

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG063020\
 Data File : BG045897.D
 Acq On : 30 Jun 2020 23:28
 Operator : CG/JU
 Sample : L2819-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BU-03-062620

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BG061520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.496	402	410	426	rBV	781488	1413645	22.29%	4.155%
2	7.118	678	686	697	rBV	869867	1557904	24.57%	4.579%
3	7.893	811	818	827	rVB	232087	401650	6.33%	1.181%
4	8.216	865	873	884	rBV	728661	1295415	20.43%	3.808%
5	9.056	1009	1016	1028	rBV	546683	1024765	16.16%	3.012%
6	10.701	1288	1296	1307	rBV	309185	557871	8.80%	1.640%
7	12.099	1526	1534	1544	rBV	49237	104365	1.65%	0.307%
8	13.168	1708	1716	1722	rBV	1591589	2493480	39.32%	7.329%
9	13.227	1722	1726	1734	rVB	38453	67749	1.07%	0.199%
10	14.002	1852	1858	1863	rBV	124801	186628	2.94%	0.549%
11	14.549	1945	1951	1957	rVB	493548	758216	11.96%	2.229%
12	16.047	2196	2206	2217	rBV	1082965	1715657	27.05%	5.043%
13	17.298	2413	2419	2424	rBV	525539	839723	13.24%	2.468%
14	17.973	2528	2534	2540	rVB	1025591	1297876	20.47%	3.815%
15	18.214	2571	2575	2582	rBV3	106843	158092	2.49%	0.465%
16	18.960	2698	2702	2707	rBV	64853	82595	1.30%	0.243%
17	19.113	2722	2728	2731	rBV	4903474	6341480	100.00%	18.640%
18	19.148	2731	2734	2743	rVB2	3746481	4685090	73.88%	13.771%
19	19.278	2751	2756	2762	rVB	742907	901760	14.22%	2.651%
20	19.360	2765	2770	2775	rBV	141496	215091	3.39%	0.632%
21	19.718	2823	2831	2839	rBV	115310	227863	3.59%	0.670%
22	19.918	2859	2865	2872	rBV	2299054	3101878	48.91%	9.118%
23	20.259	2920	2923	2929	rVB5	81434	115406	1.82%	0.339%
24	20.370	2938	2942	2945	rBV2	86341	101892	1.61%	0.299%
25	20.529	2966	2969	2972	rBV3	64194	66642	1.05%	0.196%
26	21.034	3051	3055	3059	rVB	182331	238749	3.76%	0.702%
27	21.216	3081	3086	3095	rVB3	240969	396129	6.25%	1.164%
28	21.369	3109	3112	3117	rVB2	67094	87539	1.38%	0.257%
29	21.557	3137	3144	3149	rBV	538346	906971	14.30%	2.666%
30	22.362	3274	3281	3288	rVB5	101391	276176	4.36%	0.812%
31	23.789	3518	3524	3531	rVB	365312	759961	11.98%	2.234%
32	24.676	3667	3675	3688	rVB2	324922	938115	14.79%	2.757%
33	25.780	3856	3863	3875	rVB2	240384	704709	11.11%	2.071%

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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-BG061520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

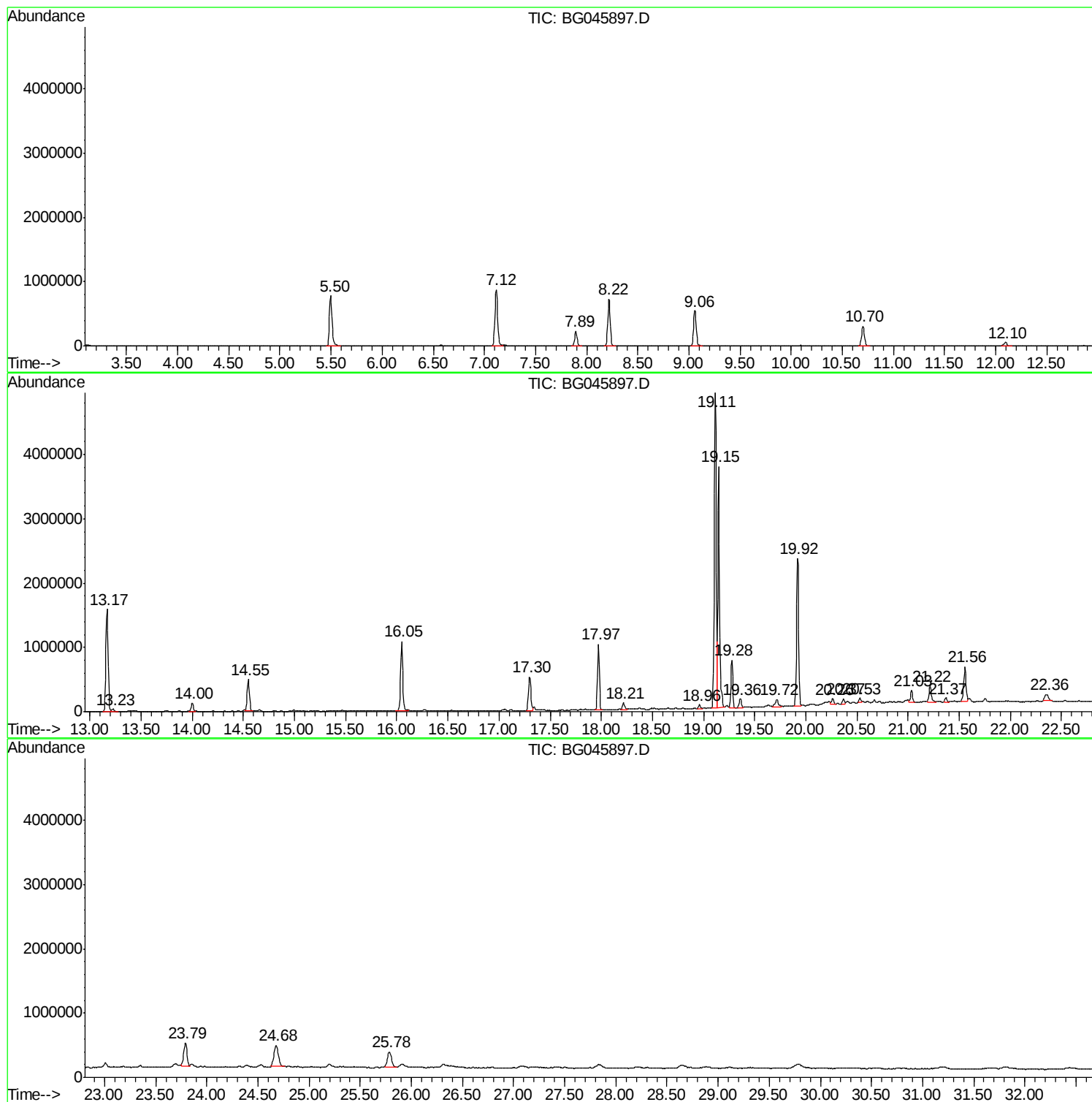
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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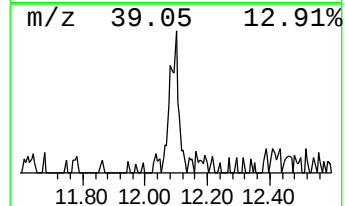
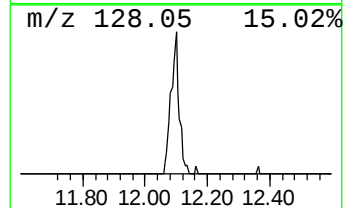
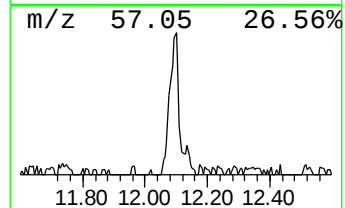
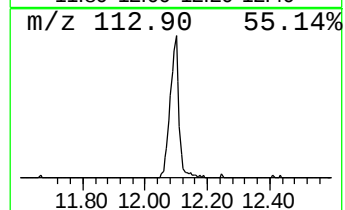
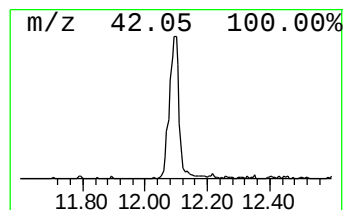
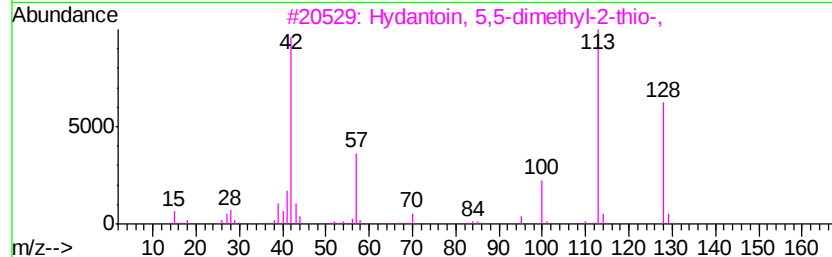
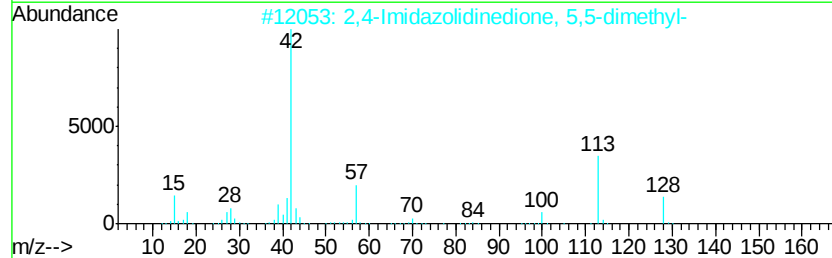
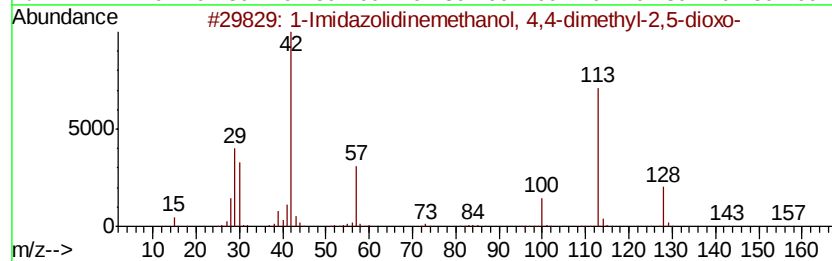
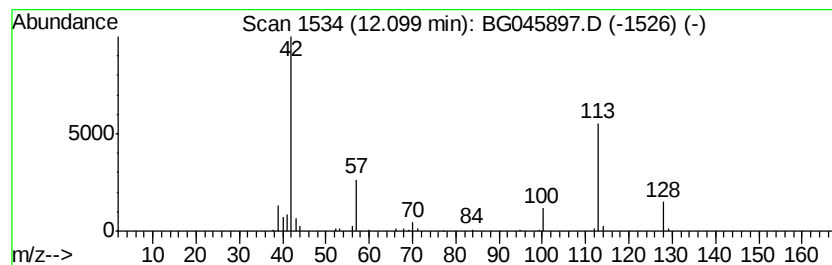
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Imidazolidinemethanol, 4,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.10	3.74 ng	104365	Naphthalene-d8	10.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Imidazolidinemethanol, 4,4-dim...	158	C6H10N2O3	016228-00-5	64
2		2,4-Imidazolidinedione, 5,5-dime...	128	C5H8N2O2	000077-71-4	64
3		Hvdantoin, 5,5-dimethyl-2-thio-	144	C5H8N2OS	015998-93-3	38
4		1H-Pyrazole, 4-nitro-	113	C3H3N3O2	002075-46-9	14
5		1-Amino-2,6-dimethylpiperidine	128	C7H16N2	039135-39-2	10



