

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
 Data File : BG048400.D
 Acq On : 17 Mar 2021 16:28
 Operator : CG/JU
 Sample : M1688-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 R-LA-4-1-WC

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-BG031621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048400.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.192	309	315	323	rVB	49146	73921	1.92%	0.284%
2	5.662	387	395	402	rBV	1027653	1639890	42.54%	6.298%
3	7.254	658	666	678	rVB	1092439	1928211	50.02%	7.405%
4	8.112	806	812	819	rVB	211469	362471	9.40%	1.392%
5	9.281	1003	1011	1020	rBV	679660	1203897	31.23%	4.624%
6	10.938	1284	1293	1301	rBV	289075	521175	13.52%	2.002%
7	12.683	1585	1590	1597	rBV3	22290	46393	1.20%	0.178%
8	13.376	1701	1708	1715	rVB	1766066	2676004	69.42%	10.277%
9	14.199	1840	1848	1852	rBV	50769	75328	1.95%	0.289%
10	14.751	1936	1942	1950	rVB	510389	798951	20.73%	3.068%
11	16.237	2188	2195	2203	rBV	1625714	2443950	63.40%	9.386%
12	17.377	2385	2389	2393	rBV3	32980	49962	1.30%	0.192%
13	17.501	2404	2410	2416	rBV	667866	1003078	26.02%	3.852%
14	18.264	2535	2540	2547	rBV7	36385	69138	1.79%	0.266%
15	18.388	2555	2561	2571	rBV	787622	1175019	30.48%	4.513%
16	18.682	2606	2611	2617	rBV8	23710	45184	1.17%	0.174%
17	19.158	2688	2692	2696	rVB	51970	68540	1.78%	0.263%
18	19.551	2753	2759	2765	rVB3	96948	202467	5.25%	0.778%
19	19.657	2772	2777	2785	rBV	411470	590662	15.32%	2.268%
20	19.915	2817	2821	2824	rVB	55041	72830	1.89%	0.280%
21	20.109	2849	2854	2861	rBV	2864281	3854733	100.00%	14.804%
22	21.384	3065	3071	3075	rBV	273222	541790	14.06%	2.081%
23	21.449	3080	3082	3087	rVV	459767	668043	17.33%	2.566%
24	21.514	3087	3093	3103	rVV	1636536	2326070	60.34%	8.933%
25	21.596	3103	3107	3113	rVB	86102	128908	3.34%	0.495%
26	21.796	3135	3141	3147	rVB	634970	1044918	27.11%	4.013%
27	21.995	3172	3175	3181	rBV8	38286	70589	1.83%	0.271%
28	22.642	3281	3285	3295	rVB6	63516	164542	4.27%	0.632%
29	23.723	3464	3469	3477	rBV4	78312	157234	4.08%	0.604%
30	24.210	3548	3552	3556	rBV4	54737	92157	2.39%	0.354%
31	24.263	3556	3561	3571	rVB6	98562	216139	5.61%	0.830%
32	25.133	3700	3709	3718	rBV	349099	981406	25.46%	3.769%
33	25.750	3809	3814	3816	rBV5	30495	61333	1.59%	0.236%
34	26.531	3941	3947	3957	rVB7	69600	197138	5.11%	0.757%
35	29.569	4455	4464	4477	rVB7	118120	485578	12.60%	1.865%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

