

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
 Data File : BG037563.D
 Acq On : 26 Oct 2018 3:28
 Operator : JU/SJ
 Sample : J5633-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-2

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-BG101818.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	5.644	394	401	413	rVB	435328	731431	18.71%	3.350%
2	7.242	666	673	686	rBV2	301267	630458	16.12%	2.888%
3	7.624	731	738	748	rBV	802169	1478179	37.80%	6.771%
4	8.106	812	820	835	rBV2	198658	407047	10.41%	1.865%
5	8.423	866	874	885	rBV	721087	1317766	33.70%	6.036%
6	9.281	1011	1020	1028	rBV	655249	1227155	31.38%	5.621%
7	10.673	1249	1257	1266	rBV2	27506	57918	1.48%	0.265%
8	10.926	1289	1300	1311	rBV	301260	578597	14.80%	2.650%
9	11.584	1406	1412	1417	rBV2	23855	39618	1.01%	0.181%
10	12.706	1597	1603	1609	rBV2	30216	53970	1.38%	0.247%
11	13.082	1661	1667	1678	rVB3	32438	70345	1.80%	0.322%
12	13.359	1703	1714	1721	rBV	1789846	2956096	75.60%	13.541%
13	14.181	1848	1854	1858	rBV	34824	56603	1.45%	0.259%
14	14.240	1859	1864	1866	rVV5	22394	41518	1.06%	0.190%
15	14.263	1866	1868	1880	rVB5	30115	56752	1.45%	0.260%
16	14.481	1894	1905	1911	rBV2	24183	55209	1.41%	0.253%
17	14.733	1940	1948	1958	rBV2	483792	846470	21.65%	3.877%
18	14.927	1975	1981	1989	rBV	140606	217736	5.57%	0.997%
19	15.497	2073	2078	2083	rBV	120204	158452	4.05%	0.726%
20	15.909	2143	2148	2152	rBV2	21554	40371	1.03%	0.185%