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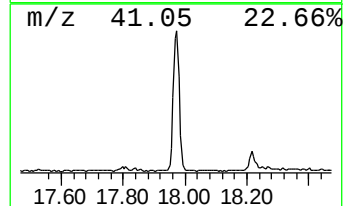
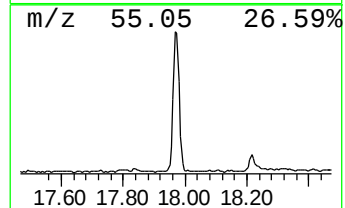
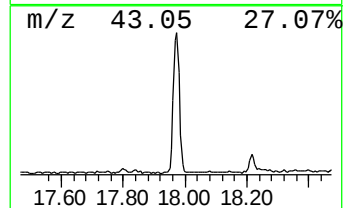
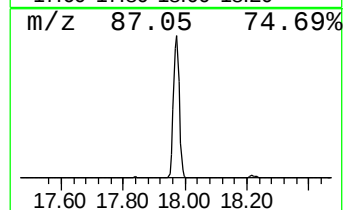
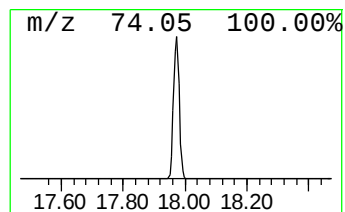
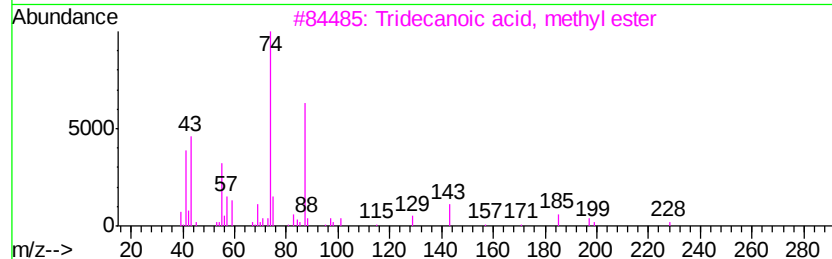
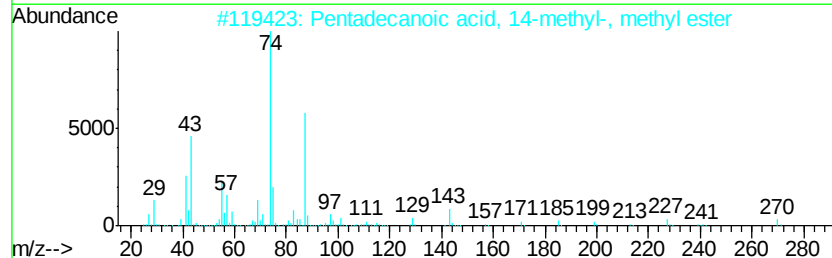
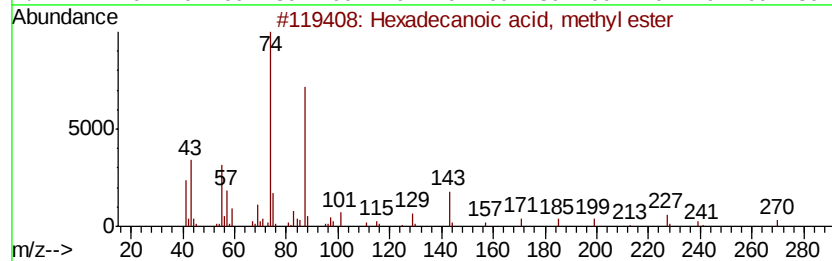
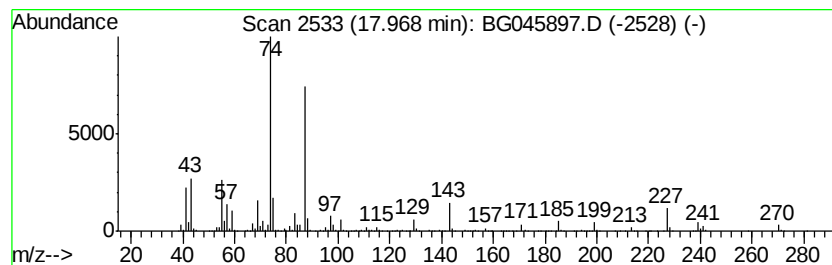
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TIC Library : C:\Database\NIST11.L
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 Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	30.91 ng	1297880	Phenanthrene-d10	17.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	89
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
5		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80