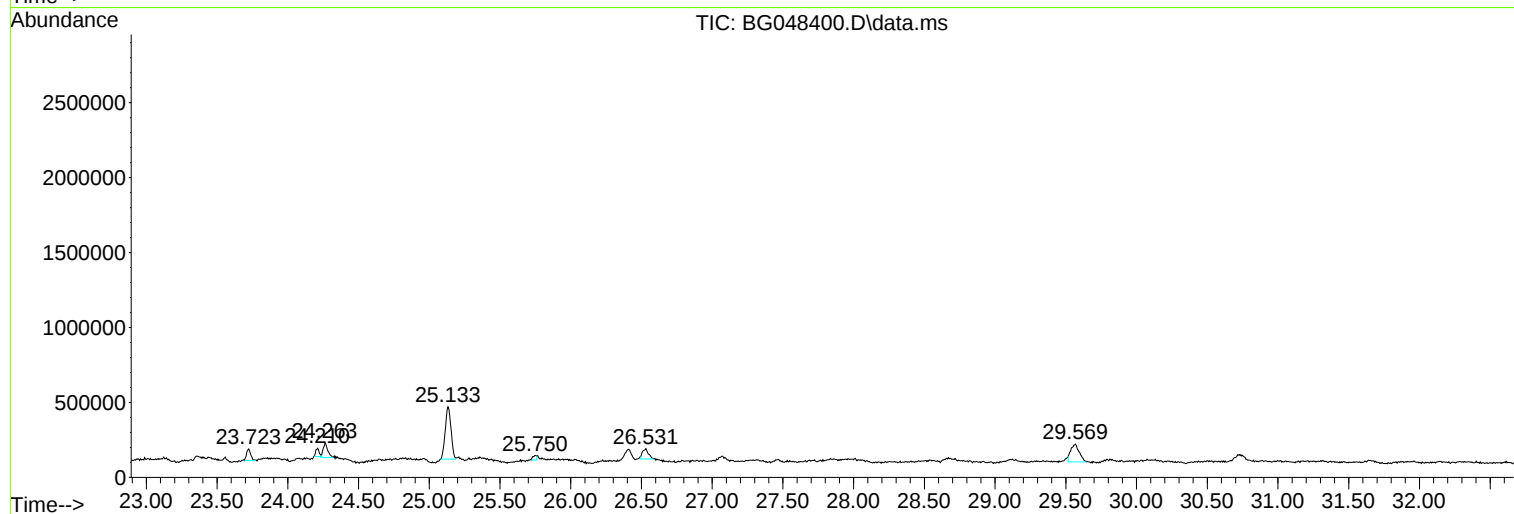
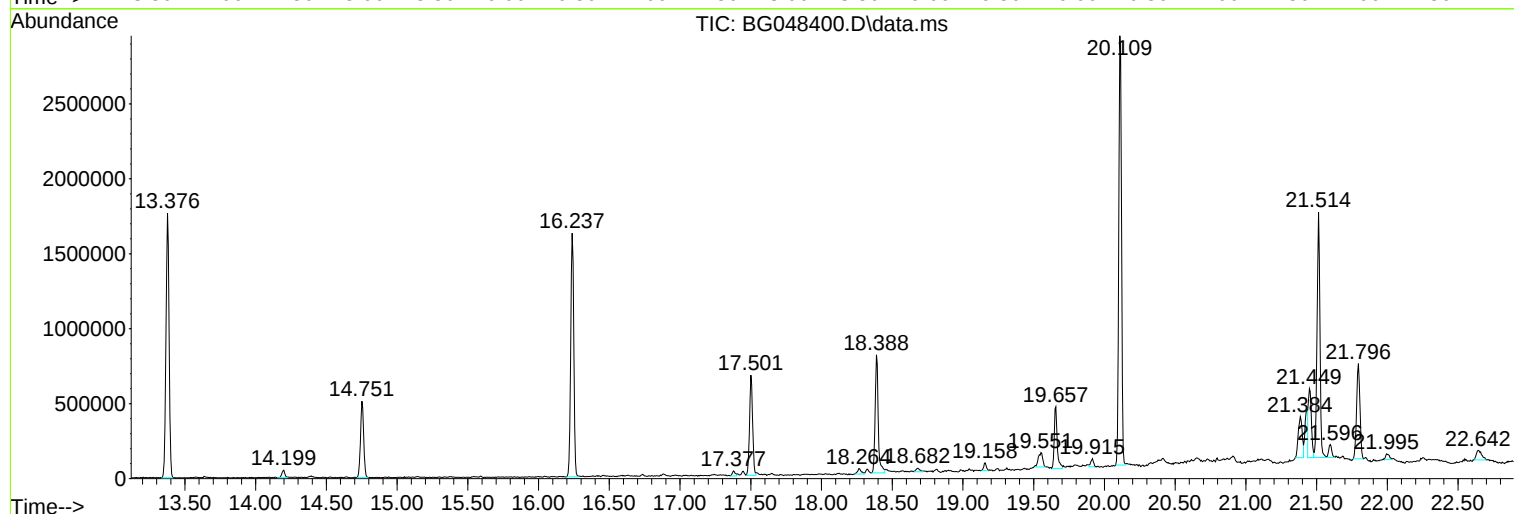
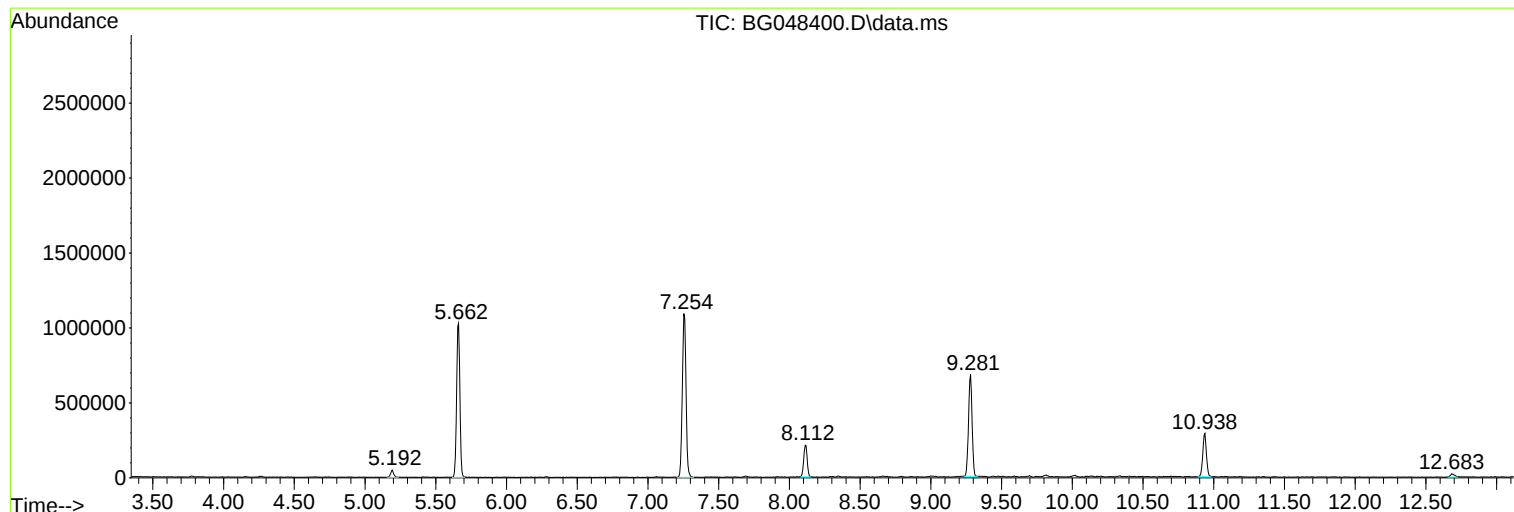
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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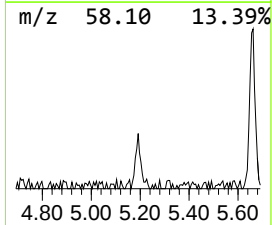
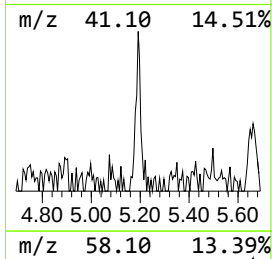
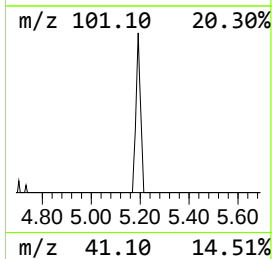
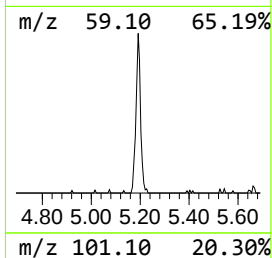
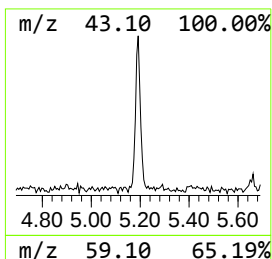
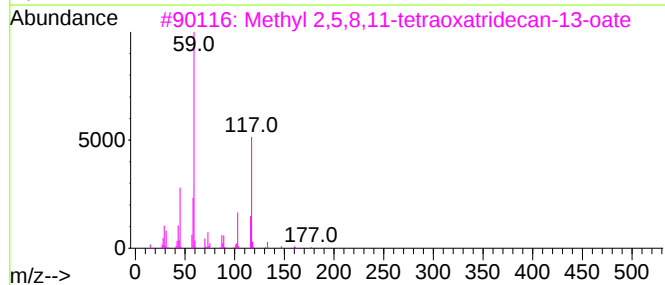
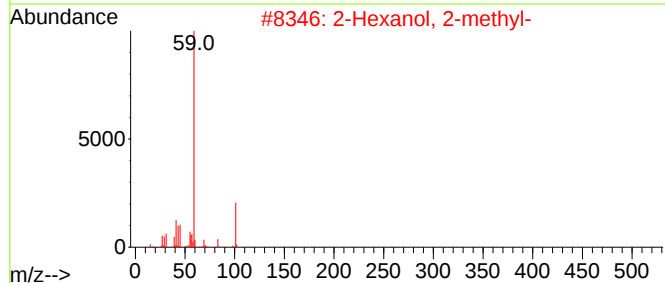
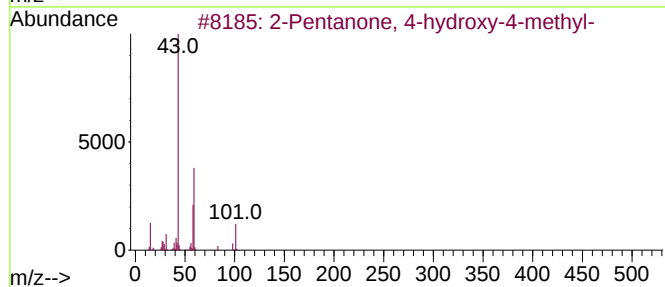
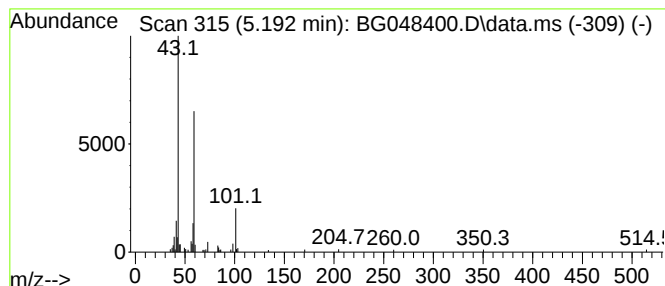
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	4.08 ng	73921	1,4-Dichlorobenzene-d4	8.112

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	45
3			Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	37
4			3-Hexanol	102	C6H14O	000623-37-0	32
5			3-Octanol	130	C8H18O	000589-98-0	25