21	16.220	2194	2201	2210	rBV2	1373403	2159514	55.23%	9.892%
22	16.543	2251	2256	2259	rBV	28373	44552	1.14%	0.204%
23	16.596	2260	2265	2272	rVB3	27867	59580	1.52%	0.273%
24	16.860	2303	2310	2317	rVB6	32725	80875	2.07%	0.370%
25	16.925	2317	2321	2325	rBV	30030	45723	1.17%	0.209%
26	17.483	2410	2416	2422	rBV	615712	949688	24.29%	4.350%
27	17.742	2455	2460	2464	rBV	83757	114628	2.93%	0.525%
28	18.129	2520	2526	2532	rVB2	261259	378368	9.68%	1.733%
29	18.341	2558	2562	2566	rBV2	132271	195664	5.00%	0.896%
30	18.558	2595	2599	2607	rVB2	43323	76325	1.95%	0.350%
31	18.682	2616	2620	2625	rBV2	35821	54095	1.38%	0.248%
32	19.604	2773	2777	2785	rBV2	80581	126105	3.23%	0.578%
33	20.080	2849	2858	2866	rBV	2735518	3910029	100.00%	17.910%
34	20.762	2971	2974	2983	rVB3	68243	99524	2.55%	0.456%

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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

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35	21.379	3073	3079	3085	rBV3	71245	137305	3.51%	0.629%
36	21.766	3138	3145	3157	rVB2	573111	1029347	26.33%	4.715%
37	22.548	3274	3278	3283	rVB5	21604	41372	1.06%	0.190%
38	23.259	3394	3399	3405	rVB2	33041	67543	1.73%	0.309%
39	24.081	3534	3539	3548	rVB3	32986	70585	1.81%	0.323%
40	25.098	3699	3712	3729	rBV2	314706	1075218	27.50%	4.925%
41	26.232	3897	3905	3916	rVB5	28015	93564	2.39%	0.429%

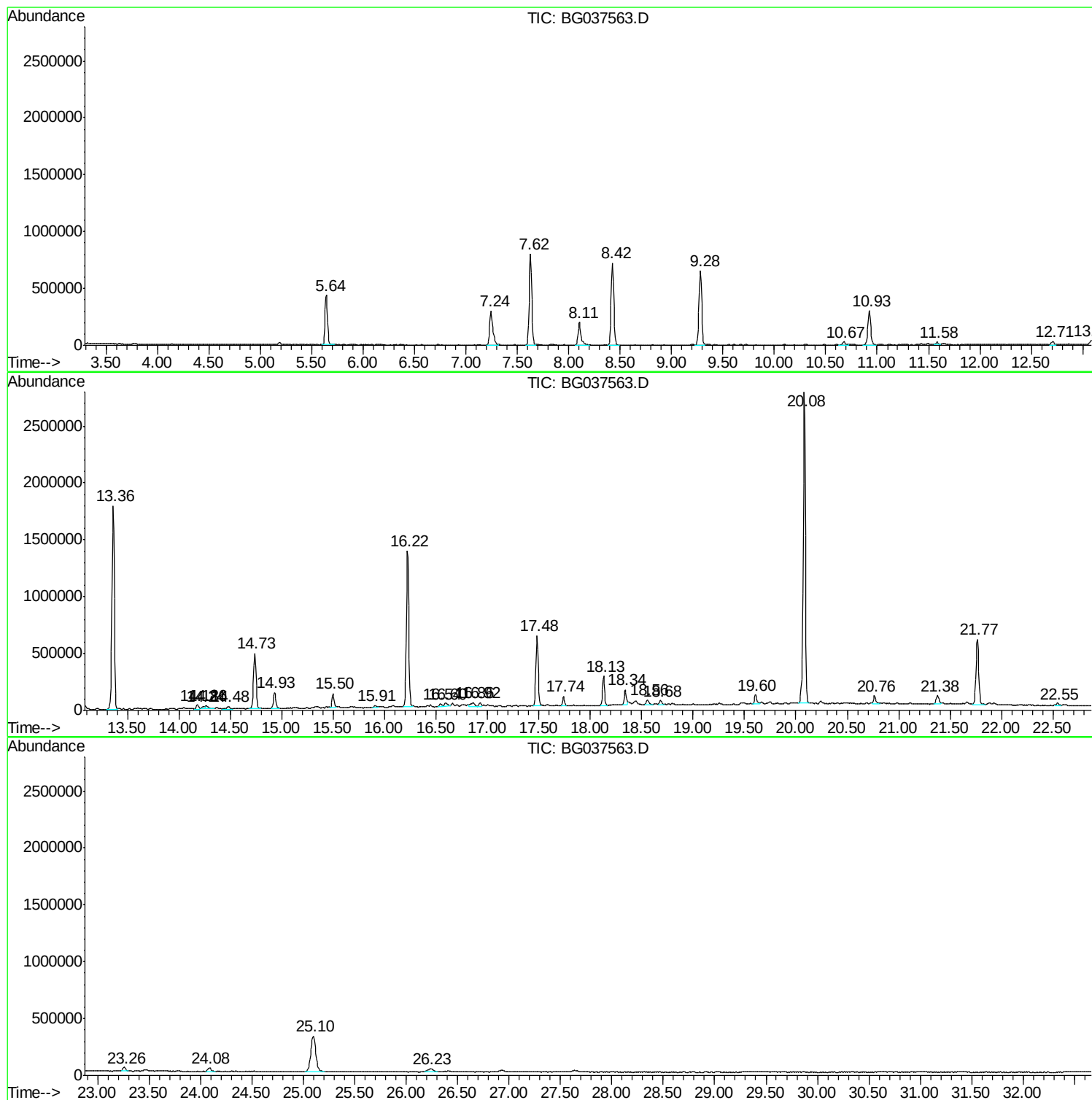