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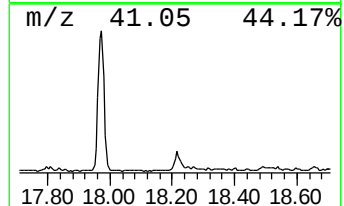
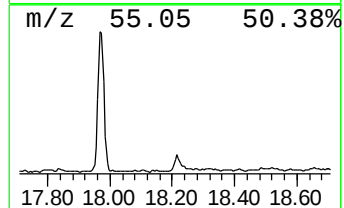
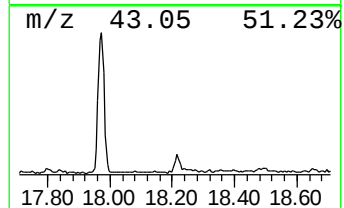
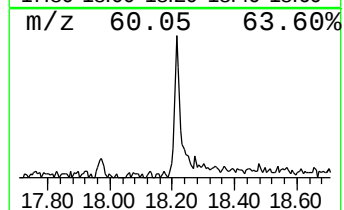
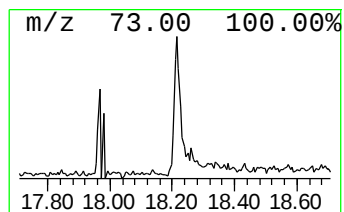
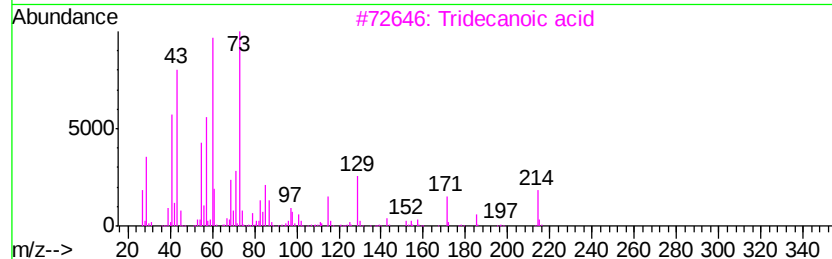
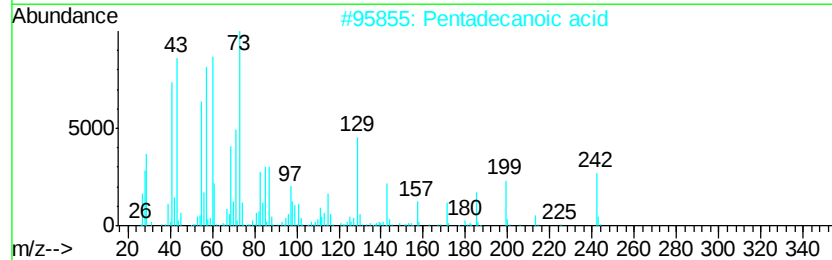
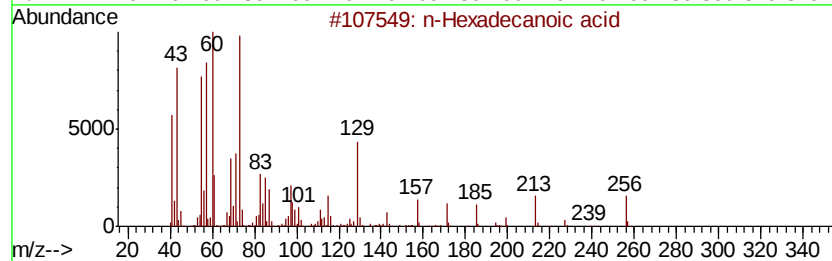
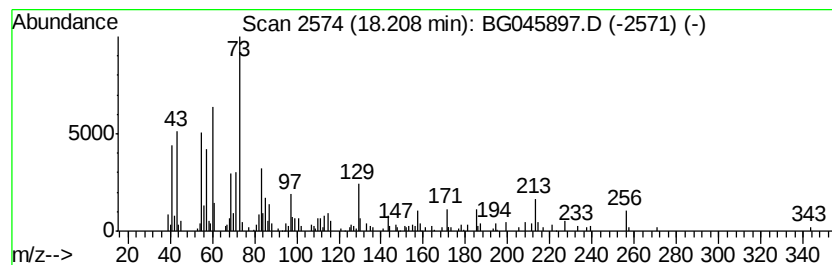
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.21	3.77 ng	158092	Phenanthrene-d10	17.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tridecanoic acid	214	C13H26O2	000638-53-9	70
4		n-Decanoic acid	172	C10H20O2	000334-48-5	62
5		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	18



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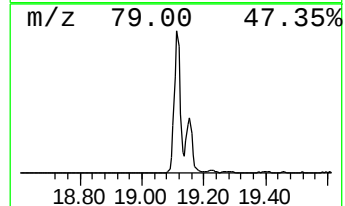
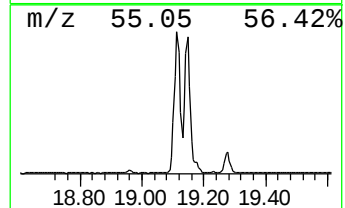
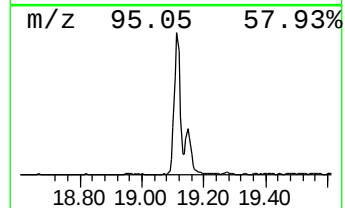
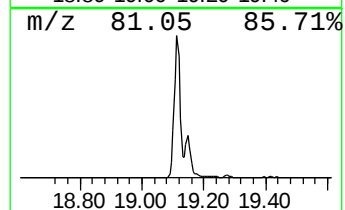
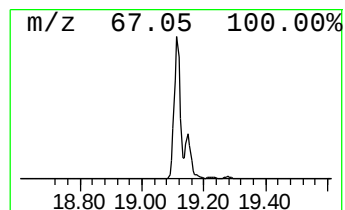
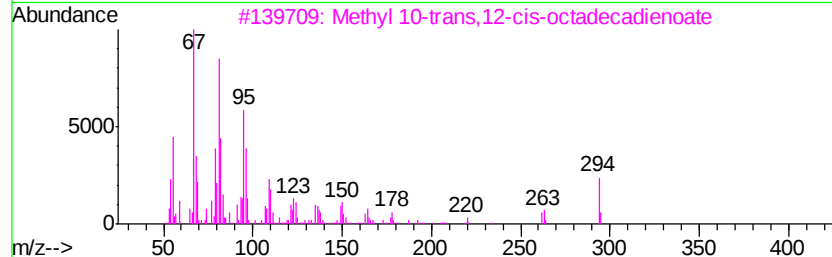
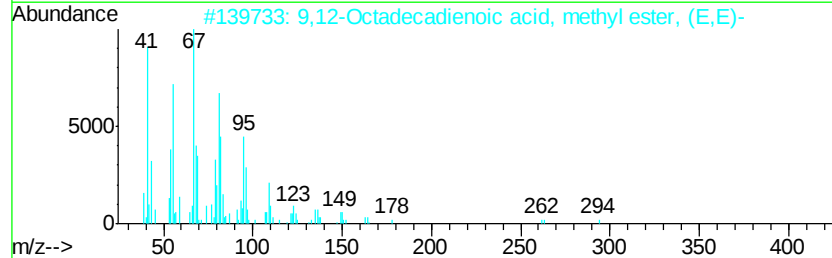
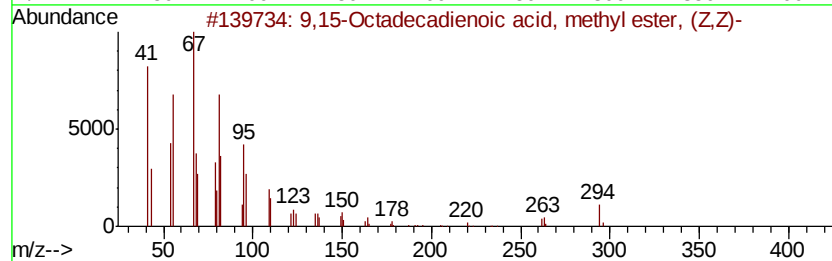
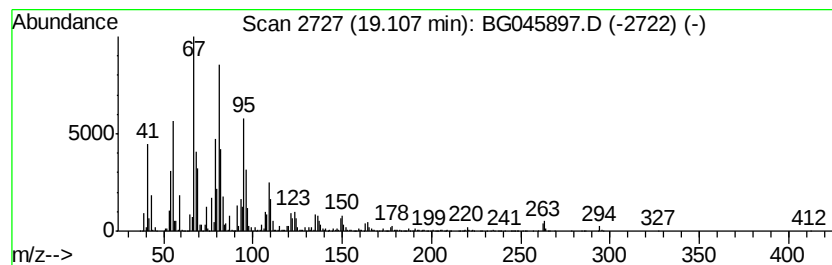
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 9,15-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.11	151.04 ng	6341480	Phenanthrene-d10	17.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99	
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98	
3	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98	
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	97	
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95	