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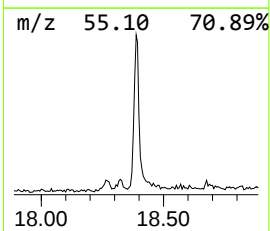
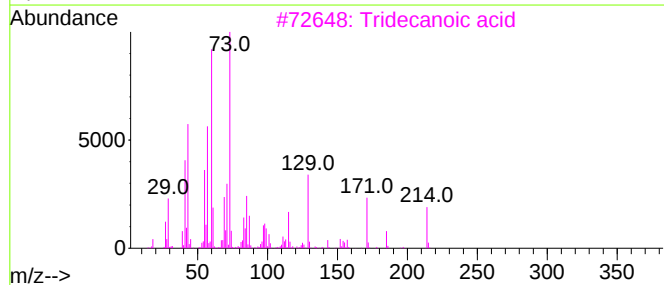
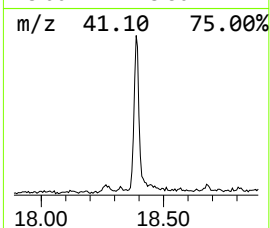
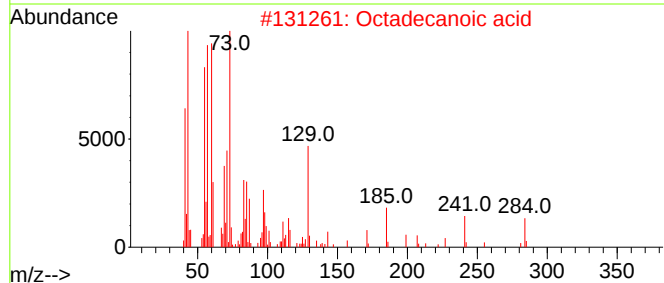
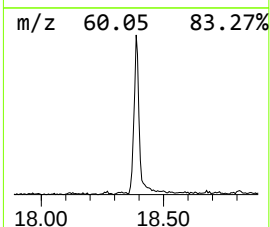
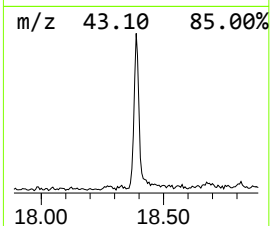
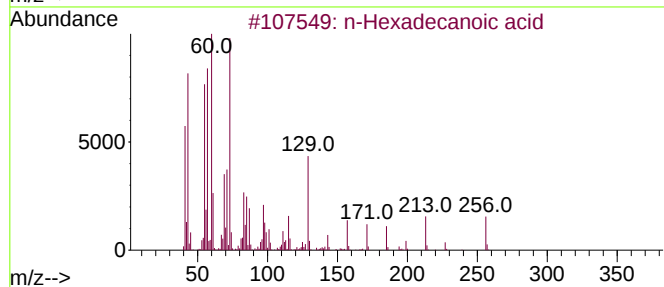
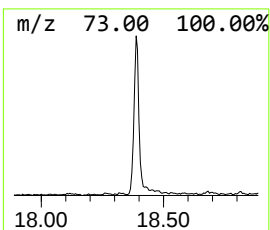
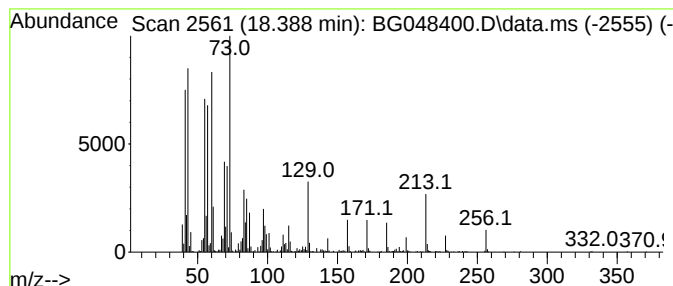
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.388	23.43 ng	1175020	Phenanthrene-d10	17.501

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Octadecanoic acid	284	C18H36O2	000057-11-4	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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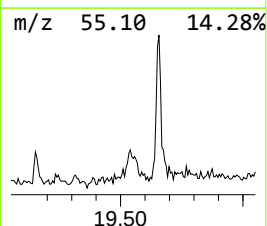
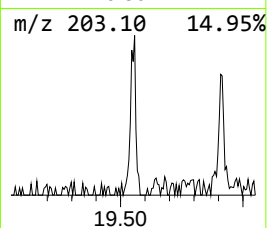
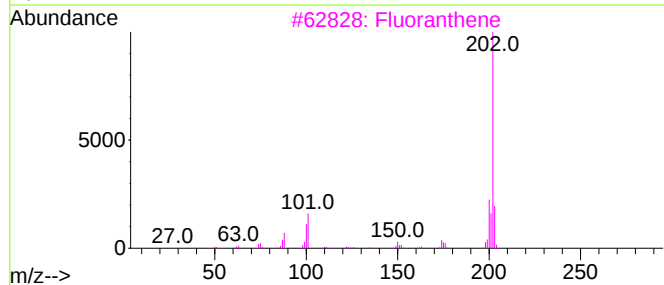
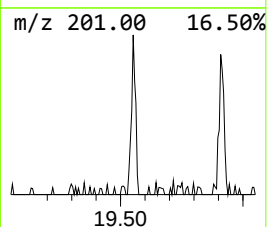
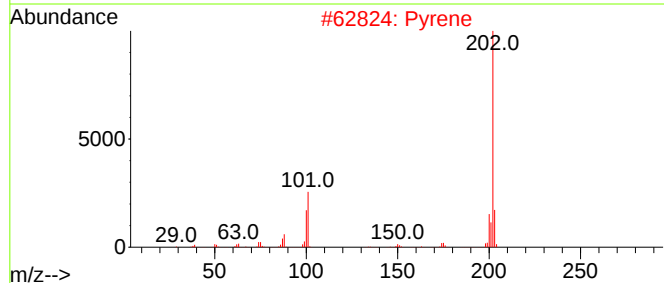
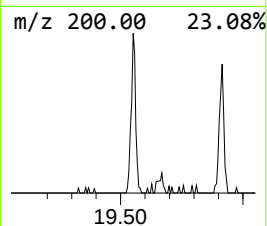
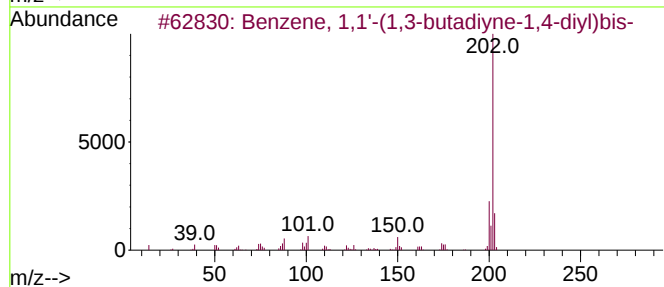
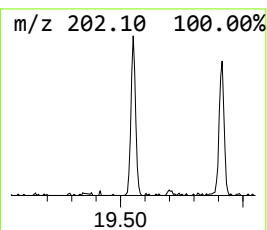
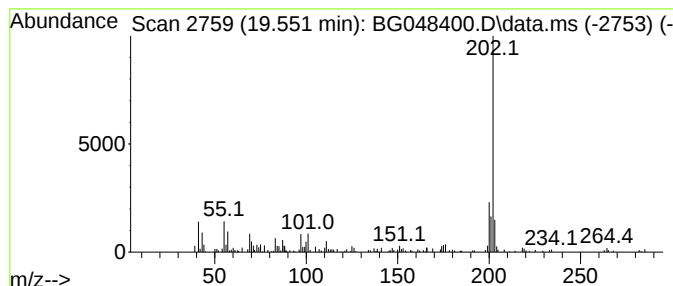
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	4.04 ng	202467	Phenanthrene-d10	17.501

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
2			Pyrene	202	C16H10	000129-00-0	62
3			Fluoranthene	202	C16H10	000206-44-0	58
4			Pyrimidine, 4-methoxy-6-(2-hydro...	202	C11H10N2O2	097630-79-0	58
5			7H-Furo[3,2-g][1]benzopyran-7-on...	202	C11H6O4	002009-24-7	50