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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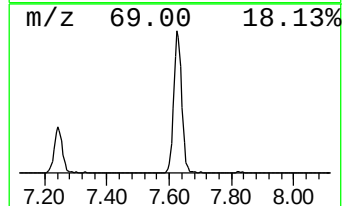
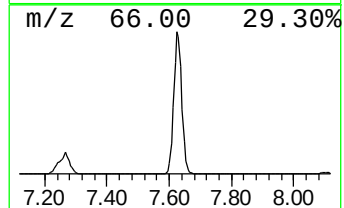
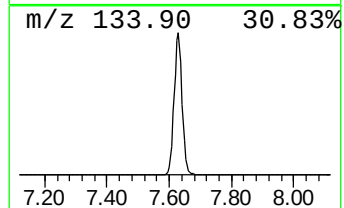
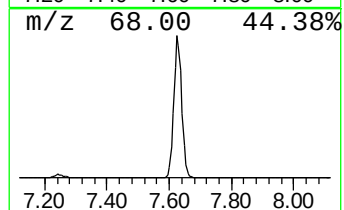
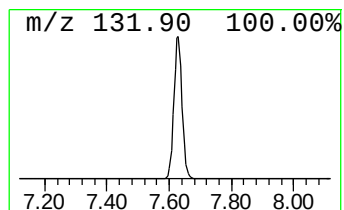
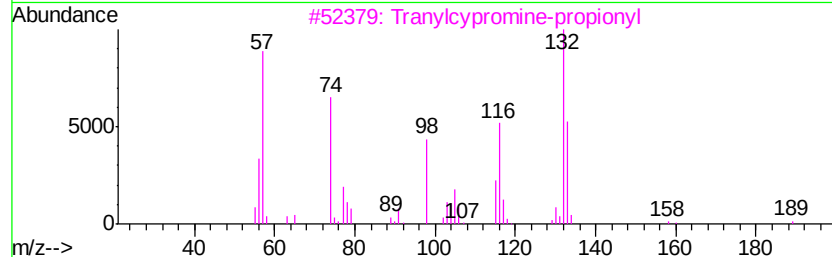
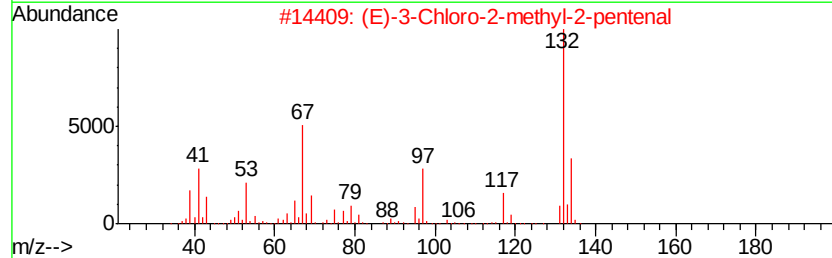
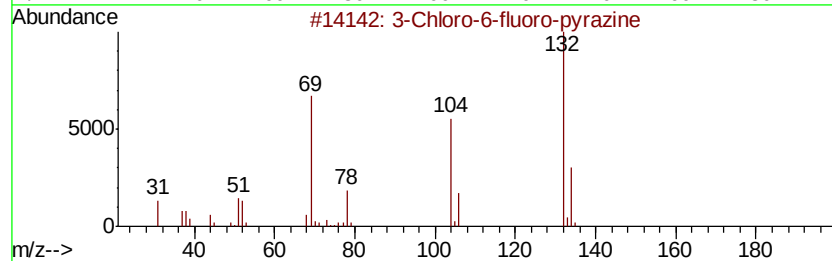
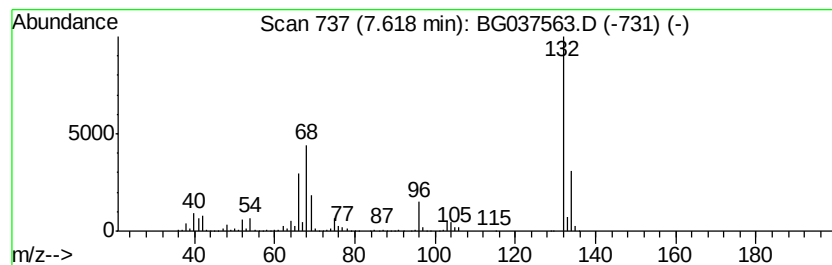
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	72.63 ng	1478180	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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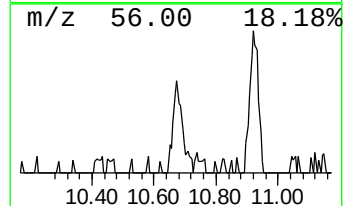
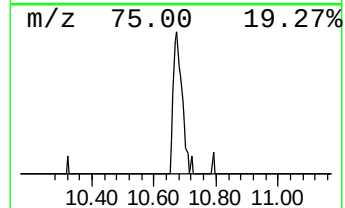
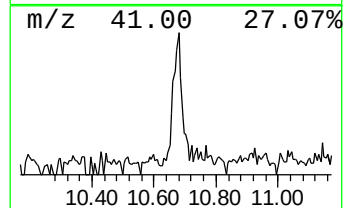
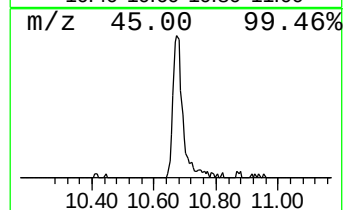
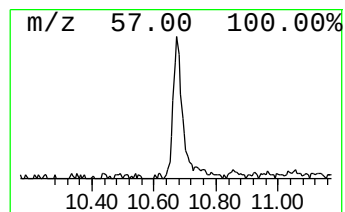
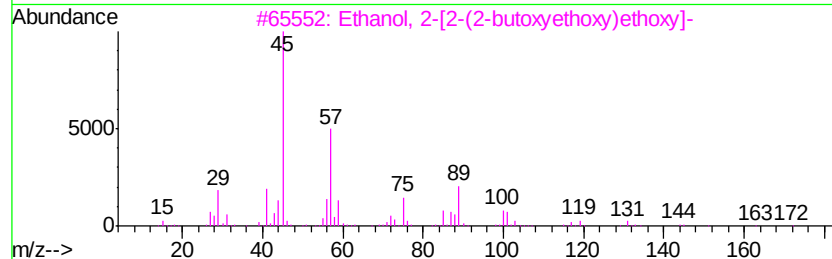
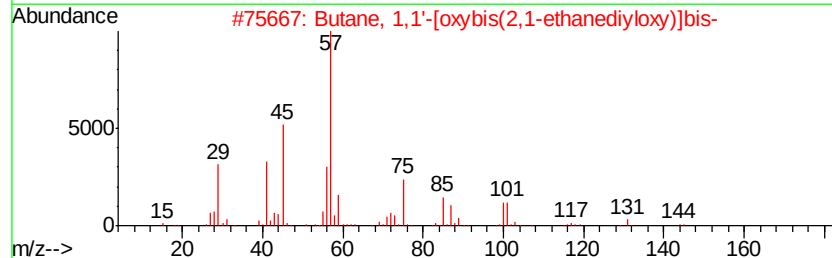
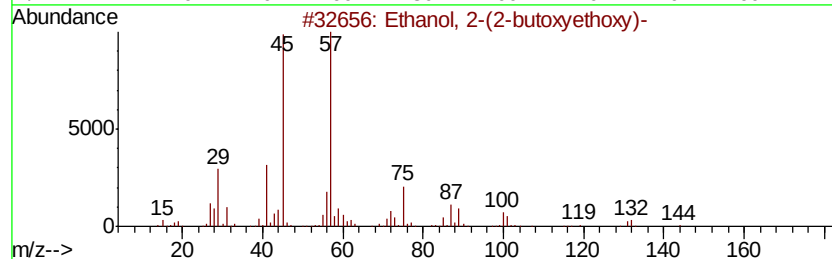
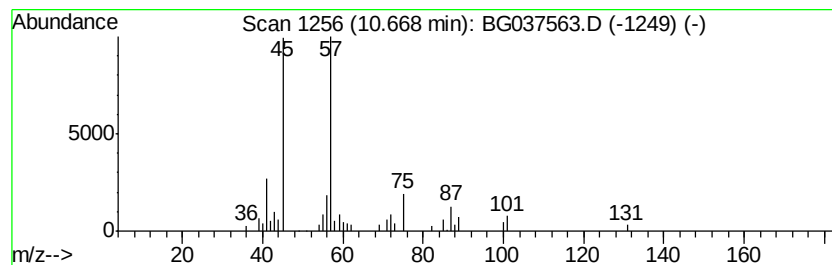
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.00 ng	57918	Naphthalene-d8	10.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2		Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50
3		Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4		Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50
5		Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50