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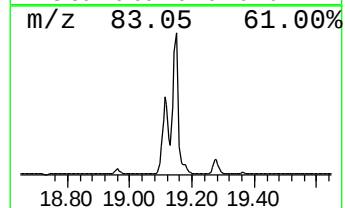
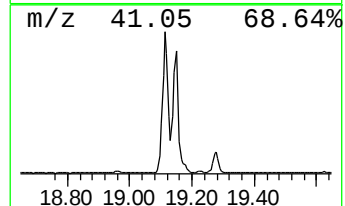
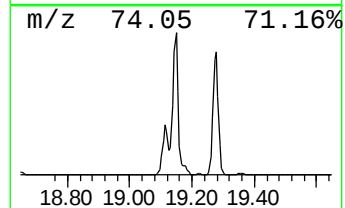
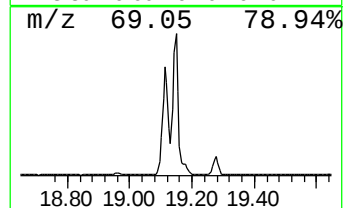
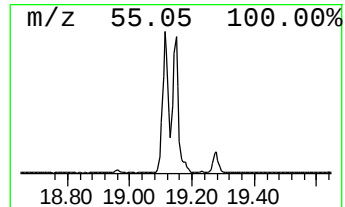
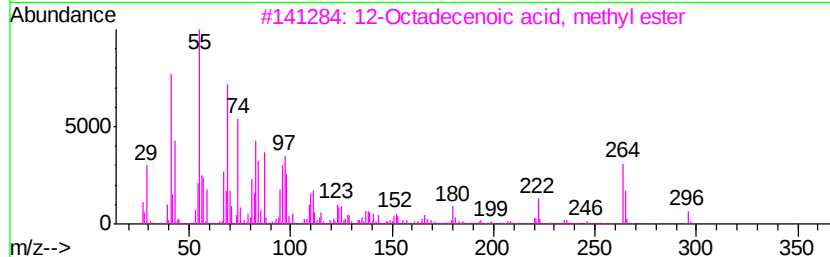
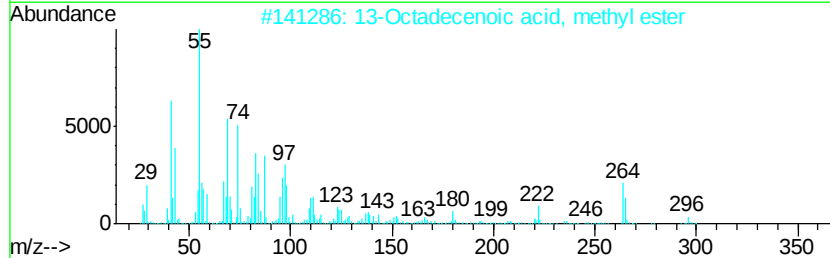
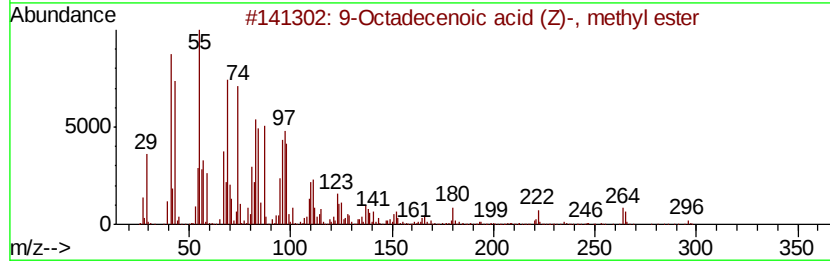
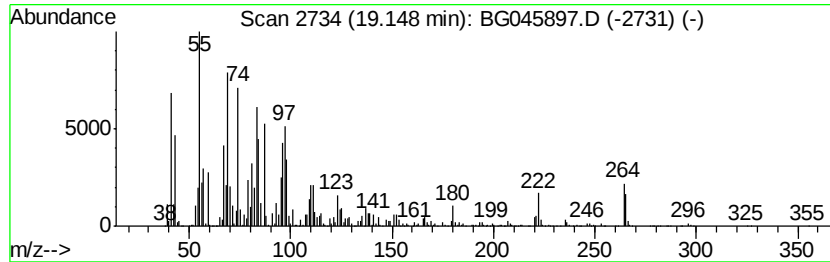
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Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.15	111.59 ng	4685090	Phenanthrene-d10	17.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
4		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
5		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99



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Data File : BG045897.D
Acq On : 30 Jun 2020 23:28
Operator : CG/JU
Sample : L2819-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-03-062620