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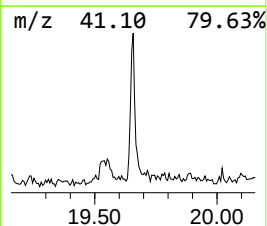
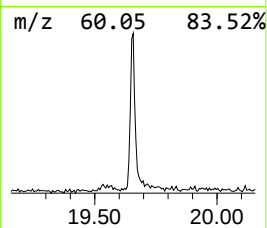
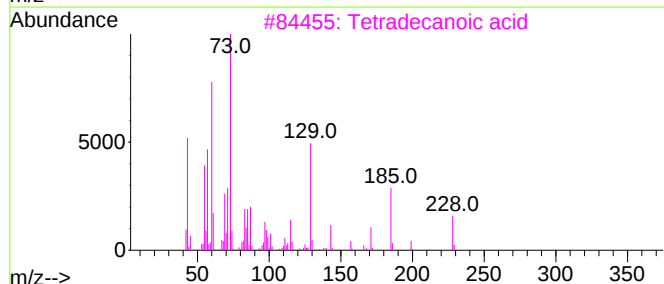
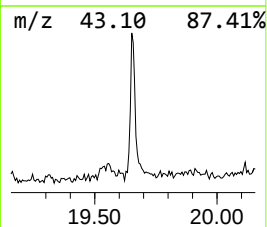
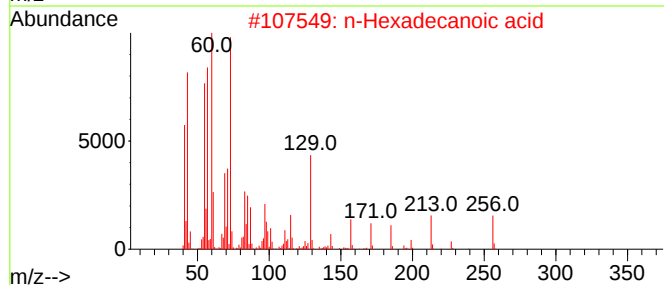
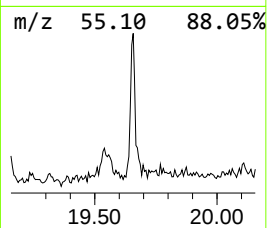
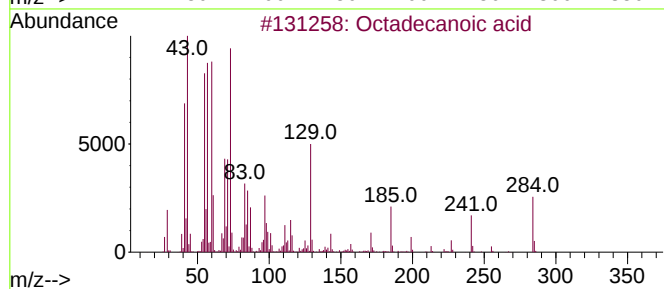
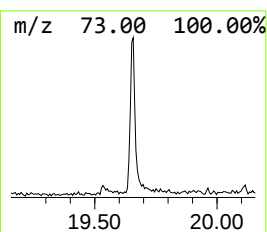
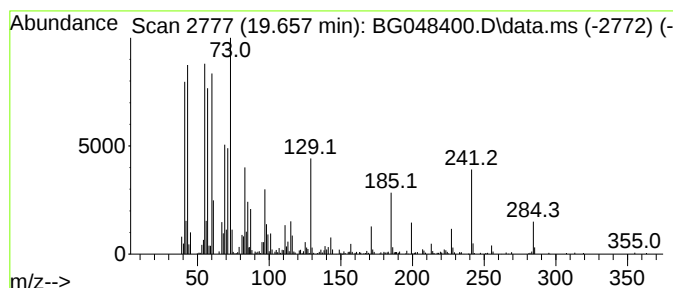
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.657	11.31 ng	590662	Chrysene-d12	21.796

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			Tridecanoic acid	214	C13H26O2	000638-53-9	49



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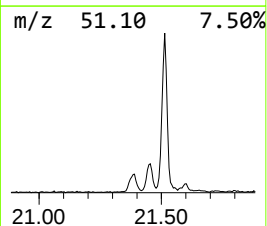
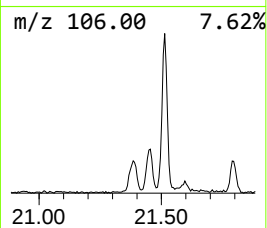
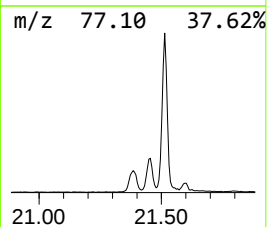
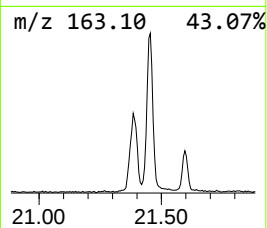
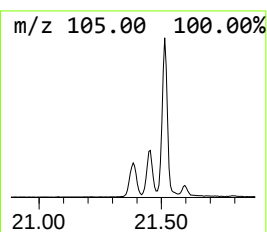
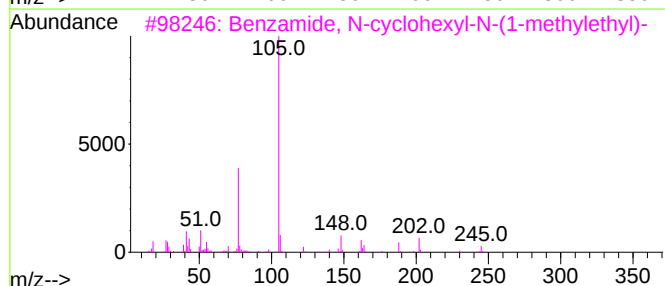
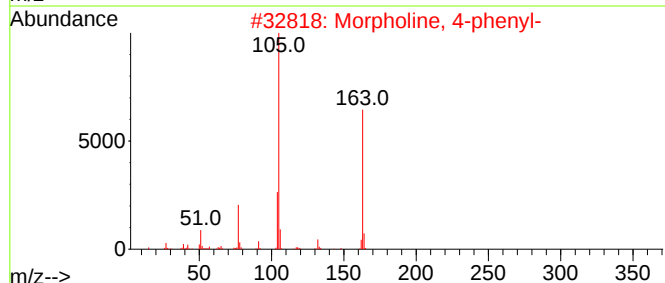
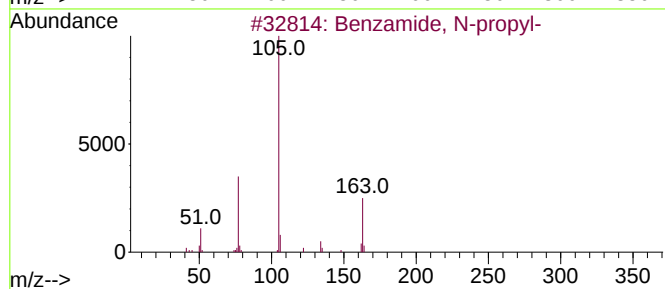
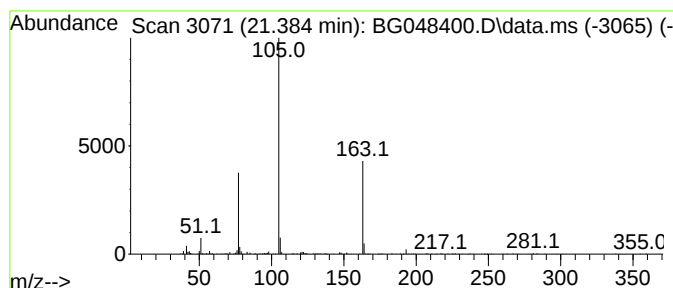
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown21.38 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.384	10.37 ng	541790	Chrysene-d12	21.796	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	56
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
3	Benzamide, N-cyclohexyl-N-(1-met...	245	C16H23NO	052812-84-7	32
4	Benzo[b]thiophene-3-carboxylic a...	343	C18H17NO4S	096334-43-9	27
5	Isopropyl phenyl ketone	148	C10H12O	000611-70-1	27



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Data File : BG048400.D
Acq On : 17 Mar 2021 16:28
Operator : CG/JU
Sample : M1688-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
R-LA-4-1-WC