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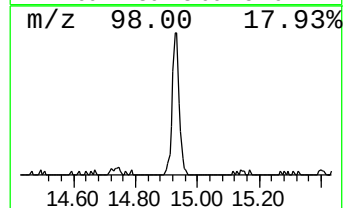
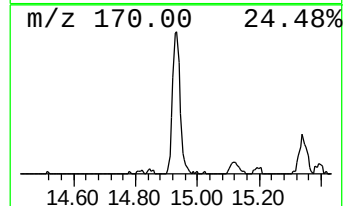
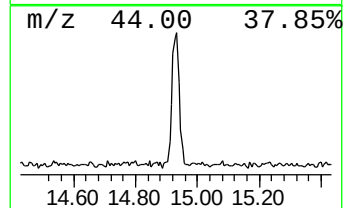
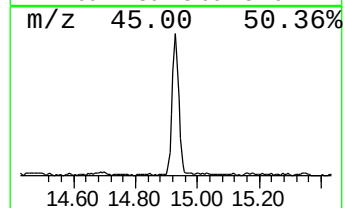
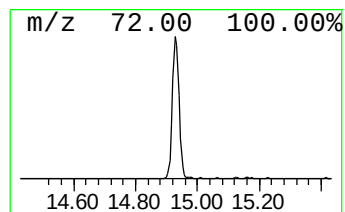
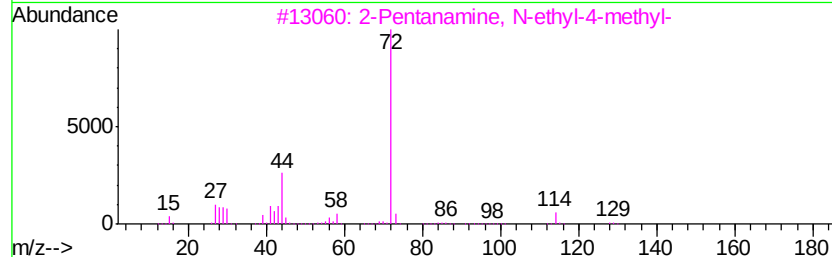
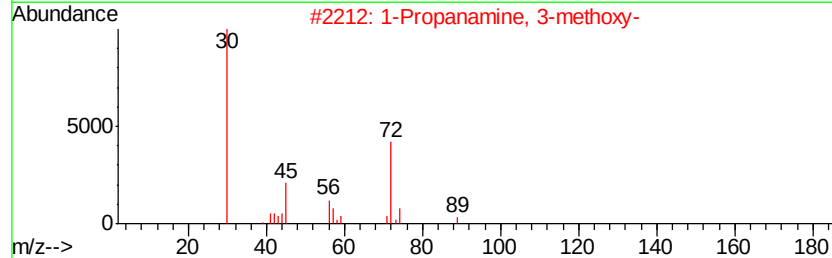
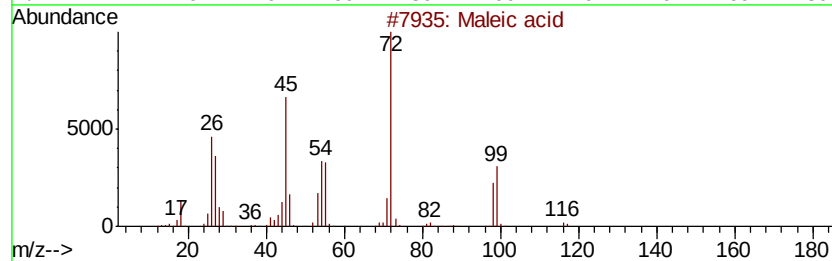
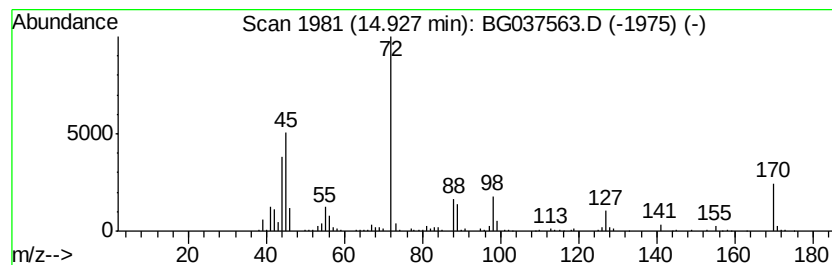
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Maleic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	5.14 ng	217736	Acenaphthene-d10	14.73
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Maleic acid	116 C4H4O4	000110-16-7	50
2	1-Propanamine, 3-methoxy-	89 C4H11NO	005332-73-0	50
3	2-Pentanamine, N-ethyl-4-methyl-	129 C8H19N	042966-64-3	35
4	N-Isopropylethylenediamine	102 C5H14N2	019522-67-9	35
5	2,3,N,N-Tetramethyl-4-nitro-buty...	188 C8H16N2O3	1000187-66-9	32



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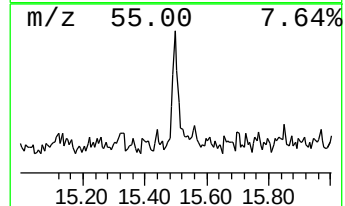
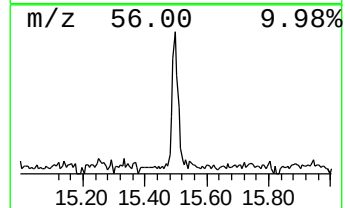
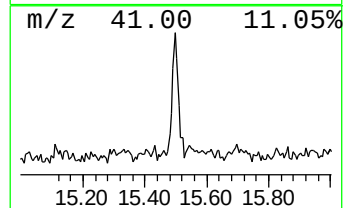
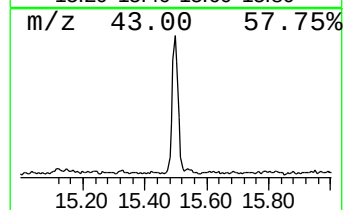
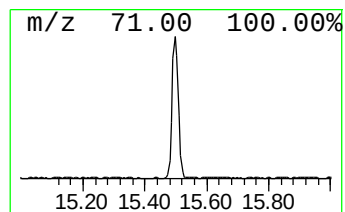
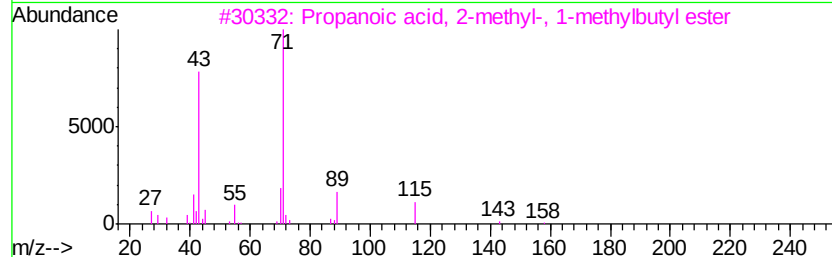
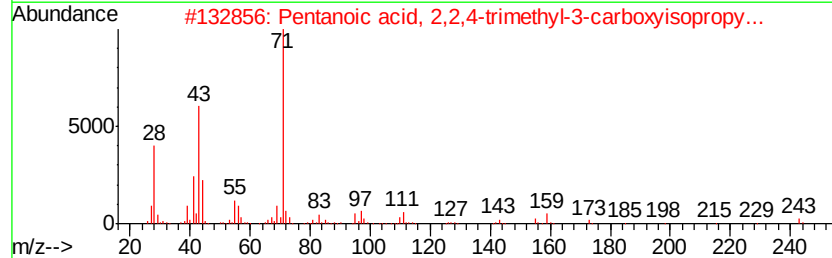
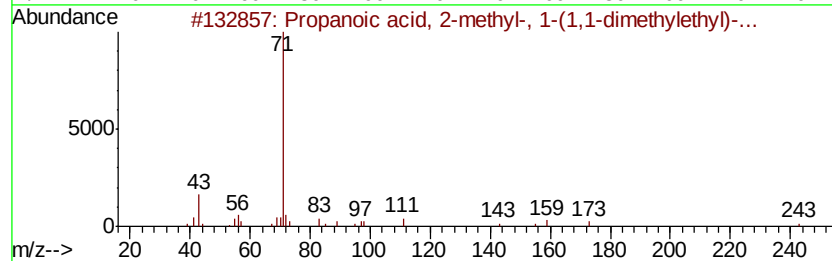
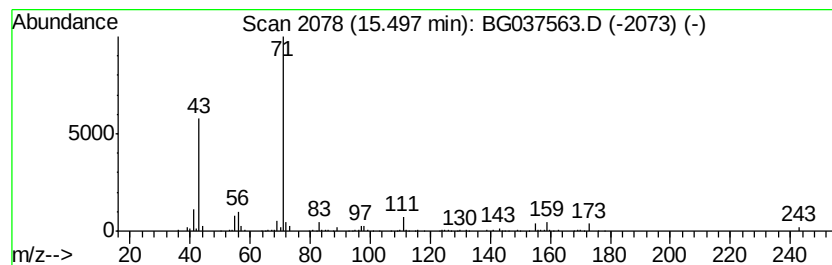