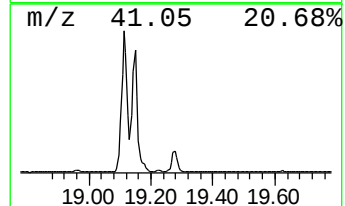
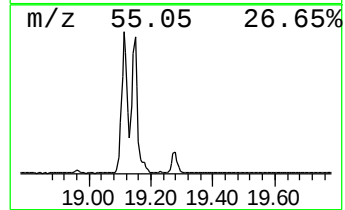
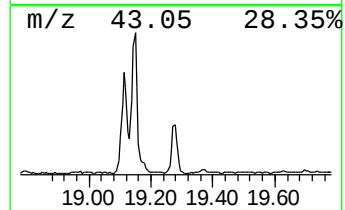
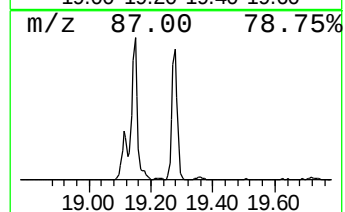
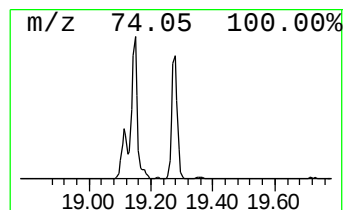
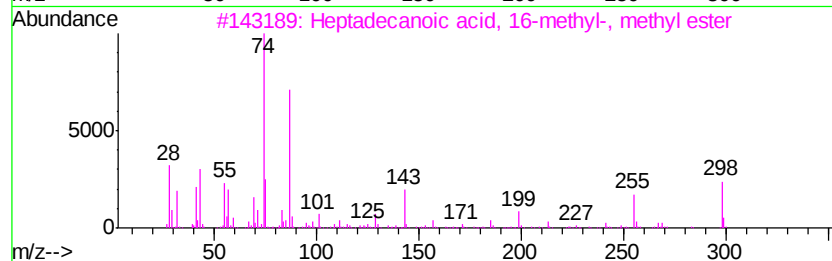
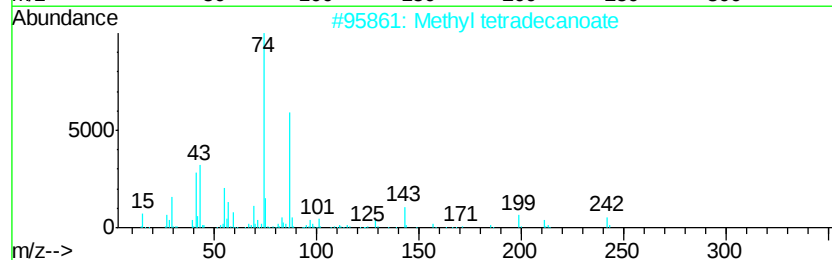
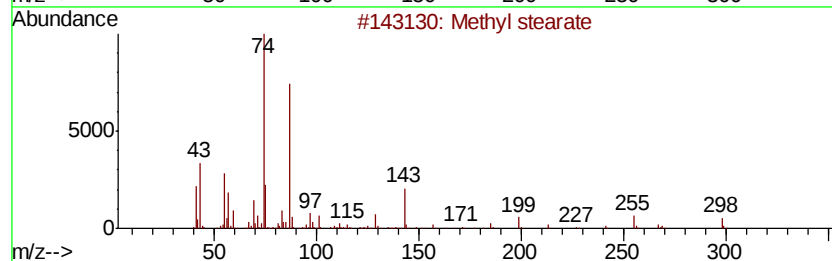
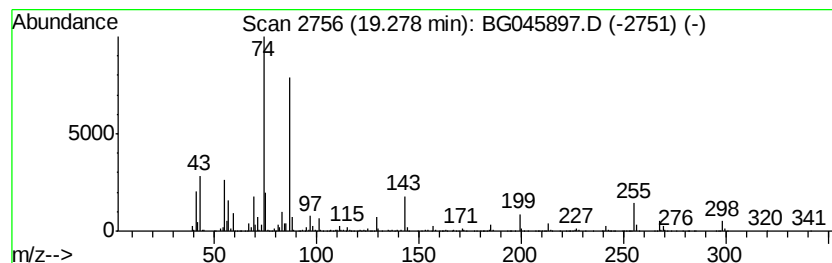
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.28	21.48 ng	901760	Phenanthrene-d10	17.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl stearate	298	C19H38O2	000112-61-8	98
2		Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
3		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
4		Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	90
5		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG063020\
Data File : BG045897.D
Acq On : 30 Jun 2020 23:28
Operator : CG/JU
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ClientSampleId :
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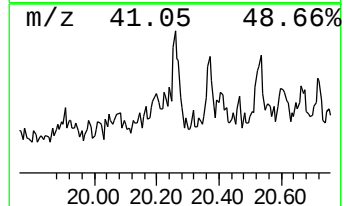
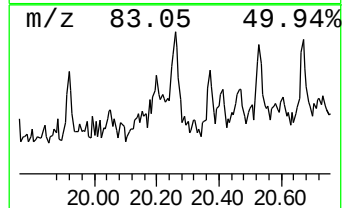
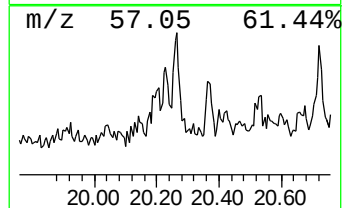
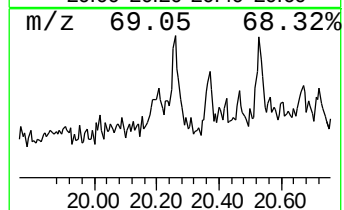
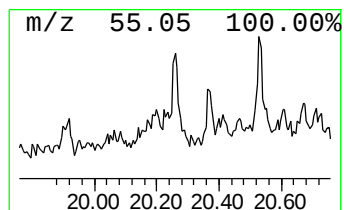
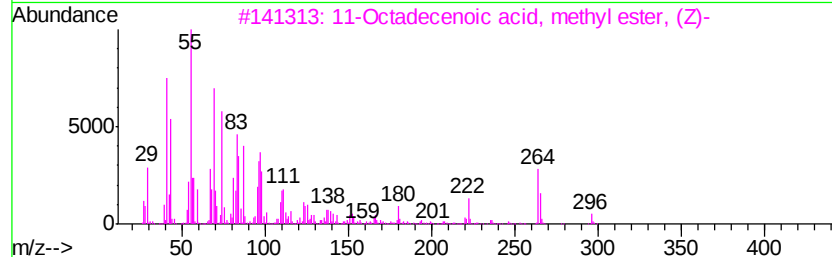
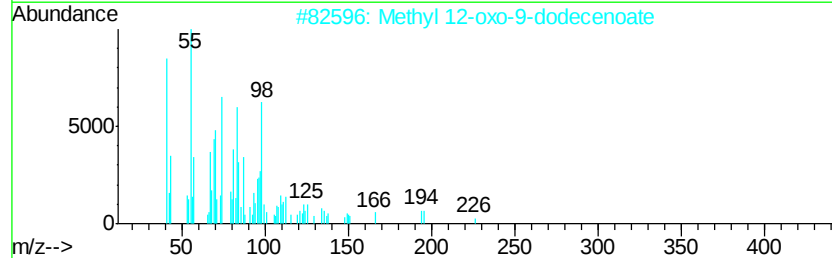
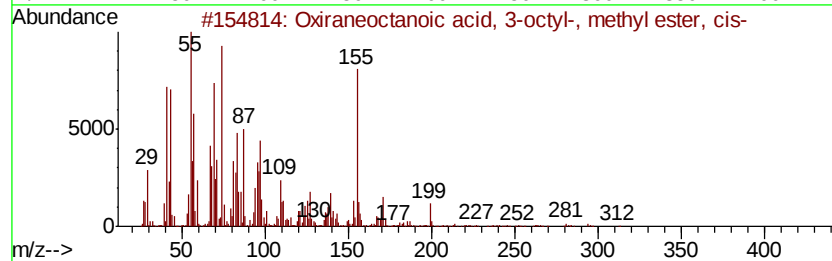
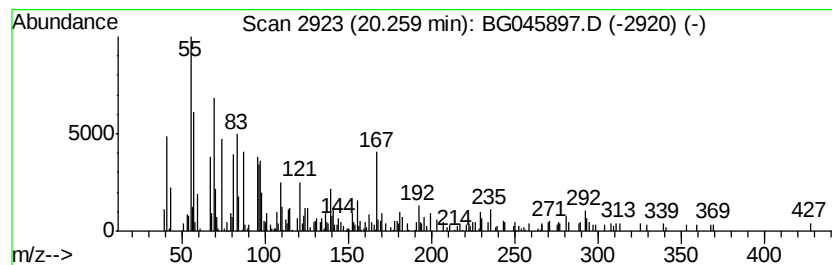
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown20.26 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.26	2.54 ng	115406	Chrysene-d12	21.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxiraneoctanoic acid, 3-octyl-, ...	312	C19H36O3	002566-91-8	30
2		Methyl 12-oxo-9-dodecenoate	226	C13H22O3	022418-58-2	15
3		11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	15
4		Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	14
5		Methyl 9-heptadecenoate or 9-17:1	282	C18H34O2	1000336-38-0	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG063020\
Data File : BG045897.D
Acq On : 30 Jun 2020 23:28
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ClientSampleId :
BU-03-062620

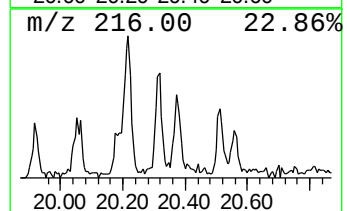
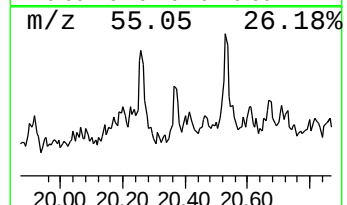
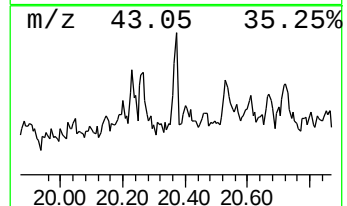
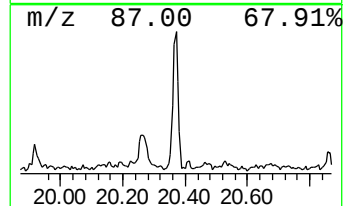
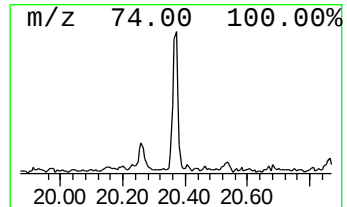
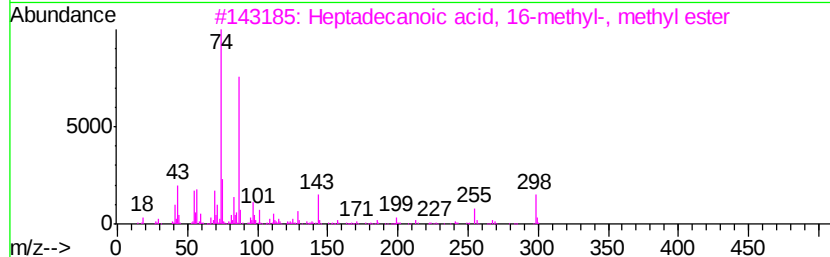
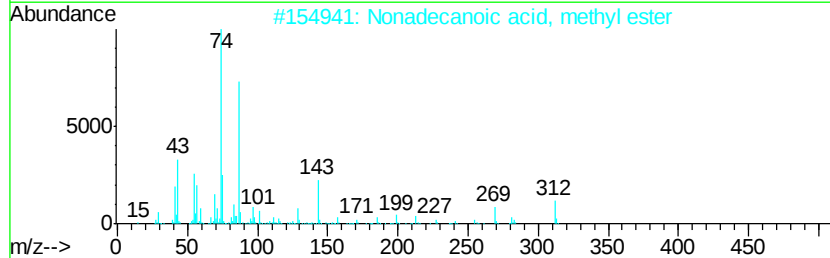
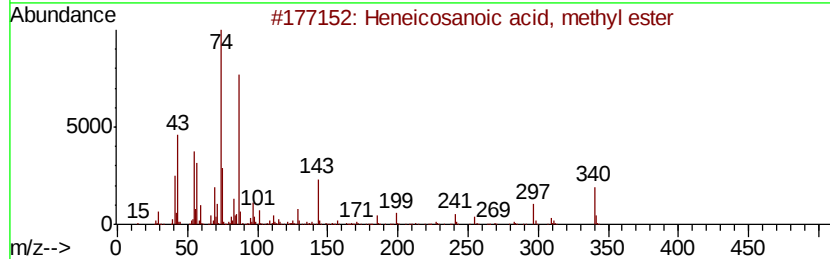
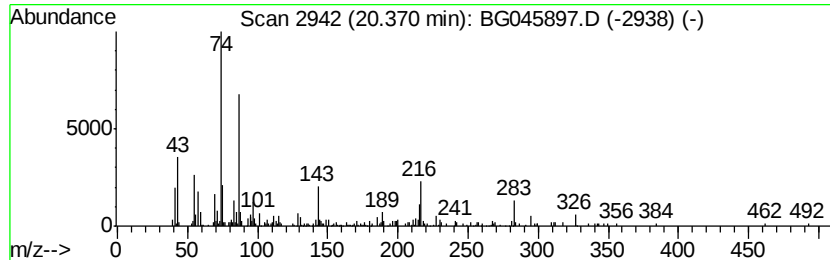
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosanoic acid, methyl ... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.37	2.25 ng	101892	Chrysene-d12	21.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	96
2		Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	92
3		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
4		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86
5		Methyl stearate	298	C19H38O2	000112-61-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG063020\
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ClientSampleId :
BU-03-062620

