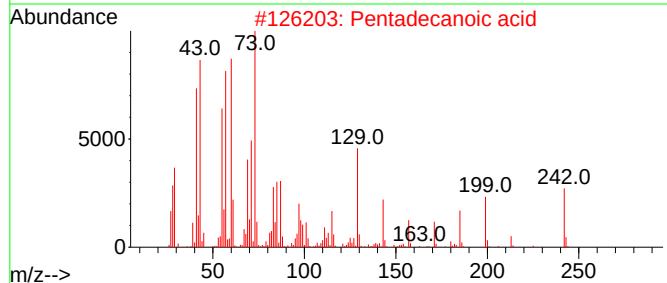
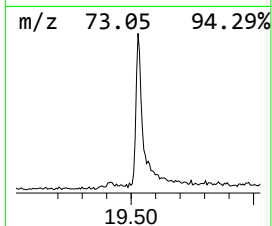
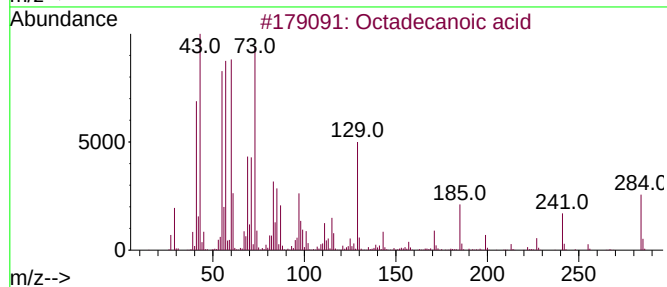
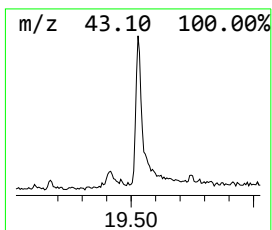
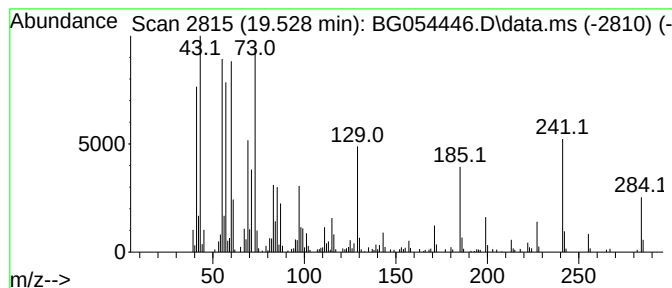
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.528	21.60 ng	417943	Chrysene-d12	21.631	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	78
5	Undecanoic acid	186	C11H22O2	000112-37-8	55



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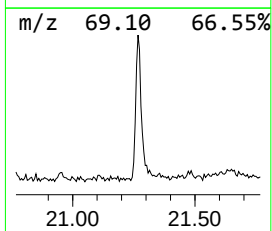
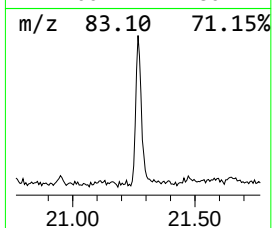
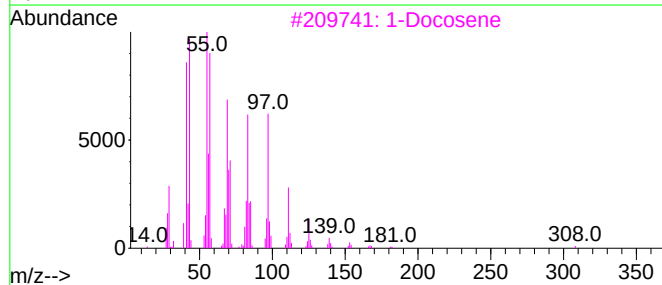
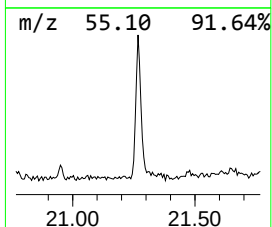
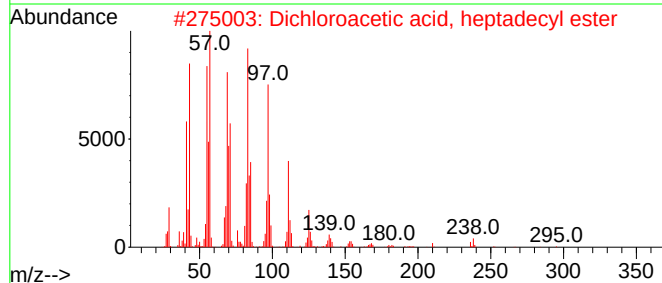
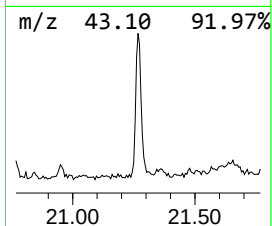
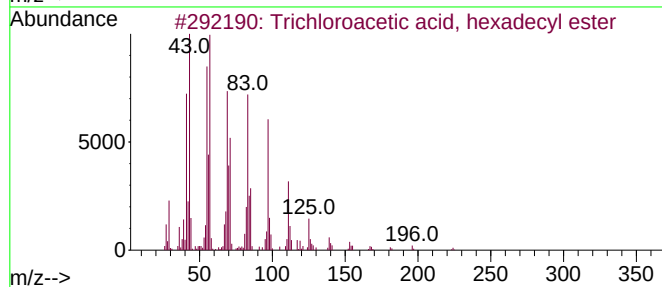
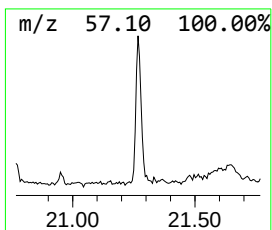
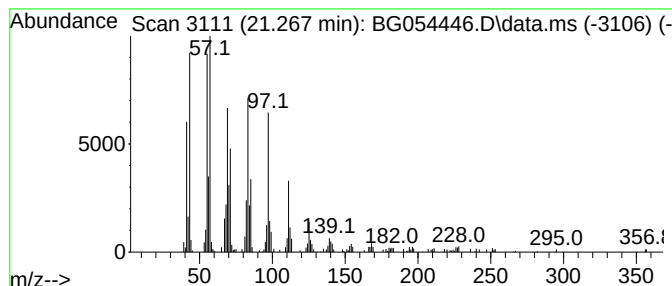
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.267	11.34 ng	219378	Chrysene-d12		21.631	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	95
2	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	95
3	1-Docosene		308	C22H44	001599-67-3	95
4	1-Tricosene		322	C23H46	018835-32-0	95
5	Pentafluoropropionic acid, penta...		374	C18H31F5O2	959092-08-1	94



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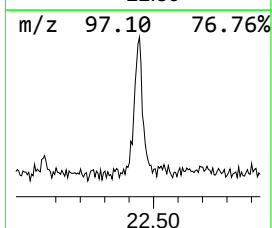
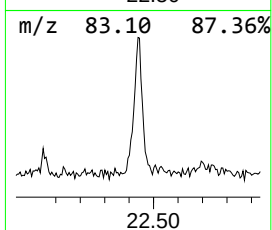
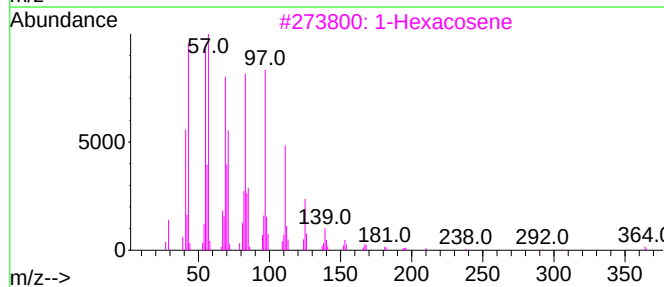
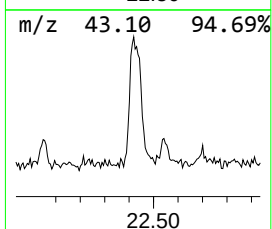