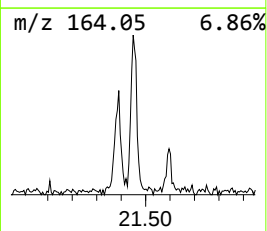
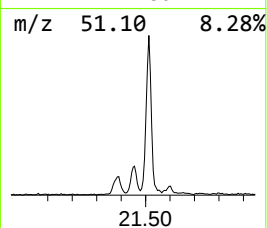
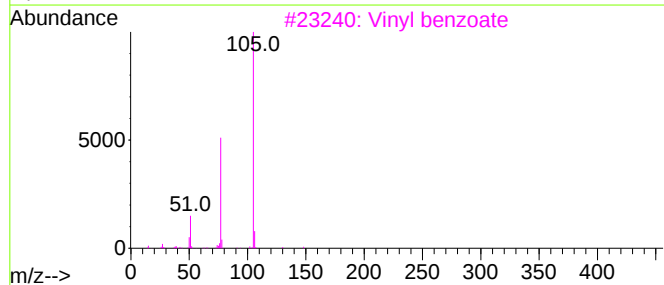
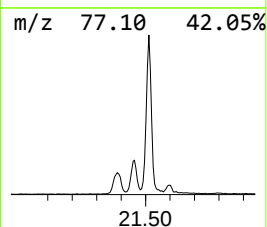
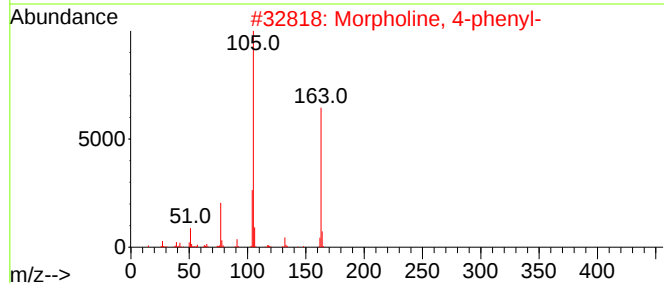
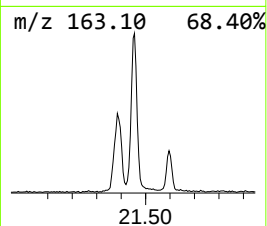
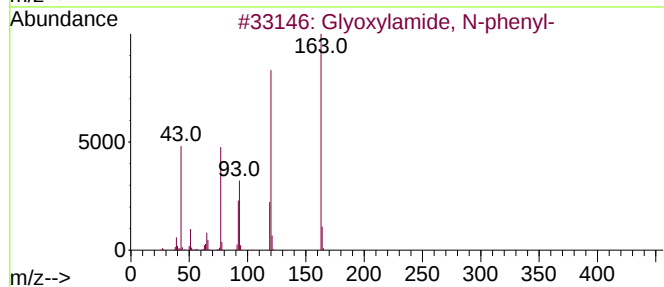
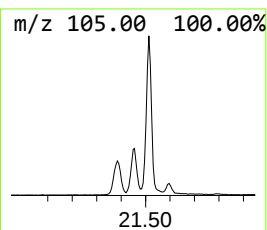
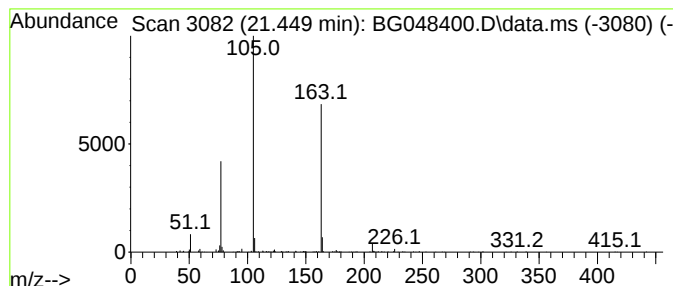
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown21.44 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.449	12.79 ng	668043	Chrysene-d12	21.796

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
2		Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	47
3		Vinyl benzoate	148	C9H8O2	000769-78-8	38
4		Benzoyl chloride	140	C7H5ClO	000098-88-4	38
5		4'-Nitrobenzanilide	242	C13H10N2O3	003393-96-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
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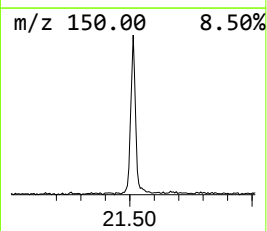
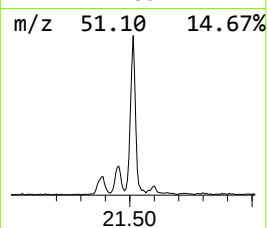
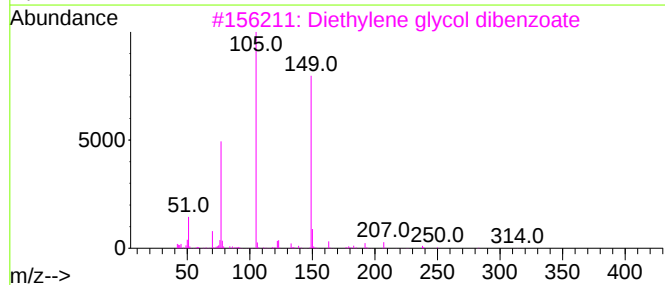
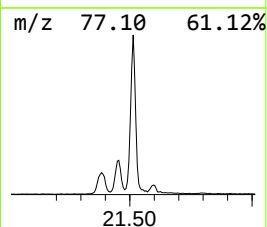
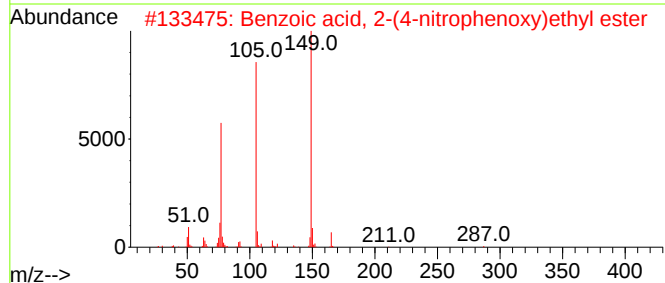
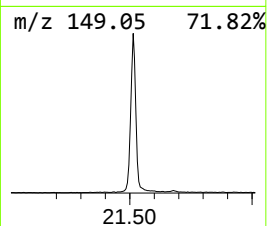
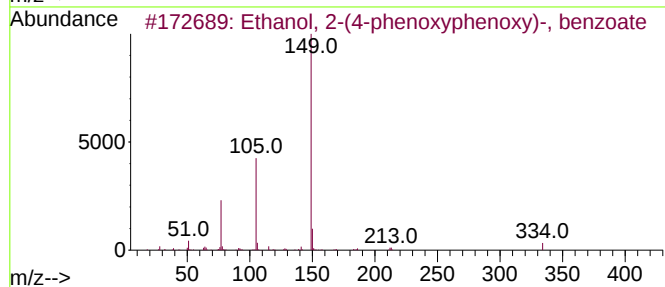
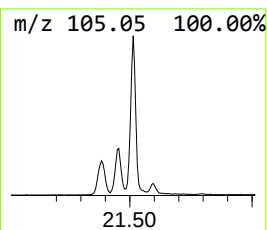
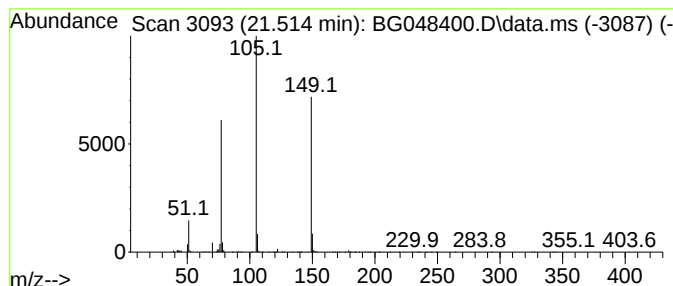
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Ethanol, 2-(4-phenoxyphenox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.514	44.52 ng	2326070	Chrysene-d12	21.796