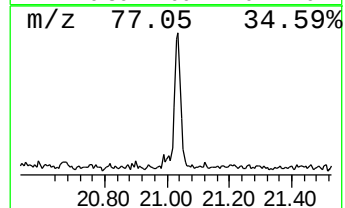
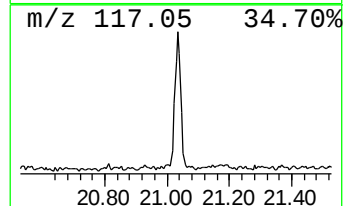
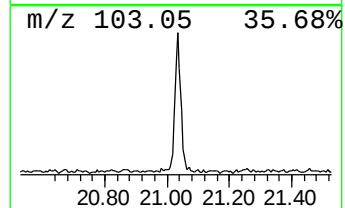
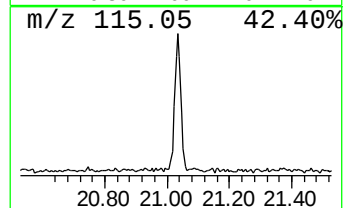
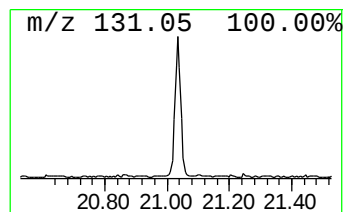
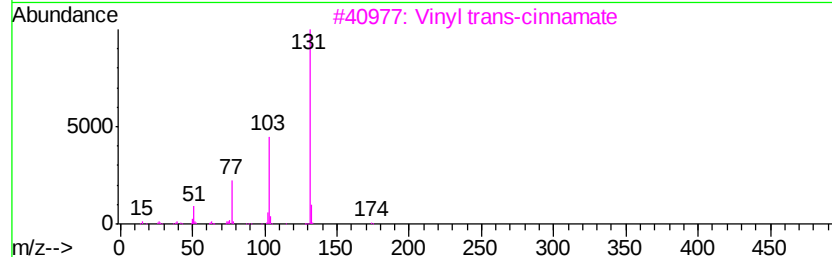
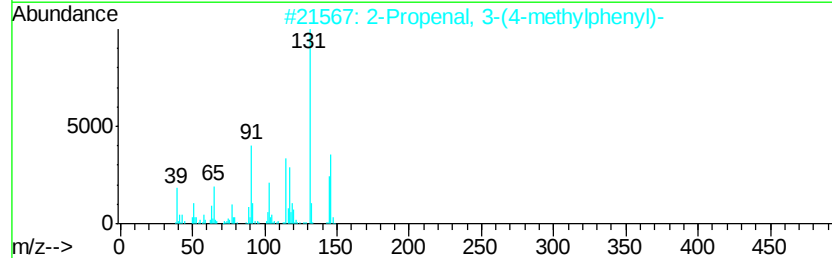
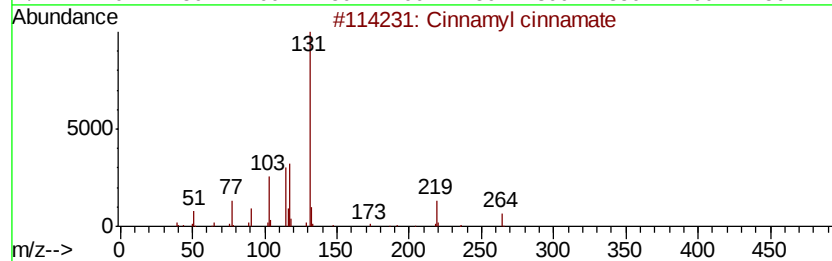
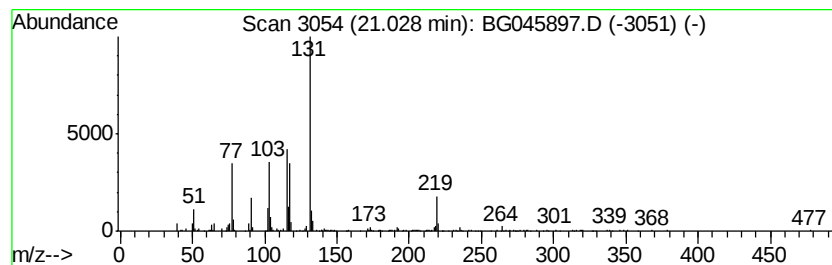
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cinnamyl cinnamate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	5.26 ng	238749	Chrysene-d12	21.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	86
2		2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	50
3		Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	45
4		2-Propenoic acid, 3-phenyl-, met...	162	C10H10O2	001754-62-7	43
5		Propenoic acid, 3-phenyl-, 2-(3-...	311	C17H13NO5	1000264-14-5	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG063020\
Data File : BG045897.D
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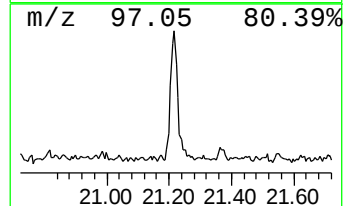
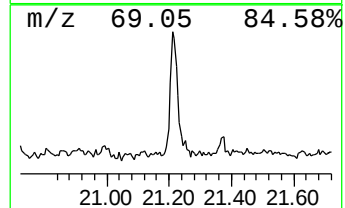
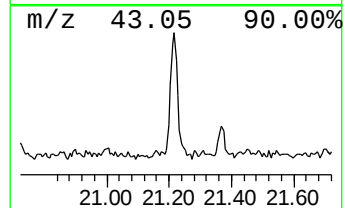
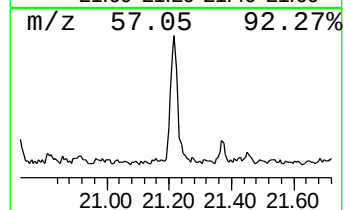
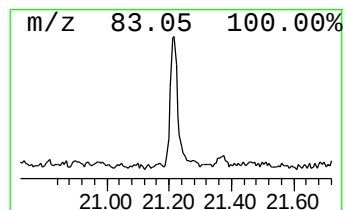
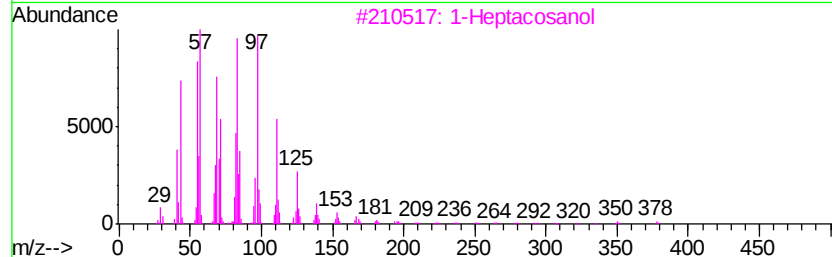
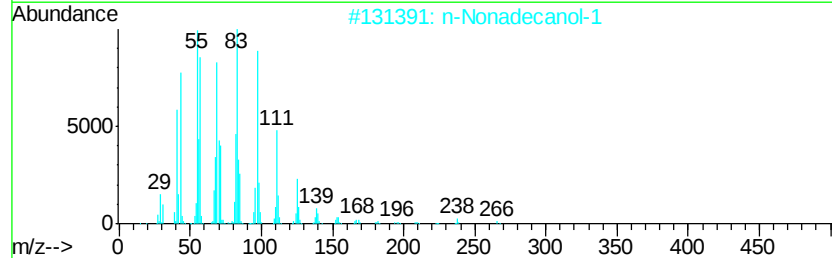
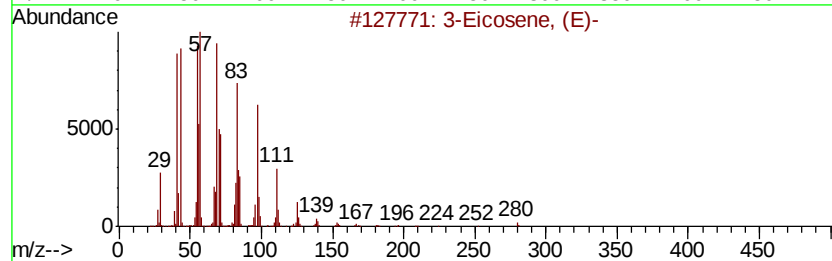
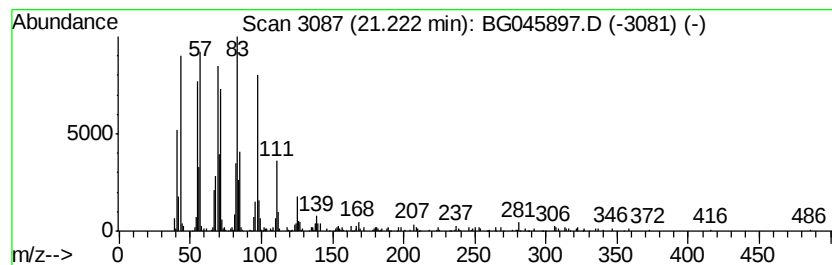
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.22	8.74 ng	396129	Chrysene-d12	21.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
3		1-Heptacosanol	396	C27H56O	002004-39-9	90
4		Behenic alcohol	326	C22H46O	000661-19-8	87
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG063020\
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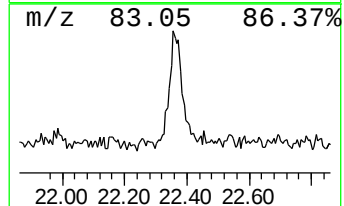
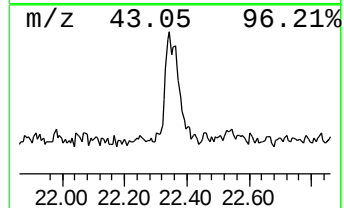
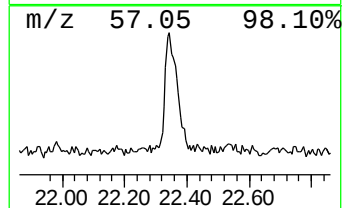
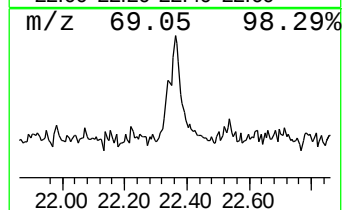
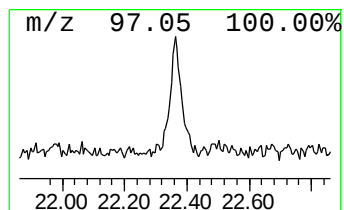
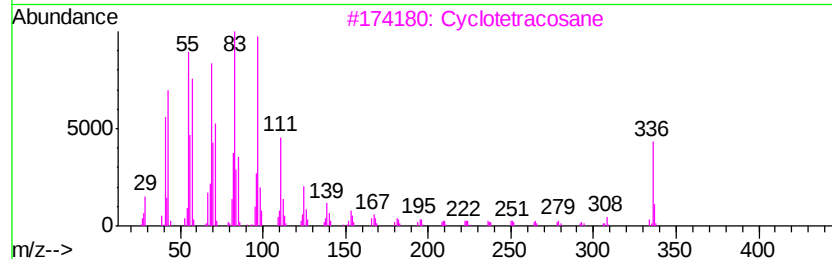
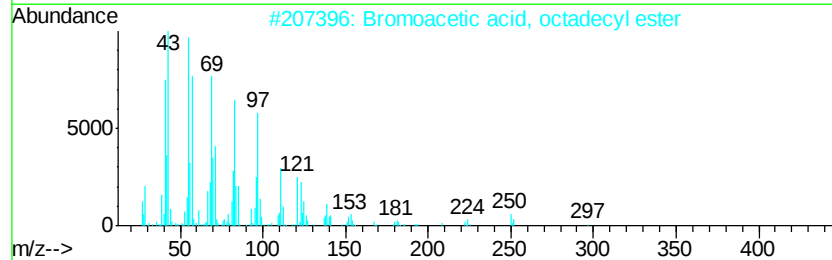
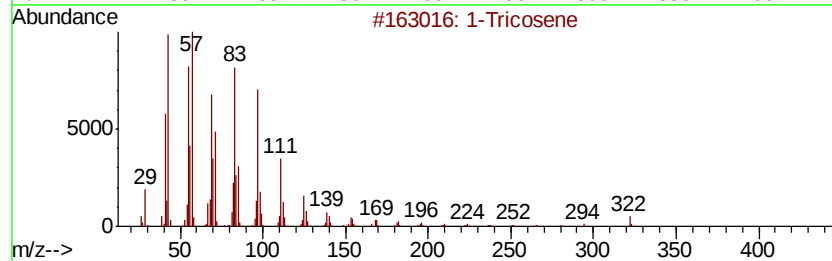
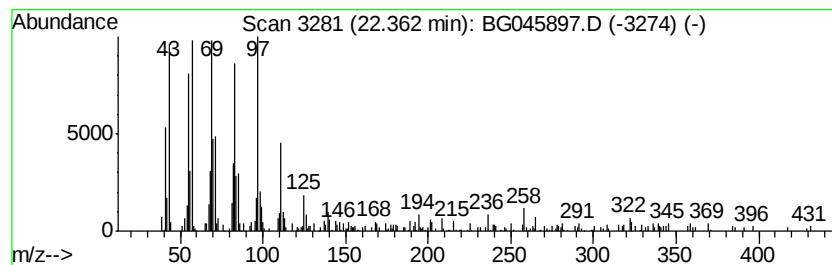
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Tricosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.36	6.09 ng	276176	Chrysene-d12	21.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Tricosene	322	C23H46	018835-32-0	93
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3		Cyclotetracosane	336	C24H48	000297-03-0	91
4		9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	90