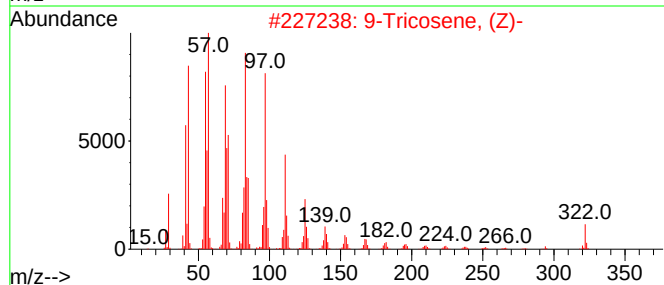
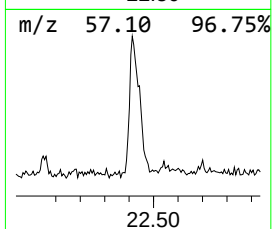
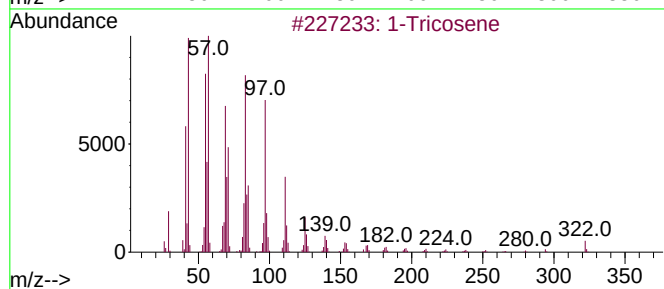
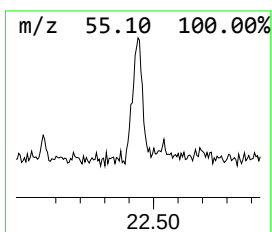
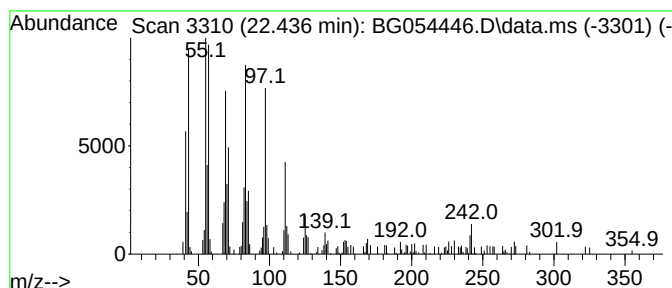
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Tricosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.436	10.21 ng	197545	Chrysene-d12	21.631

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene			322	C23H46	018835-32-0	96
2	9-Tricosene, (Z)-			322	C23H46	027519-02-4	95
3	1-Hexacosene			364	C26H52	018835-33-1	95
4	2-Methyl-2-docosene			322	C23H46	1000131-16-9	95
5	Pentafluoropropionic acid, penta...			374	C18H31F5O2	959092-08-1	94



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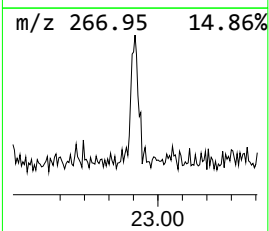
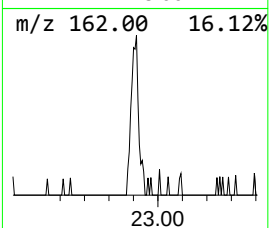
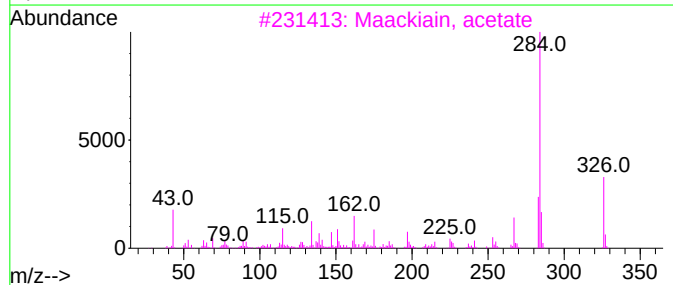
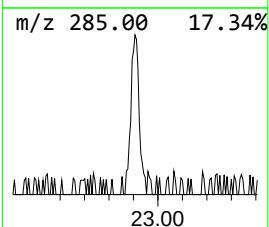
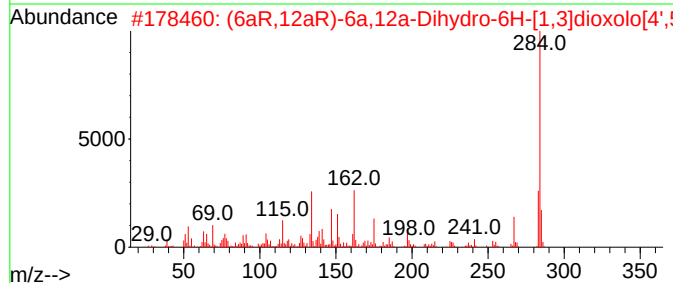
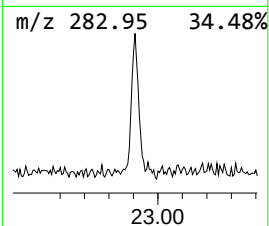
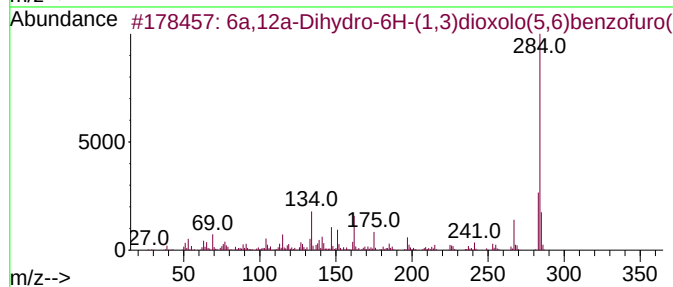
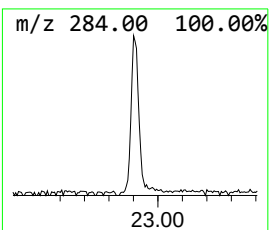
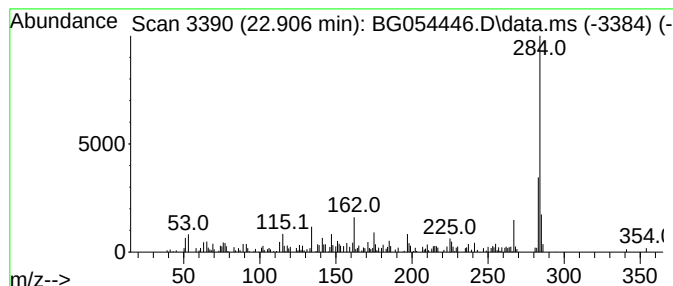
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.906	5.18 ng	100346	Chrysene-d12	21.631

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6a,12a-Dihydro-6H-(1,3)dioxolo(5...	284	C16H12O5	076496-57-6	95
2			(6aR,12aR)-6a,12a-Dihydro-6H-[1,...	284	C16H12O5	002035-15-6	94