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(4-phenoxyphenoxy)-, ...	334	C21H18O4	055191-59-8	83
2			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
3			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
4			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
5			1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048400.D
Acq On : 17 Mar 2021 16:28
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Sample : M1688-01
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ClientSampleId :
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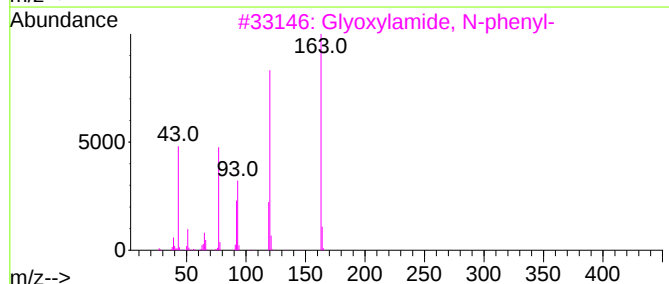
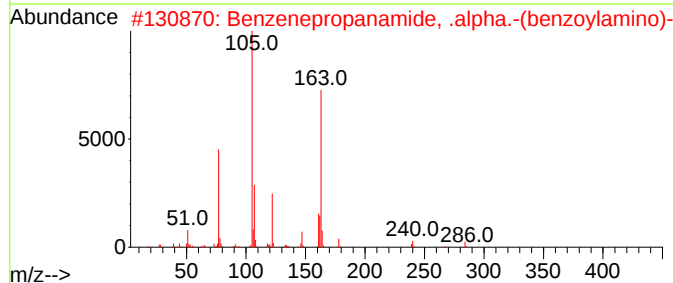
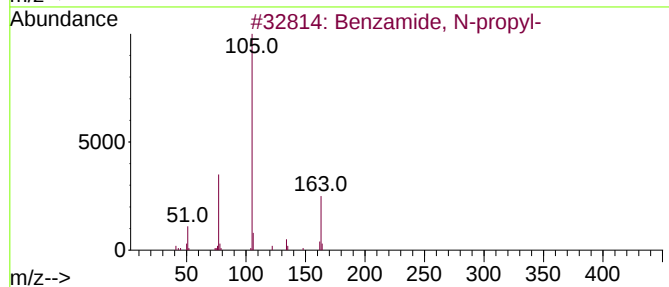
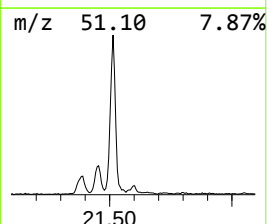
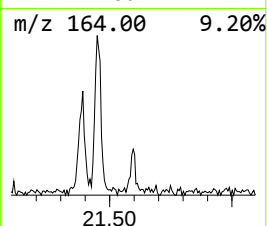
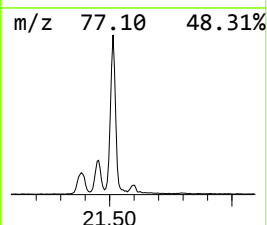
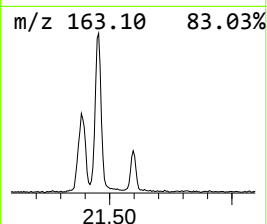
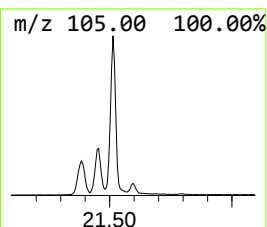
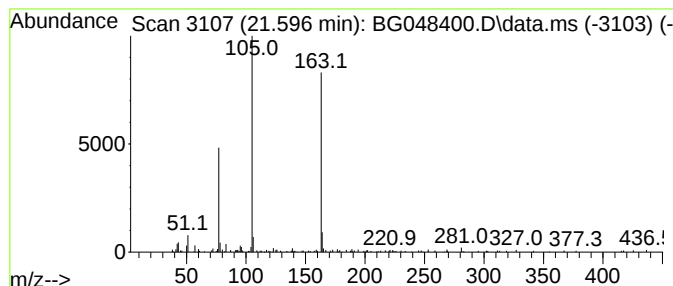
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzamide, N-propyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.596	2.47 ng	128908	Chrysene-d12	21.796

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	64
2			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	64
3			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	59
4			Benzoic acid, 2-benzoyl-, methyl...	240	C15H12O3	000606-28-0	43
5			.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048400.D
Acq On : 17 Mar 2021 16:28
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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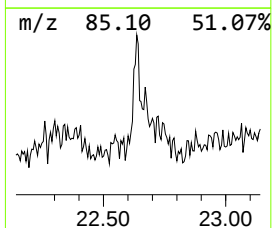
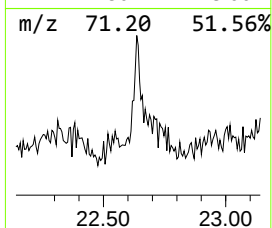
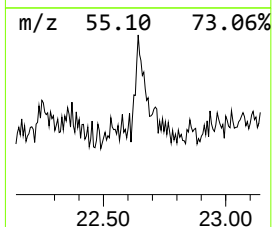
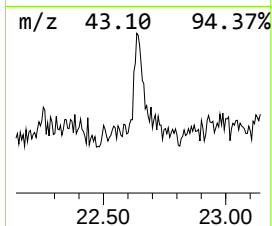
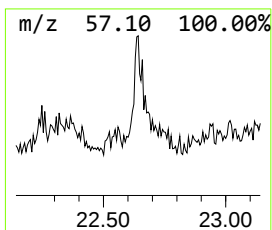
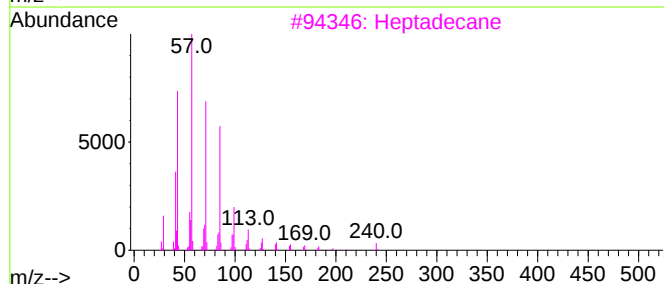
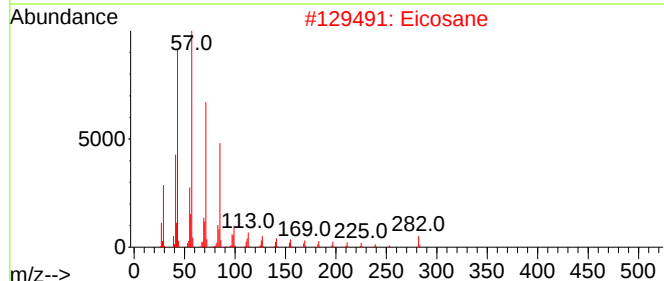
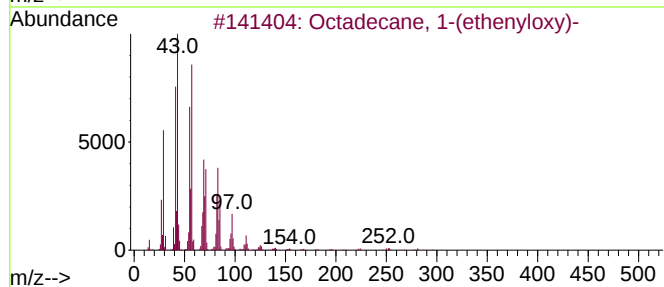
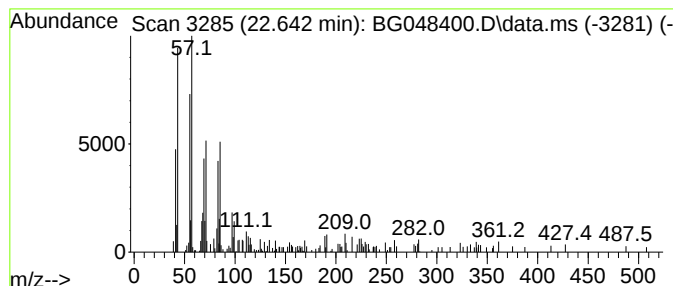
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octadecane, 1-(ethenyloxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.642	3.15 ng	164542	Chrysene-d12	21.796