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Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.50	3.74 ng	158452	Acenaphthene-d10	14.73	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	78
2	Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	64
3	Propanoic acid, 2-methyl-, 1-met...	158	C9H18O2	054340-93-1	53
4	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	50
5	Oxalic acid, neopentyl nonyl ester	286	C16H30O4	1000309-73-3	45



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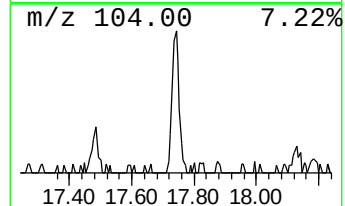
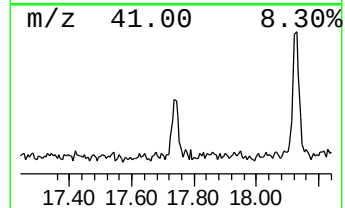
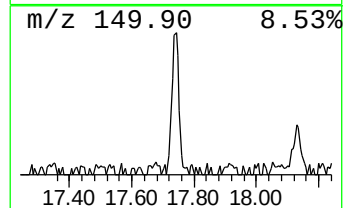
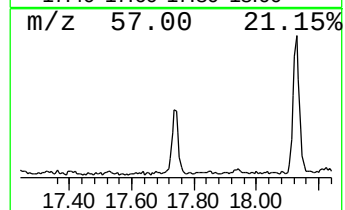
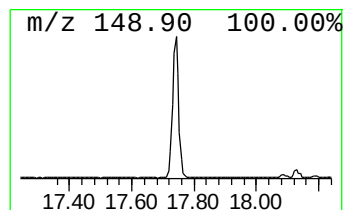
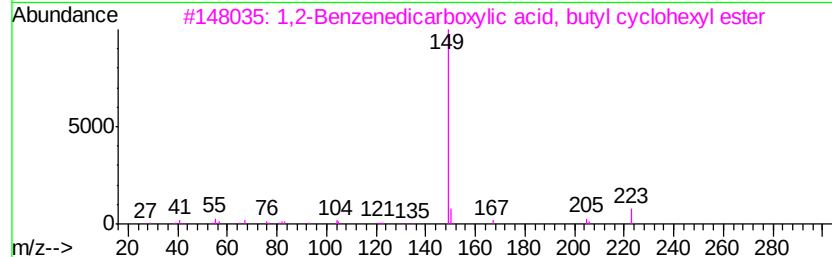
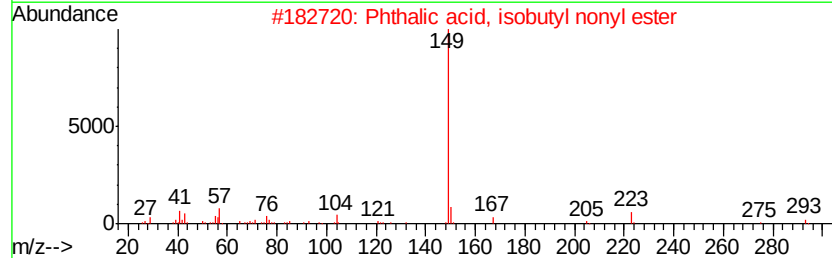
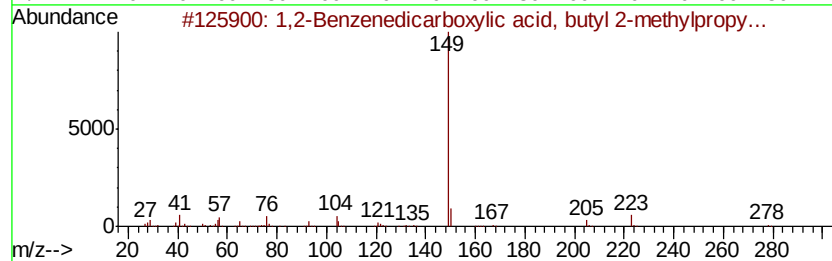
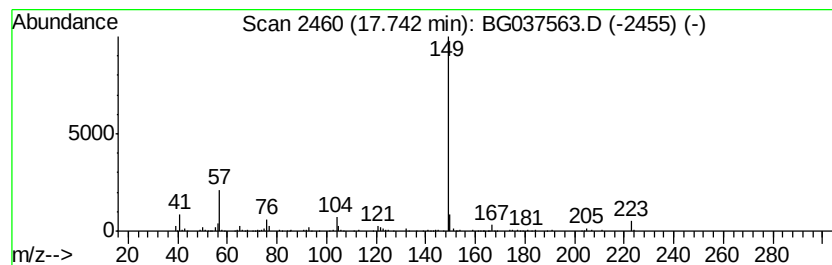
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Peak Number 6 1,2-Benzenedicarboxylic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.74	2.41 ng	114628	Phenanthrene-d10	17.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	86
2		Phthalic acid, isobutyl nonyl ester	348	C21H32O4	1000309-04-4	83
3		1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	83
4		Phthalic acid, cyclohexyl isohex...	304	C18H24O4	1000315-34-0	83
5		Phthalic acid, butyl tetradecyl ...	418	C26H42O4	1000308-91-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037563.D