3			Maackiain, acetate	326	C18H14O6	002035-16-7	91
4			Benzo-1,3,2-dioxaborolane, 2-[2'...	284	C16H17BO4	1000164-23-9	68
5			2-(9-Acridinyl)-4-methylbenzenea...	284	C20H16N2	035586-77-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072922\
Data File : BG054446.D
Acq On : 29 Jul 2022 12:43
Operator : CG/JU
Sample : N3895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

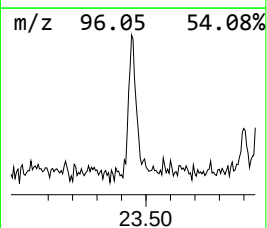
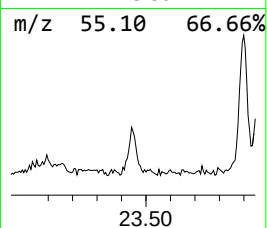
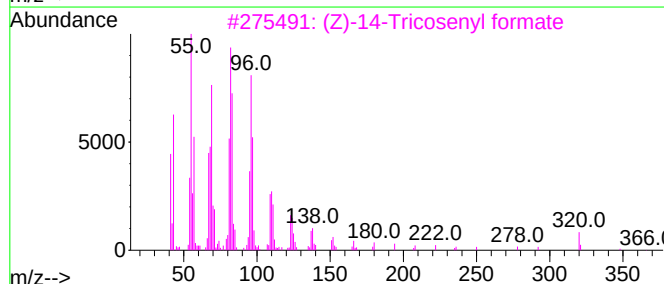
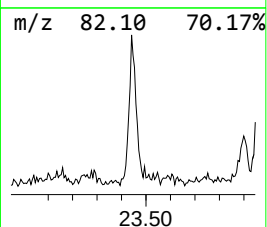
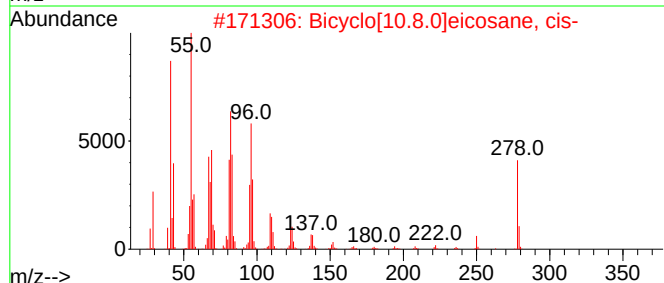
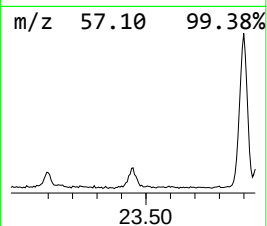
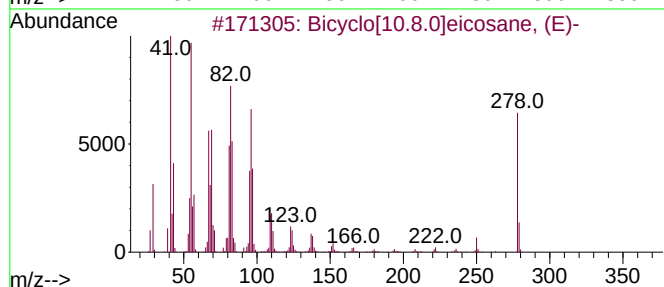
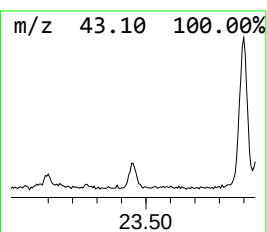
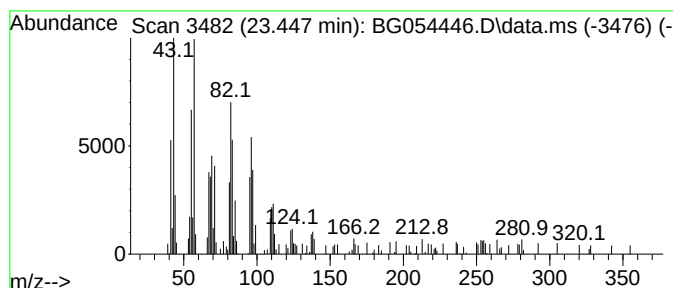
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bicyclo[10.8.0]eicosane, (E)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.447	5.24 ng	103031	Perylene-d12	24.839	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[10.8.0]eicosane, (E)-	278	C20H38	1010155-85-0	98
2	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	93
3	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	91
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
5	Tricosanal	338	C23H46O	072934-02-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072922\
Data File : BG054446.D
Acq On : 29 Jul 2022 12:43
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Instrument :