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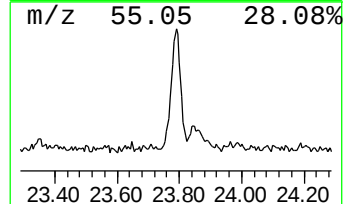
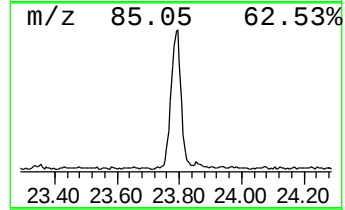
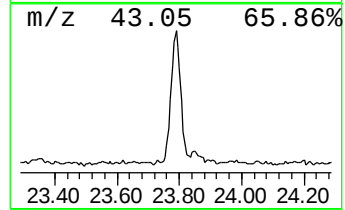
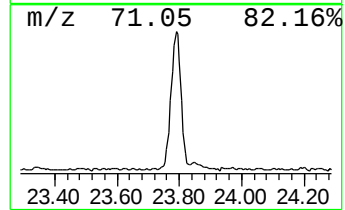
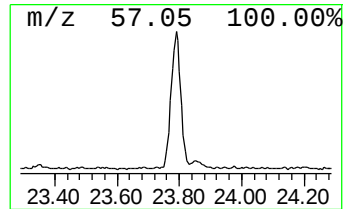
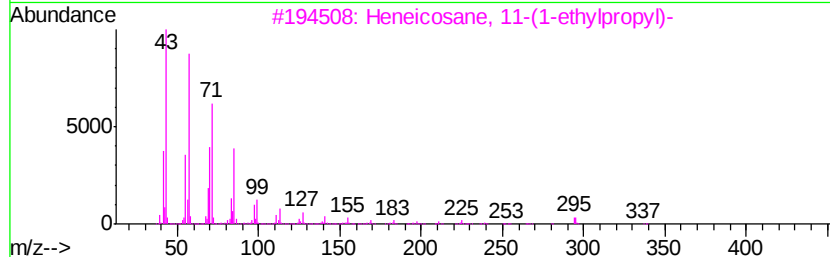
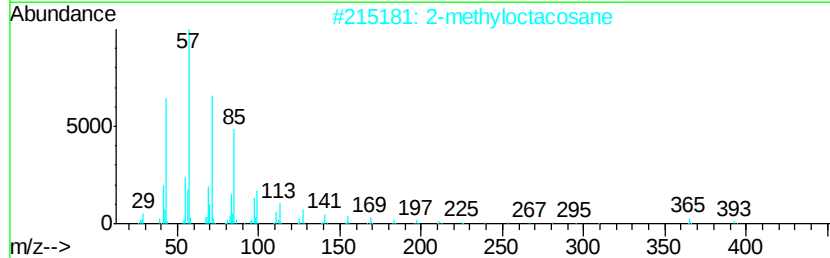
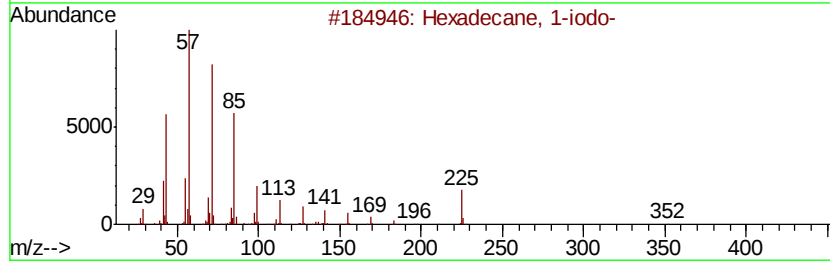
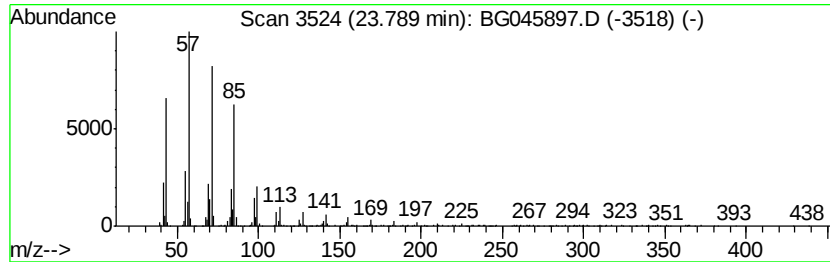
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexadecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.79	16.20 ng	759961	Perylene-d12	24.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	95
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4		Hexacosane	366	C26H54	000630-01-3	87
5		Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG063020\
Data File : BG045897.D
Acq On : 30 Jun 2020 23:28
Operator : CG/JU
Sample : L2819-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-03-062620