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	64
2			Eicosane	282	C20H42	000112-95-8	55
3			Heptadecane	240	C17H36	000629-78-7	50
4			Octadecane	254	C18H38	000593-45-3	50
5			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
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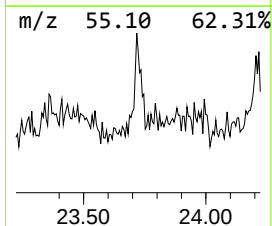
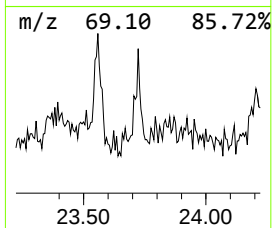
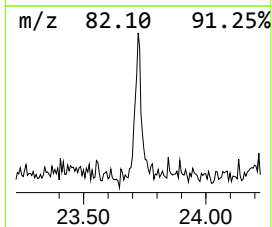
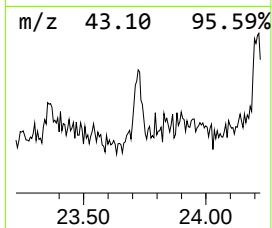
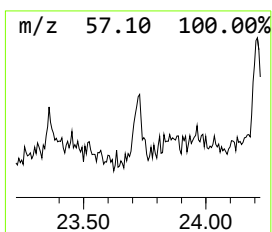
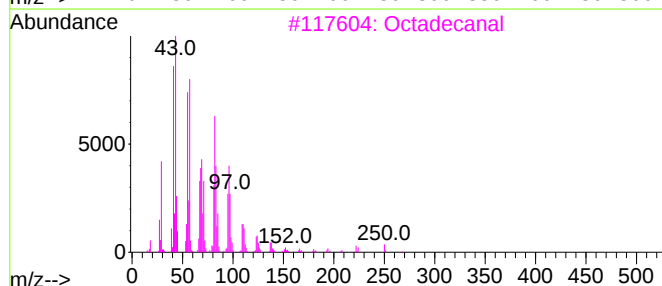
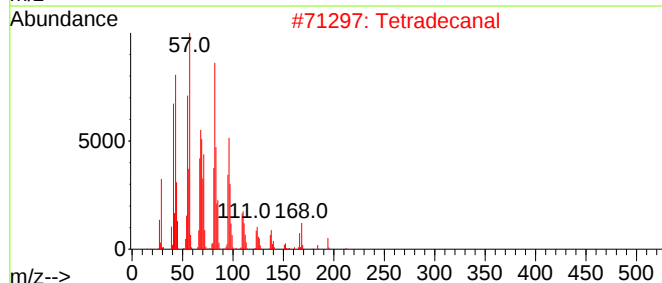
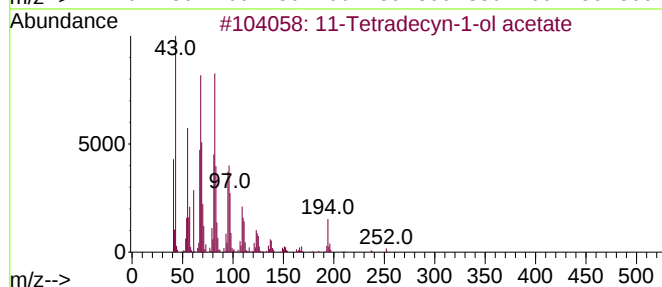
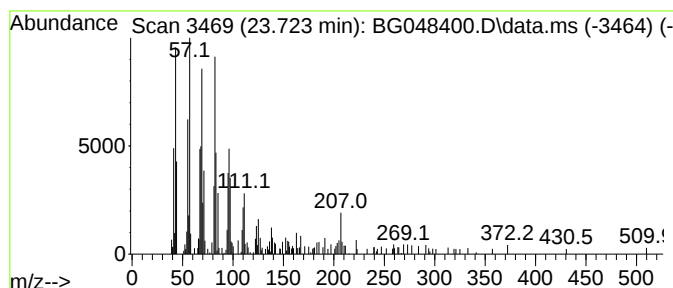
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 11-Tetradecyn-1-ol acetate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.723	3.20 ng	157234	Perylene-d12		25.133	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tetradecyn-1-ol	acetate	252	C16H28O2	033925-72-3	70
2	Tetradecanal		212	C14H28O	000124-25-4	58
3	Octadecanal		268	C18H36O	000638-66-4	58
4	1,13-Tetradecadiene		194	C14H26	021964-49-8	50
5	14-Heptadecenal		252	C17H32O	1000144-58-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
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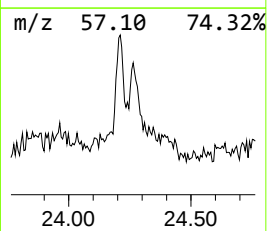
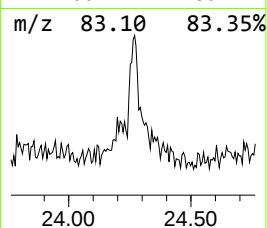
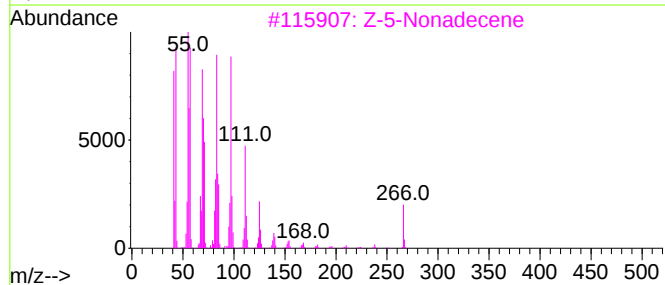
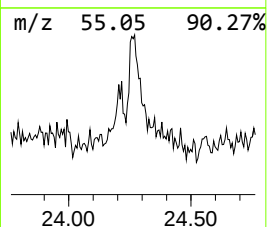
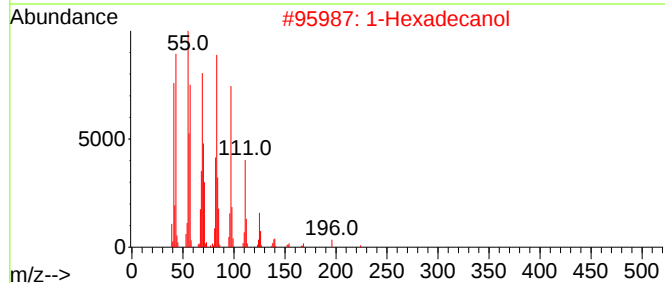
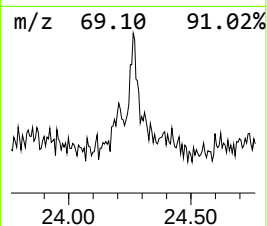
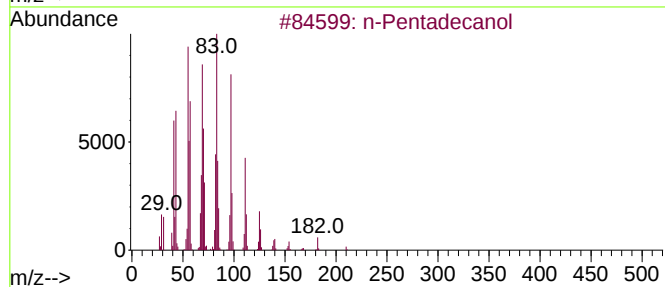
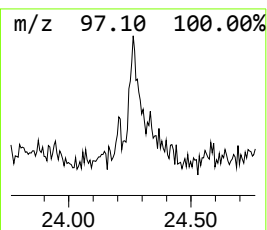
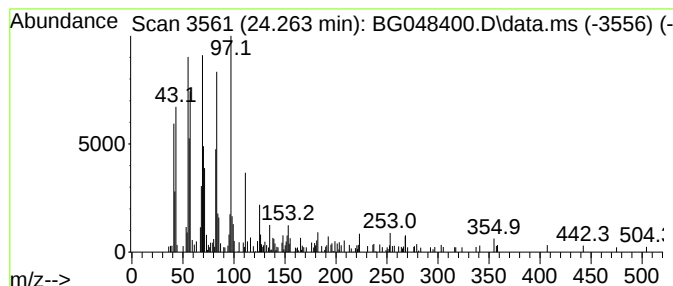
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 n-Pentadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.263	4.40 ng	216139	Perylene-d12	25.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Pentadecanol	228	C15H32O	000629-76-5	87
2			1-Hexadecanol	242	C16H34O	036653-82-4	87
3			Z-5-Nonadecene	266	C19H38	1000131-11-8	87
4			1-Nonadecene	266	C19H38	018435-45-5	78
5			Cycloundecane, (1-methylethyl)-	196	C14H28	062338-56-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048400.D
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ALS Vial : 7 Sample Multiplier: 1