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ClientSampleId :
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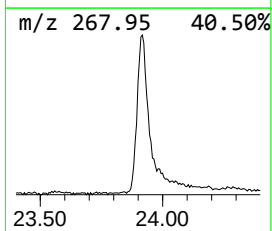
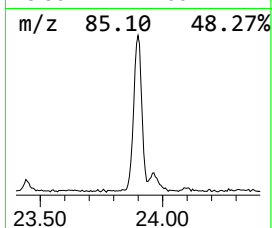
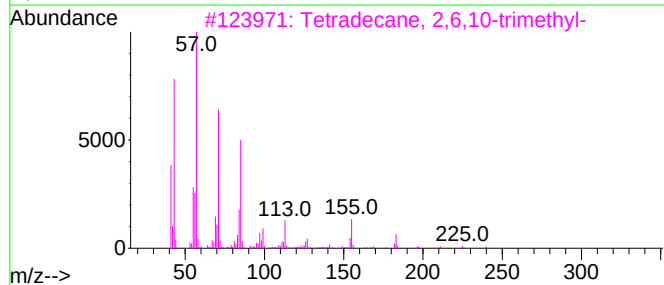
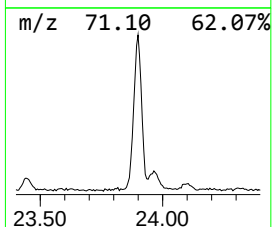
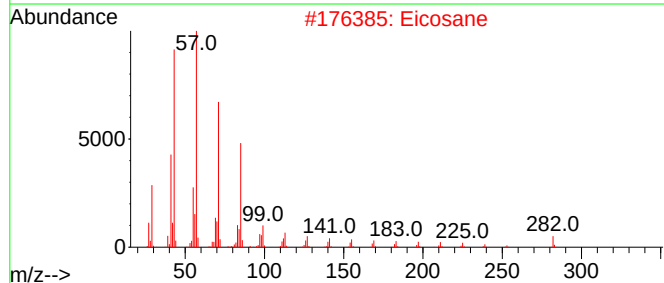
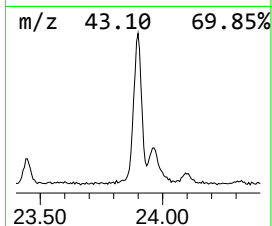
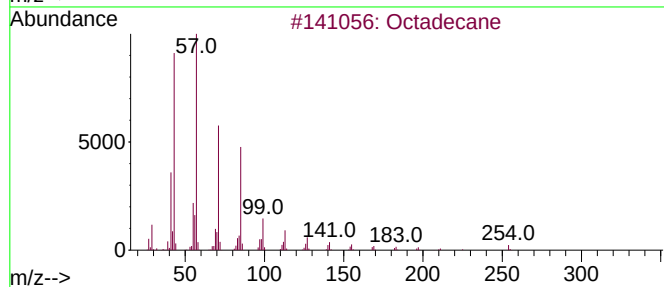
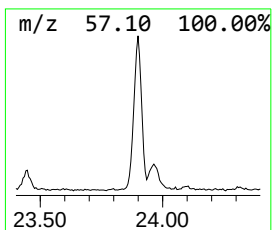
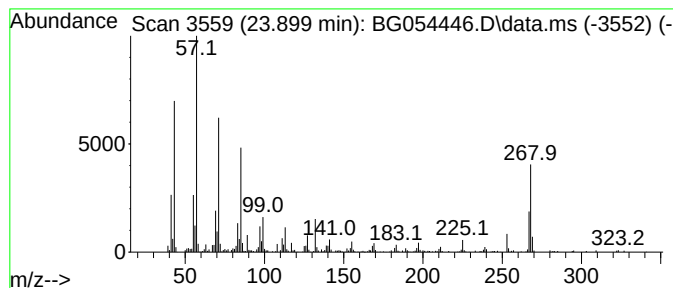
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.899	29.47 ng	579186	Perylene-d12	24.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	96
2			Eicosane	282	C20H42	000112-95-8	91
3			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	83
4			Triacontane	422	C30H62	000638-68-6	64
5			Docosane	310	C22H46	000629-97-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072922\
Data File : BG054446.D
Acq On : 29 Jul 2022 12:43
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Sample : N3895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

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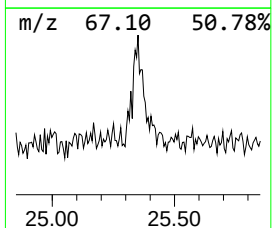
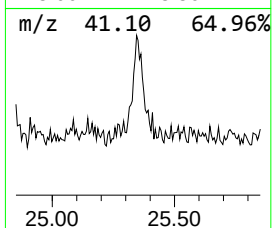
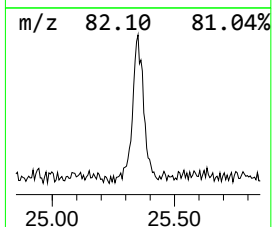
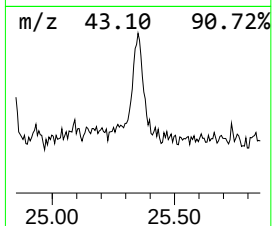
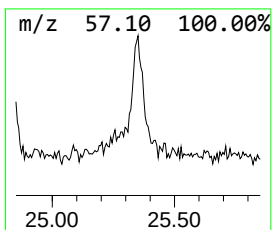
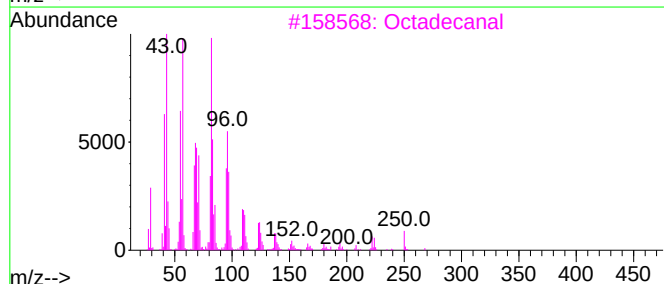
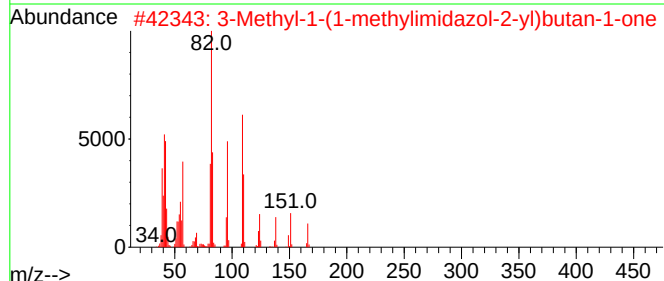