Acq On : 26 Oct 2018 3:28
Operator : JU/SJ
Sample : J5633-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

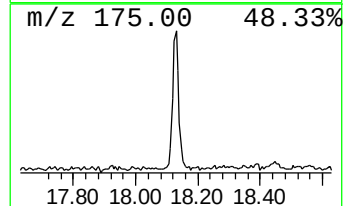
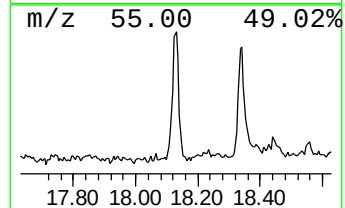
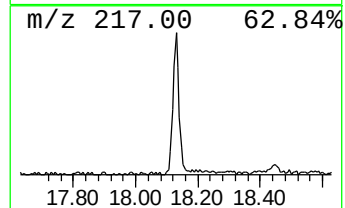
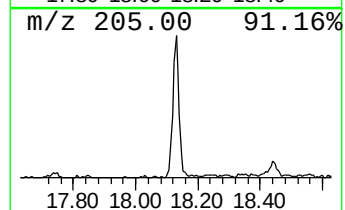
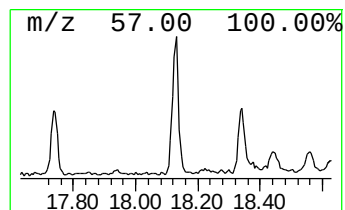
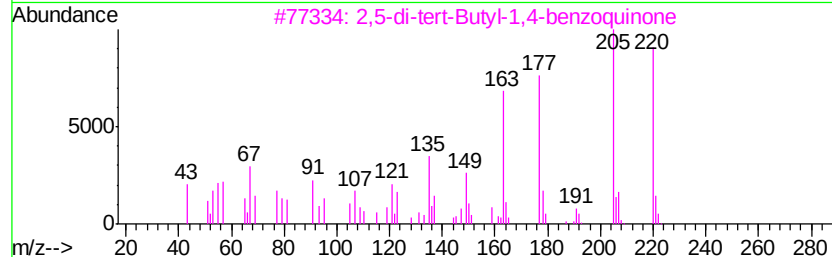
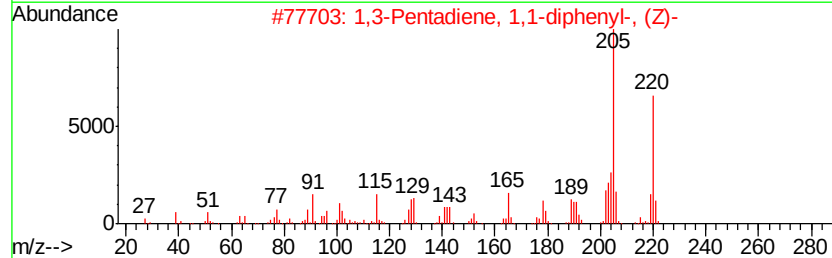
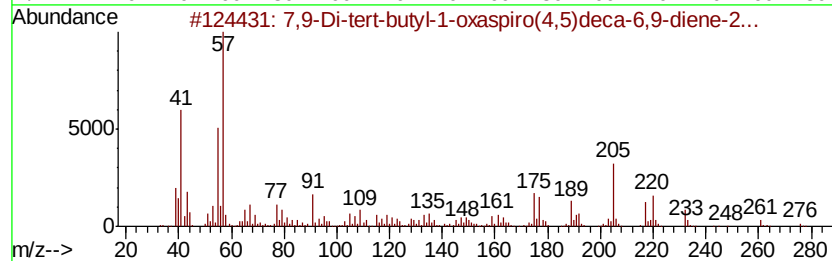
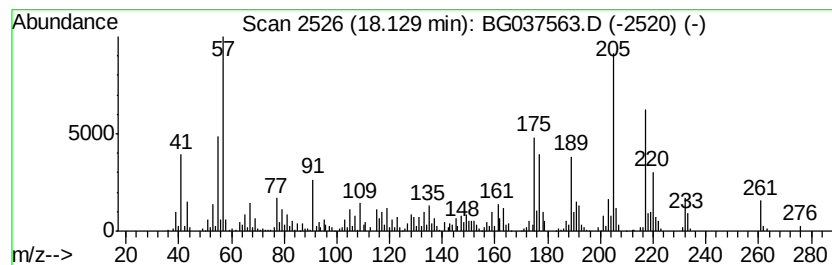
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.13	7.97 ng	378368	Phenanthrene-d10	17.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	98
2		1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	50
3		2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	45
4		2,4-Dimethyl-5,6-dimethoxy-8-ami...	232	C13H16N2O2	064993-02-8	35
5		2,4-Diamino-6-nitroquinazoline	205	C8H7N5O2	007154-34-9	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037563.D
Acq On : 26 Oct 2018 3:28
Operator : JU/SJ
Sample : J5633-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

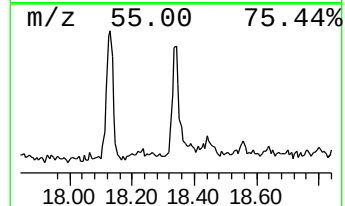
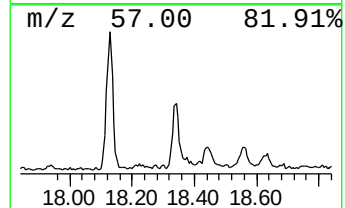
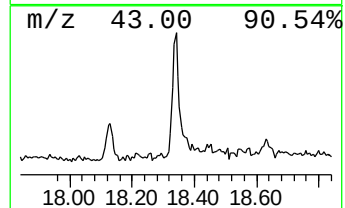
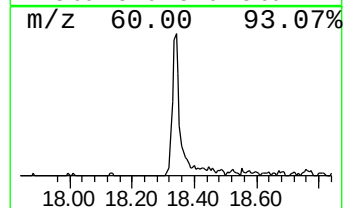
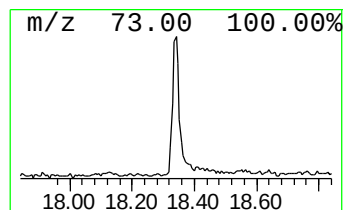
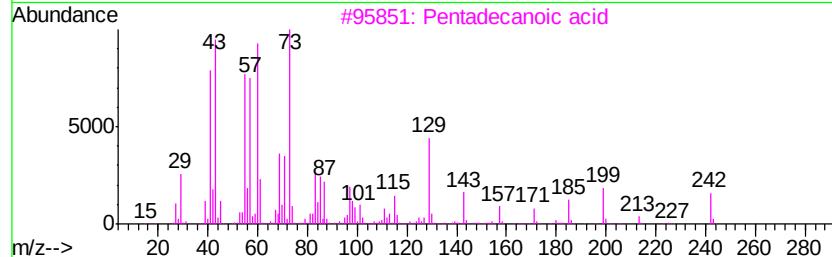
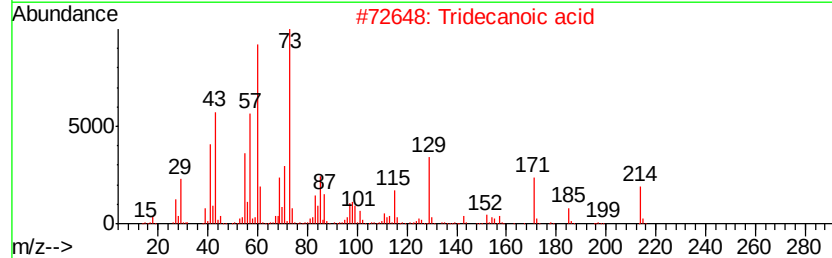
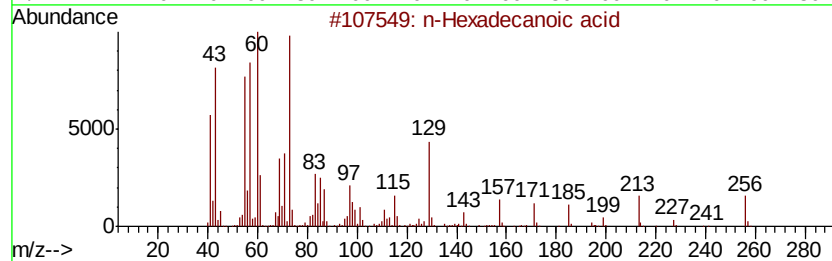