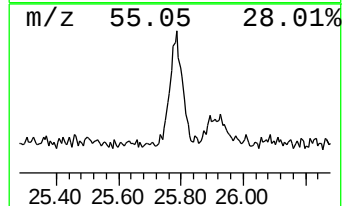
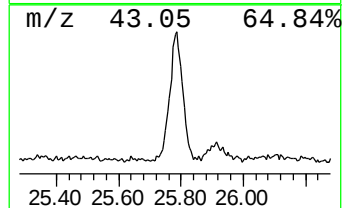
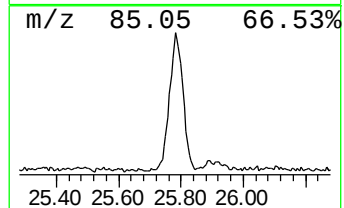
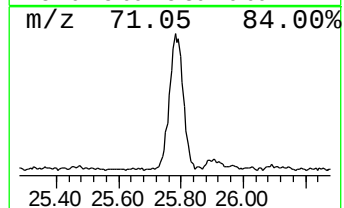
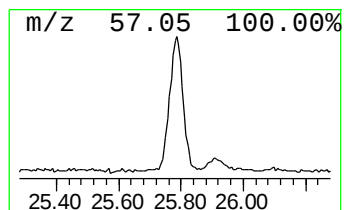
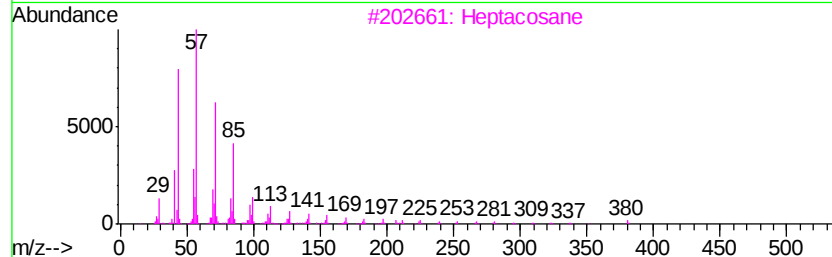
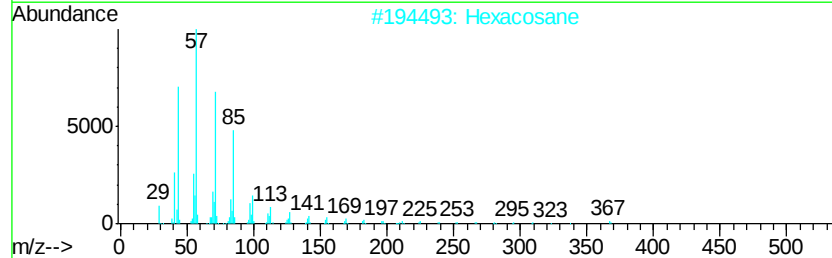
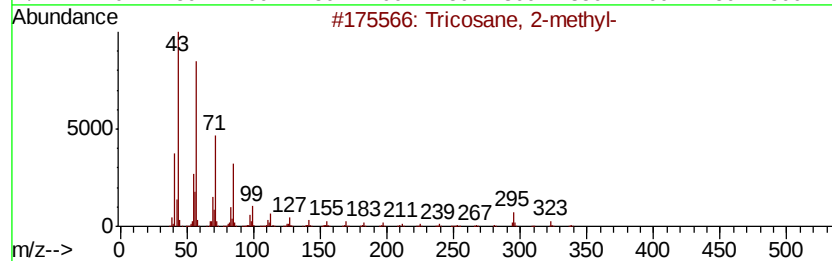
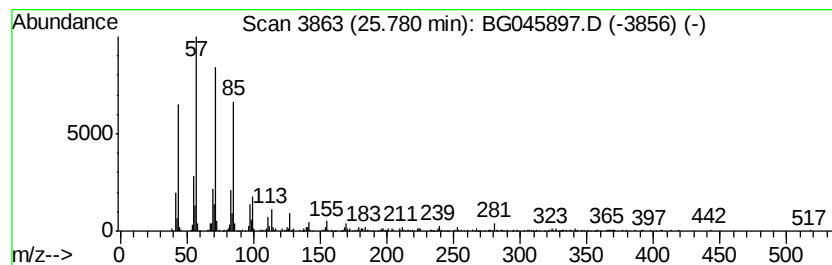
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tricosane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.78	15.02 ng	704709	Perylene-d12	24.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	87
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG063020\
 Data File : BG045897.D
 Acq On : 30 Jun 2020 23:28
 Operator : CG/JU
 Sample : L2819-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BU-03-062620

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.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
1-Imidazolidineme...	12.10	3.7	ng	104365	2	10.70	557871	20.0
Hexadecanoic acid...	17.97	30.9	ng	1297880	4	17.30	839723	20.0
n-Hexadecanoic acid	18.21	3.8	ng	158092	4	17.30	839723	20.0
9,15-Octadecadien...	19.11	151.0	ng	6341480	4	17.30	839723	20.0
9-Octadecenoic ac...	19.15	111.6	ng	4685090	4	17.30	839723	20.0
Methyl stearate	19.28	21.5	ng	901760	4	17.30	839723	20.0
unknown20.26	20.26	2.5	ng	115406	5	21.56	906971	20.0
Heneicosanoic aci...	20.37	2.3	ng	101892	5	21.56	906971	20.0
Cinnamyl cinnamate	21.03	5.3	ng	238749	5	21.56	906971	20.0
3-Eicosene, (E)-	21.22	8.7	ng	396129	5	21.56	906971	20.0
1-Tricosene	22.36	6.1	ng	276176	5	21.56	906971	20.0
Hexadecane, 1-iodo-	23.79	16.2	ng	759961	6	24.67	938115	20.0
Tricosane, 2-methyl-	25.78	15.0	ng	704709	6	24.67	938115	20.0