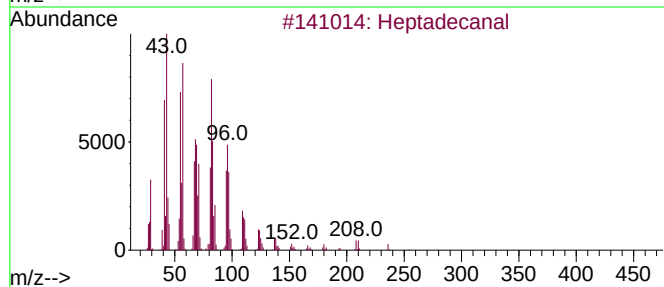
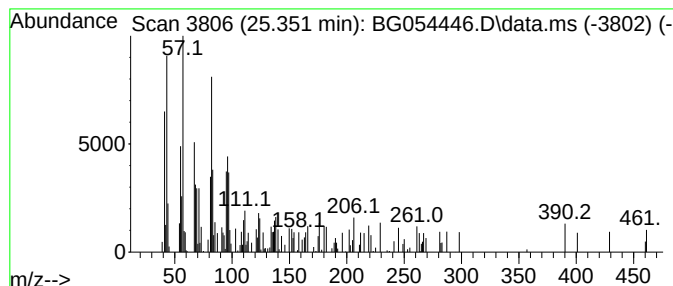
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown25.351 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.351	6.25 ng	122737	Perylene-d12	24.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanal	254	C17H34O	1000376-70-0	49
2			3-Methyl-1-(1-methylimidazol-2-yl)butan-1-one	166	C9H14N2O	1000410-03-3	49
3			Octadecanal	268	C18H36O	000638-66-4	49
4			E-6-Octadecen-1-ol acetate	310	C20H38O2	1000130-94-7	49
5			Eicosanal-	296	C20H40O	002400-66-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072922\
Data File : BG054446.D
Acq On : 29 Jul 2022 12:43
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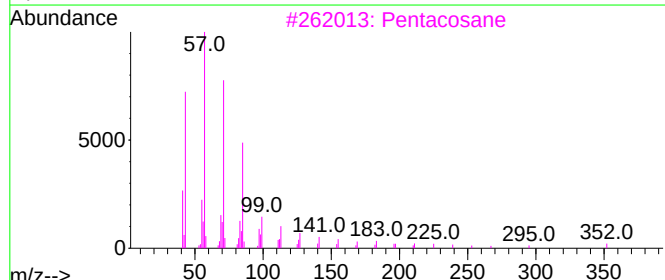
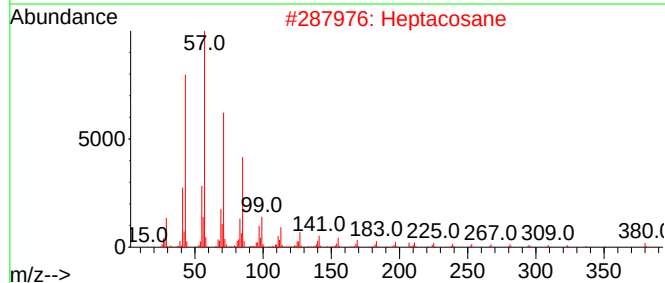
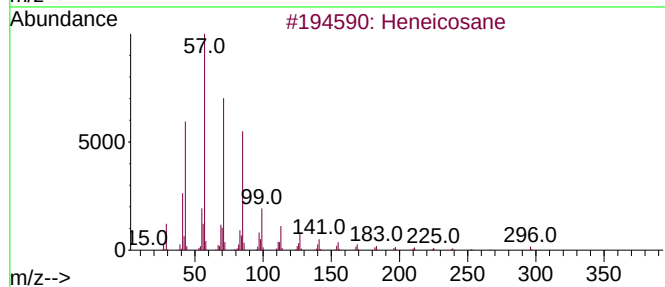
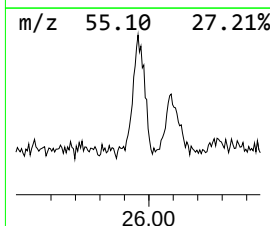
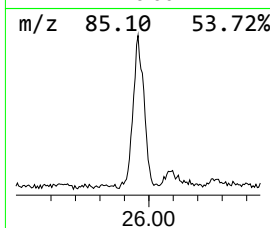
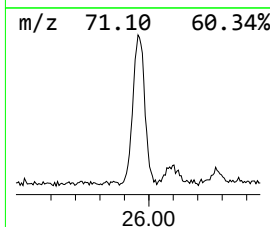
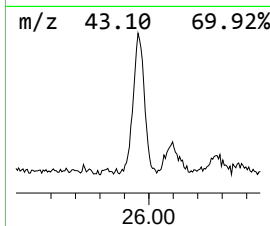
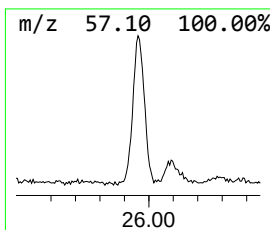
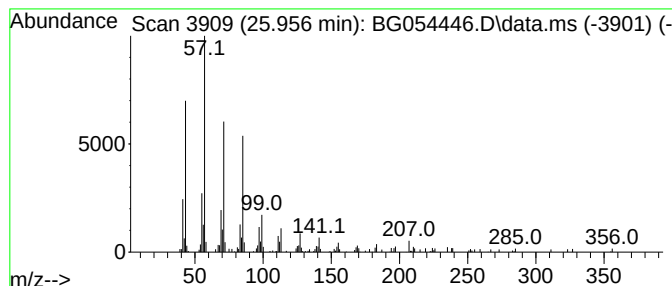
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.956	12.08 ng	237431	Perylene-d12	24.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Heptacosane	380	C27H56	000593-49-7	90
3			Pentacosane	352	C25H52	000629-99-2	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072922\
Data File : BG054446.D
Acq On : 29 Jul 2022 12:43