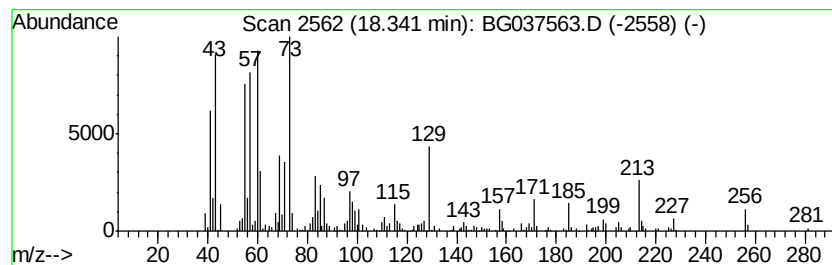
Instrument :
BNA_G
ClientSampleId :
MW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.34	4.12 ng	195664	Phenanthrene-d10	17.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	1-Phenazinecarboxylic acid, 6-[1...	506	C31H42N2O4	120464-92-8	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037563.D
Acq On : 26 Oct 2018 3:28
Operator : JU/SJ
Sample : J5633-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

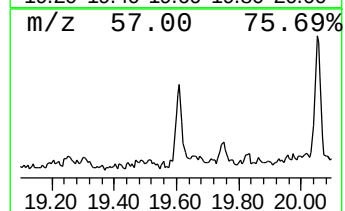
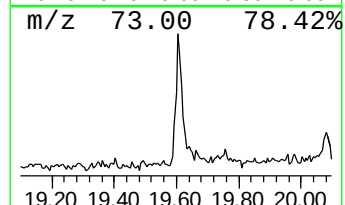
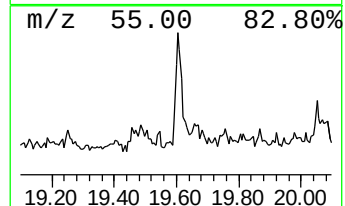
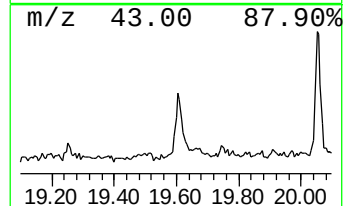
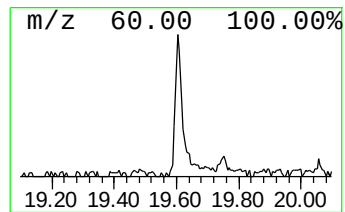
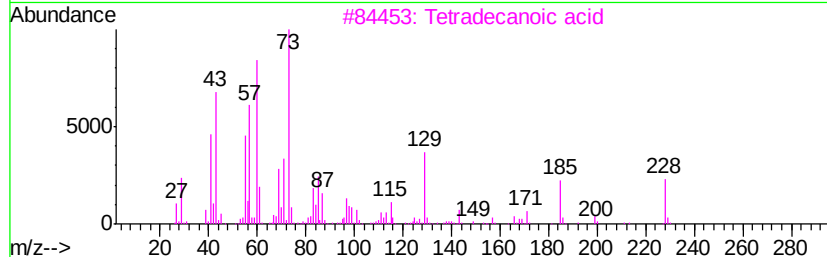
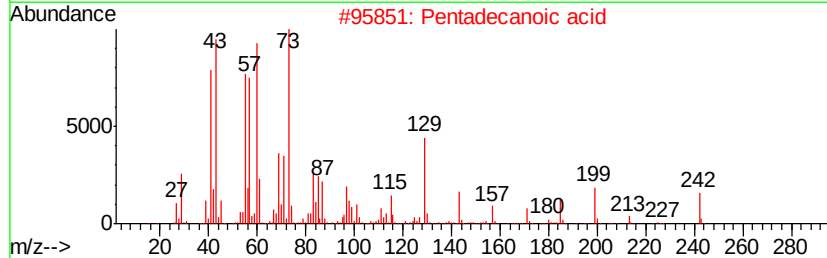
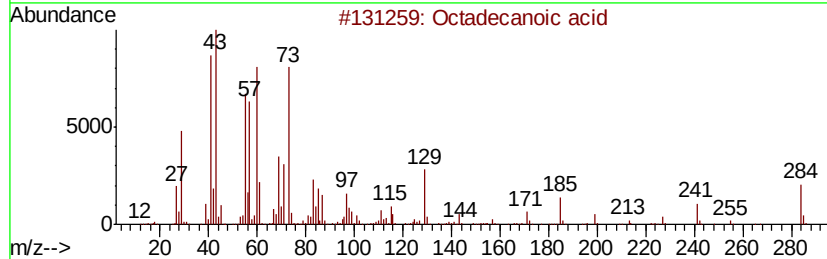
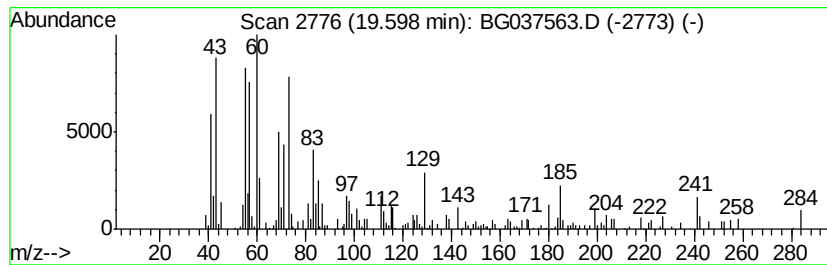
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.60	2.66 ng	126105	Phenanthrene-d10	17.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecanoic acid	284 C18H36O2	000057-11-4	95
2	Pentadecanoic acid	242 C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228 C14H28O2	000544-63-8	68
4	n-Hexadecanoic acid	256 C16H32O2	000057-10-3	64
5	n-Decanoic acid	172 C10H20O2	000334-48-5	60



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037563.D
Acq On : 26 Oct 2018 3:28
Operator : JU/SJ
Sample : J5633-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