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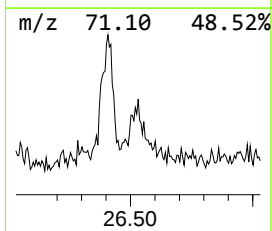
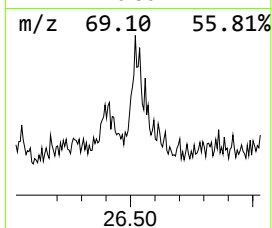
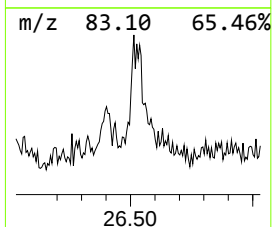
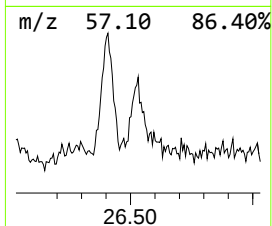
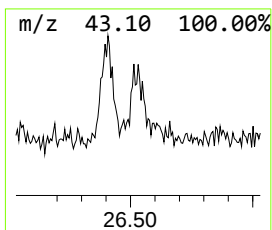
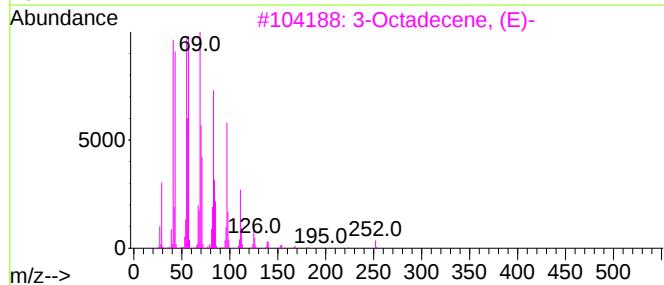
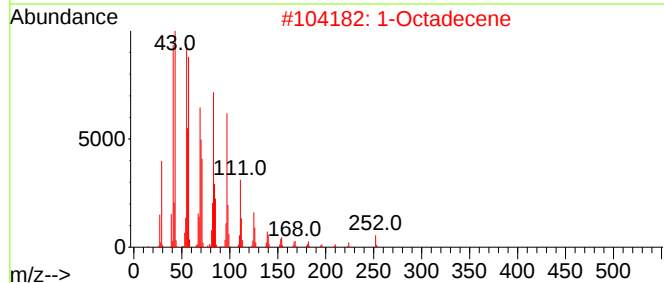
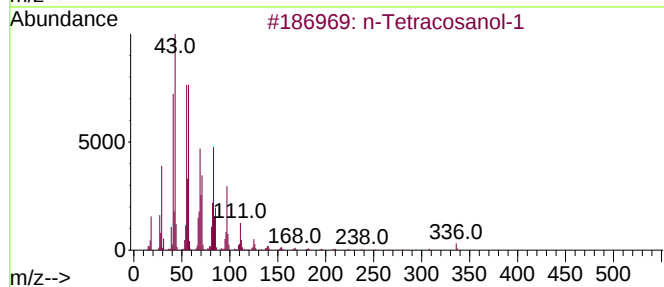
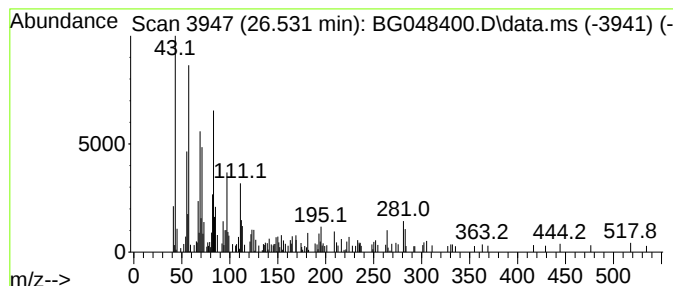
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 n-Tetracosanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.531	4.02 ng	197138	Perylene-d12	25.133

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	68
2		1-Octadecene	252	C18H36	000112-88-9	62
3		3-Octadecene, (E)-	252	C18H36	007206-19-1	62
4		E-15-Heptadecenal	252	C17H32O	1000130-97-9	62
5		Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048400.D
Acq On : 17 Mar 2021 16:28
Operator : CG/JU
Sample : M1688-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
R-LA-4-1-WC

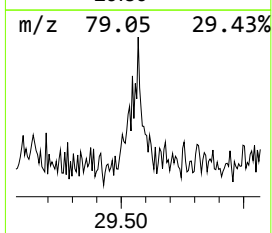
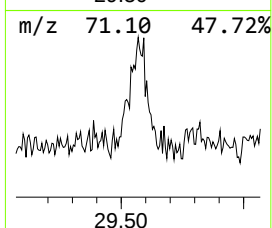
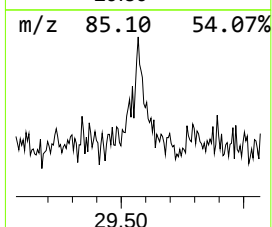
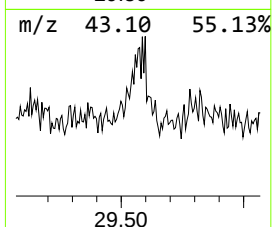
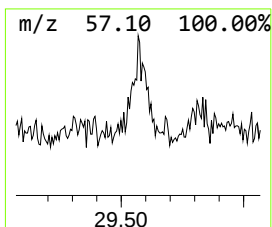
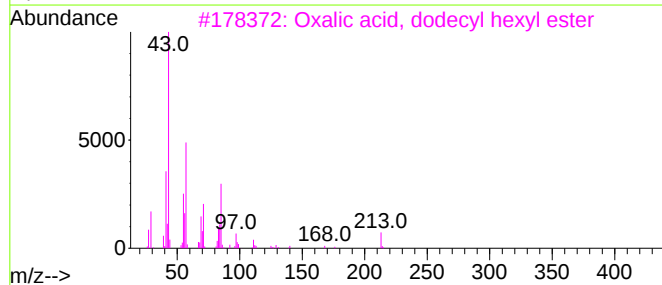
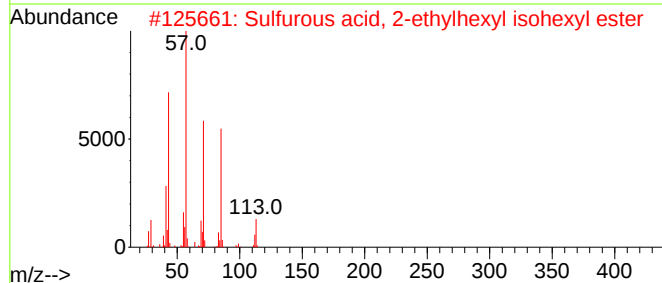
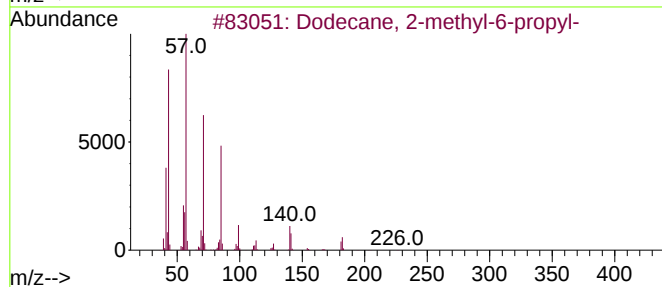
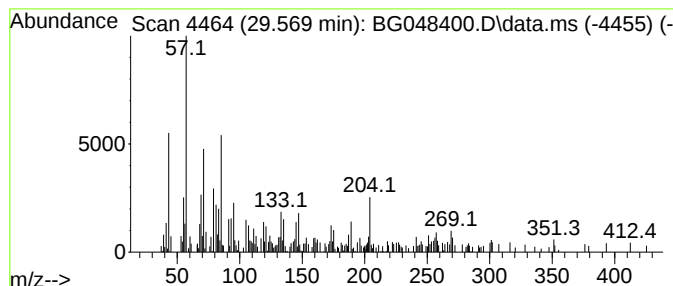
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown29.56 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.569	9.90 ng	485578	Perylene-d12	25.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	43
2			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	43
3			Oxalic acid, dodecyl hexyl ester	342	C20H38O4	1000309-24-6	43
4			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	43
5			Nonadecane	268	C19H40	000629-92-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048400.D
Acq On : 17 Mar 2021 16:28
Operator : CG/JU
Sample : M1688-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
R-LA-4-1-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.192	4.1	ng	73921	1	8.112	362471	20.0
n-Hexadecanoic ...	18.388	23.4	ng	1175020	4	17.501	1003080	20.0
Benzene, 1,1'-(...	19.551	4.0	ng	202467	4	17.501	1003080	20.0
Octadecanoic acid	19.657	11.3	ng	590662	5	21.796	1044920	20.0
unknown21.38	21.384	10.4	ng	541790	5	21.796	1044920	20.0
unknown21.44	21.449	12.8	ng	668043	5	21.796	1044920	20.0
Ethanol, 2-(4-p...	21.514	44.5	ng	2326070	5	21.796	1044920	20.0
Benzamide, N-pr...	21.596	2.5	ng	128908	5	21.796	1044920	20.0
Octadecane, 1-(...	22.642	3.1	ng	164542	5	21.796	1044920	20.0
11-Tetradecyn-1...	23.723	3.2	ng	157234	6	25.133	981406	20.0
n-Pentadecanol	24.263	4.4	ng	216139	6	25.133	981406	20.0
n-Tetracosanol-1	26.531	4.0	ng	197138	6	25.133	981406	20.0
unknown29.56	29.569	9.9	ng	485578	6	25.133	981406	20.0