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Sample : N3895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

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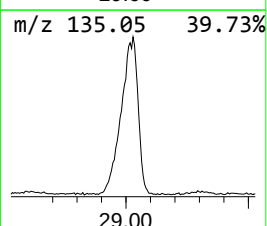
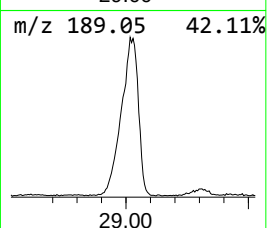
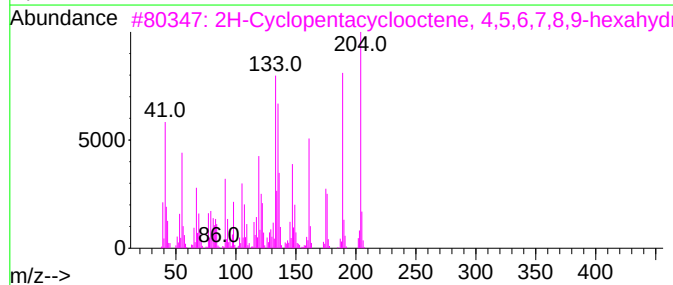
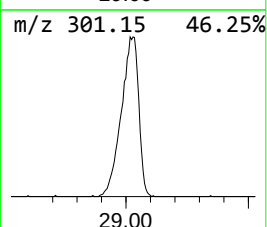
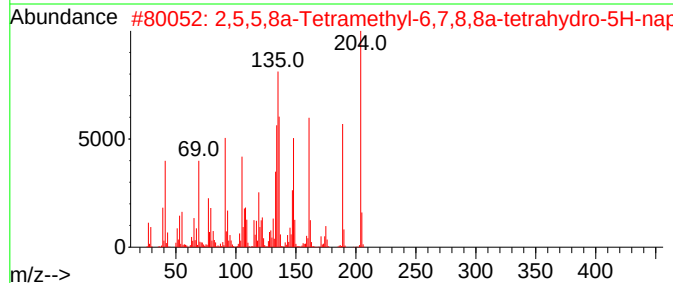
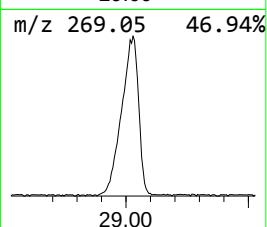
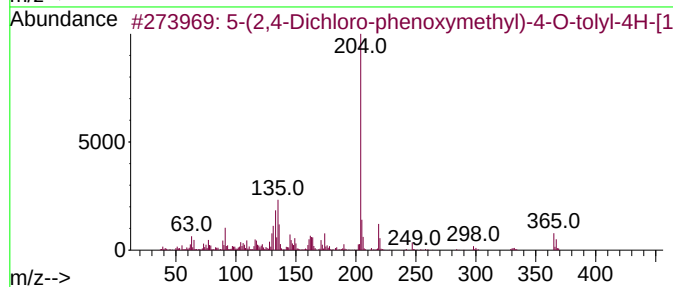
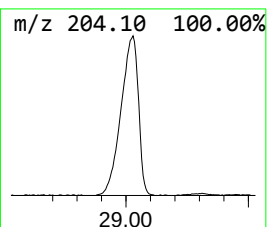
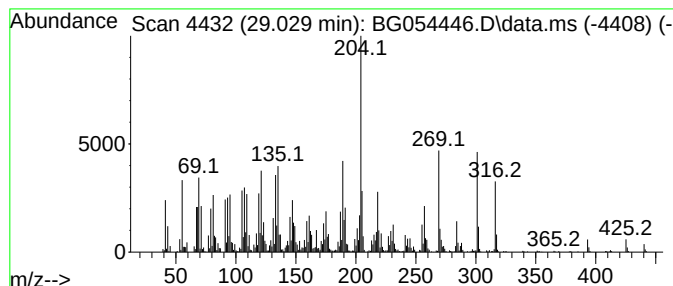
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown29.029 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.029	266.81 ng	5243240	Perylene-d12	24.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(2,4-Dichloro-phenoxy)methyl)-4...	365	C16H13Cl2N3OS	1000296-81-4	42		
2	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	38		
3	2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	38		
4	5-Amino-6,8-dimethoxyquinoline	204	C11H12N2O2	1000213-95-2	30		
5	1-(4-Amino-2-methylphenyl)-2-pip...	204	C12H16N2O	443999-53-9	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072922\
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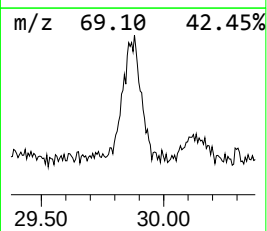
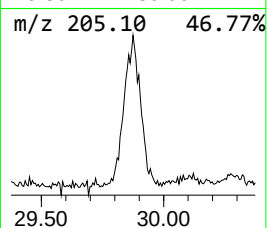
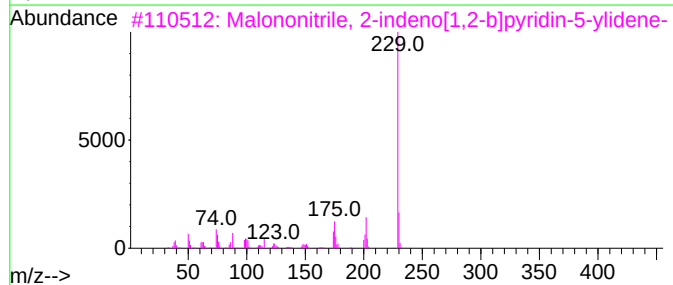
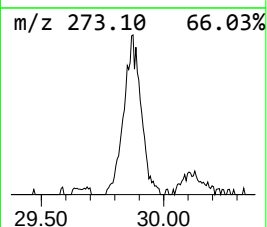
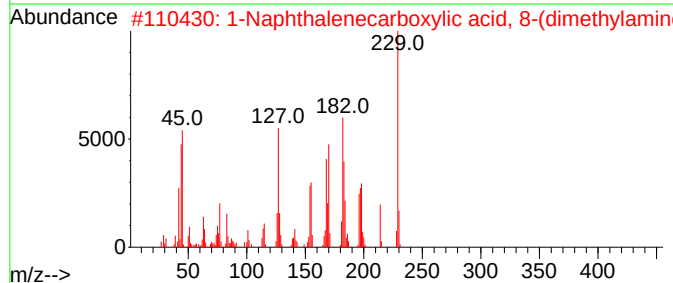