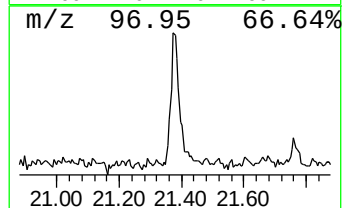
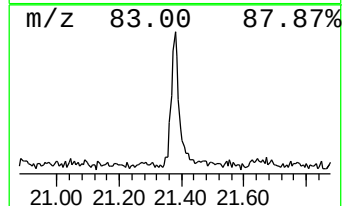
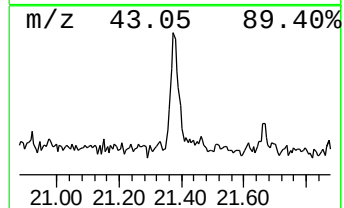
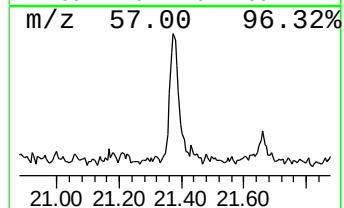
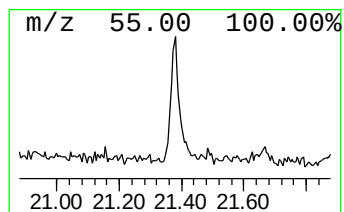
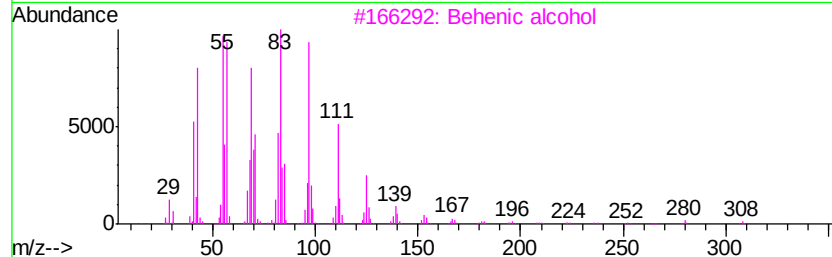
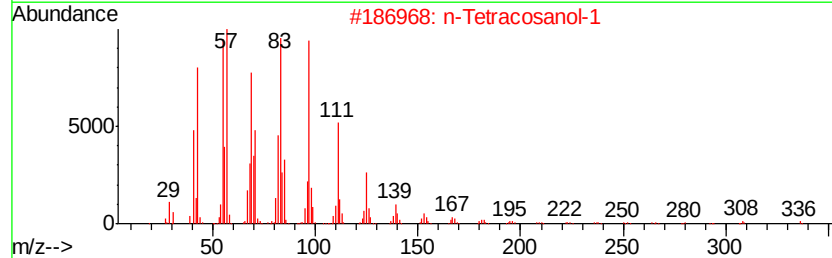
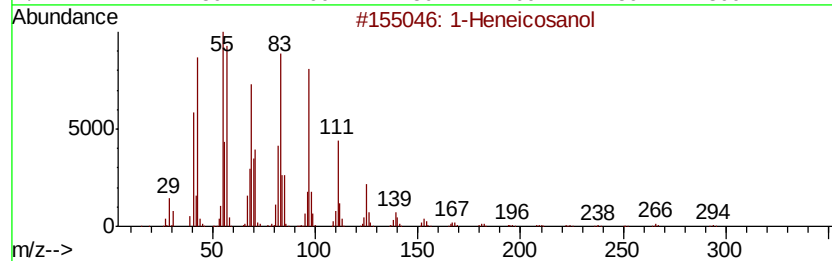
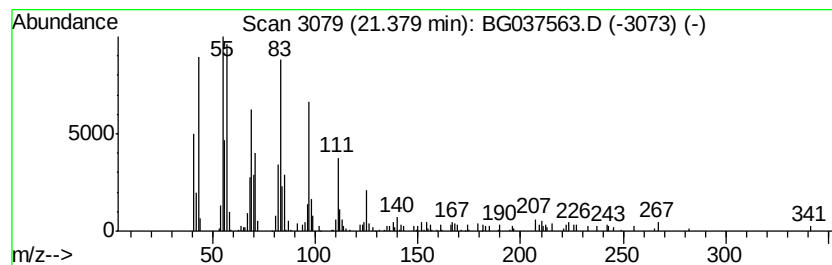
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	2.67 ng	137305	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3		Behenic alcohol	326	C22H46O	000661-19-8	90
4		1-Docosene	308	C22H44	001599-67-3	90
5		1-Tricosene	322	C23H46	018835-32-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102518\
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Sample : J5633-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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
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Ethanol, 2-(2-but...	10.67	2.0	ng	57918	2	10.93	578597	20.0
Maleic acid	14.93	5.1	ng	217736	3	14.73	846470	20.0
Propanoic acid, 2...	15.50	3.7	ng	158452	3	14.73	846470	20.0
1,2-Benzenedicarb...	17.74	2.4	ng	114628	4	17.48	949688	20.0
7,9-Di-tert-butyl...	18.13	8.0	ng	378368	4	17.48	949688	20.0
n-Hexadecanoic acid	18.34	4.1	ng	195664	4	17.48	949688	20.0
Octadecanoic acid	19.60	2.7	ng	126105	4	17.48	949688	20.0
1-Heneicosanol	21.38	2.7	ng	137305	5	21.77	1029350	20.0