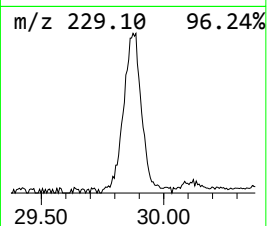
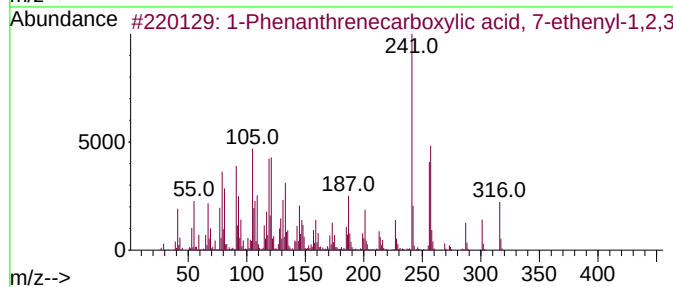
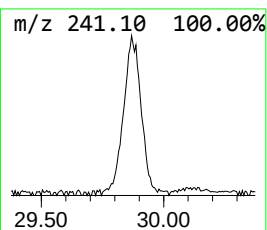
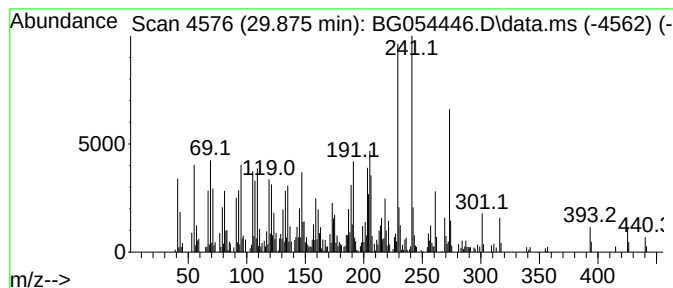
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown29.875 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.875	46.29 ng	909760	Perylene-d12	24.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenanthrenecarboxylic acid, 7...	316	C21H32O2	001686-62-0	41
2			1-Naphthalenecarboxylic acid, 8-...	229	C14H15NO2	069674-55-1	15
3			Malononitrile, 2-indeno[1,2-b]py...	229	C15H7N3	1000316-60-9	11
4			Benzo(a)acridine	229	C17H11N	000225-11-6	11
5			Phenol, 2,4-di(2-penten-4-yl)-6-...	244	C17H24O	017258-43-4	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072922\
Data File : BG054446.D
Acq On : 29 Jul 2022 12:43
Operator : CG/JU
Sample : N3895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RVE-40

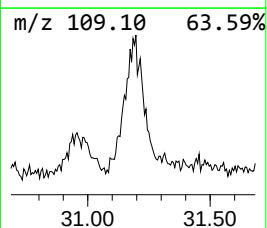
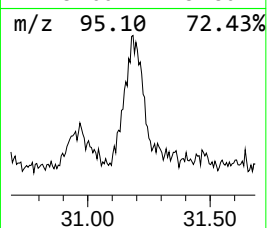
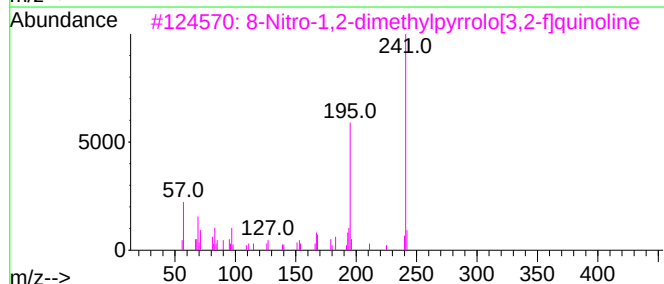
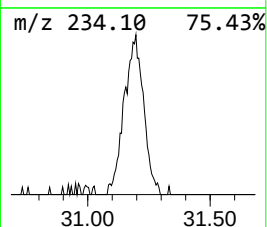
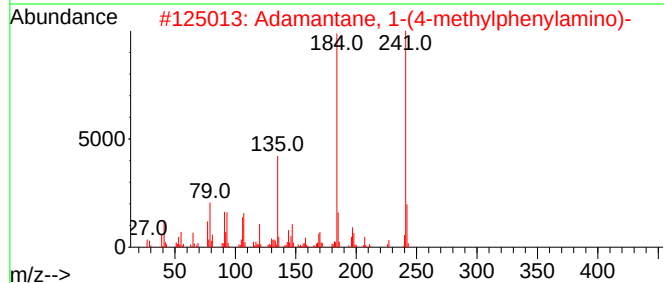
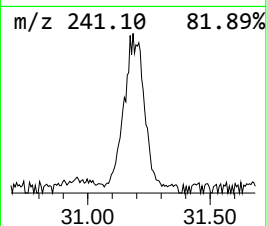
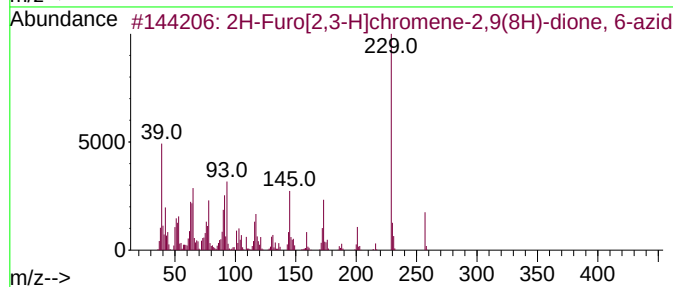
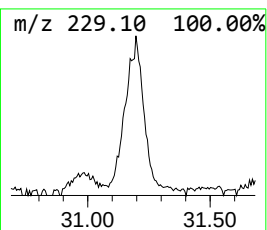
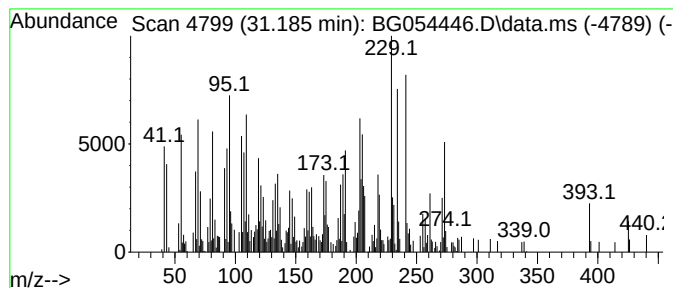
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown31.185 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.185	28.57 ng	561452	Perylene-d12	24.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Furo[2,3-H]chromene-2,9(8H)-d...	257	C12H7N3O4	1000272-56-6	25
2			Adamantane, 1-(4-methylphenylami...	241	C17H23N	019984-39-5	25
3			8-Nitro-1,2-dimethylpyrrolo[3,2-...	241	C13H11N3O2	072793-29-4	25
4			2-Amino-6-(1H-indol-3-yl)-3-pyri...	234	C14H10N4	077219-02-4	25
5			4-Methyl-6-methylthio-8-nitroqui...	234	C11H10N2O2S	1000213-15-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072922\
Data File : BG054446.D
Acq On : 29 Jul 2022 12:43
Operator : CG/JU
Sample : N3895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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
Butane, 2-metho...	3.106	33.3	ng	137725	1	7.989	82654	20.0
Tridecanoic acid	18.259	15.9	ng	208703	4	17.366	263399	20.0
Octadecanoic acid	19.528	21.6	ng	417943	5	21.631	387072	20.0
Trichloroacetic...	21.267	11.3	ng	219378	5	21.631	387072	20.0
1-Tricosene	22.436	10.2	ng	197545	5	21.631	387072	20.0
6a,12a-Dihydro-...	22.906	5.2	ng	100346	5	21.631	387072	20.0
Bicyclo[10.8.0]...	23.447	5.2	ng	103031	6	24.839	393036	20.0
Octadecane	23.899	29.5	ng	579186	6	24.839	393036	20.0
unknown25.351	25.351	6.3	ng	122737	6	24.839	393036	20.0
Heneicosane	25.956	12.1	ng	237431	6	24.839	393036	20.0
unknown29.029	29.029	266.8	ng	5243240	6	24.839	393036	20.0
unknown29.875	29.875	46.3	ng	909760	6	24.839	393036	20.0
unknown31.185	31.185	28.6	ng	561452	6	24.839	393036	20.0