

Data Path : Z:\HPCHEM1\BNA G\DATA\BG030818\
 Data File : BG033044.D
 Acq On : 8 Mar 2018 17:15
 Operator : SJ/JU
 Sample : J1825-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FK-BPM-01-C0-C0a-D0-D0a

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:\HPCHEM1\BNA_G\METHODS\8270-BG022118.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	3.517	33	39	50	rBV4	30343	78903	3.82%	0.505%
2	3.611	50	55	68	rVB	42979	83025	4.02%	0.531%
3	3.746	72	78	88	rVB	25134	44641	2.16%	0.285%
4	5.819	425	431	439	rVB2	30250	52503	2.54%	0.336%
5	6.325	510	517	527	rBV	569617	986416	47.73%	6.308%
6	8.005	795	803	817	rBV	620964	1134485	54.89%	7.255%
7	8.422	866	874	887	rBV	597785	1092054	52.84%	6.984%
8	8.909	950	957	967	rVB	183512	333839	16.15%	2.135%
9	9.250	1006	1015	1024	rVB	424231	772600	37.38%	4.941%
10	10.108	1152	1161	1175	rBV	370579	691132	33.44%	4.420%
11	11.800	1438	1449	1460	rVB	266366	507076	24.54%	3.243%
12	13.885	1798	1804	1811	rBV2	23017	37109	1.80%	0.237%
13	14.155	1838	1850	1857	rBV	998119	1585366	76.71%	10.139%
14	14.431	1892	1897	1907	rBV2	28162	45041	2.18%	0.288%
15	15.530	2076	2084	2092	rVB2	405913	686388	33.21%	4.390%
16	16.993	2326	2333	2346	rBV	780471	1209422	58.52%	7.735%
17	18.256	2541	2548	2555	rBV2	506798	819390	39.65%	5.240%
18	18.473	2580	2585	2592	rBV	62500	84420	4.08%	0.540%
19	19.054	2678	2684	2693	rBV	454411	656466	31.76%	4.198%
20	19.137	2693	2698	2704	rVB	273157	355900	17.22%	2.276%
21	19.941	2831	2835	2839	rVB	20662	26510	1.28%	0.170%
22	20.282	2888	2893	2901	rBV	56747	102853	4.98%	0.658%
23	20.500	2926	2930	2934	rBV	44332	51463	2.49%	0.329%
24	20.770	2970	2976	2985	rBV	1565953	2066672	100.00%	13.217%
25	21.022	3014	3019	3025	rBV	59462	75097	3.63%	0.480%
26	21.557	3105	3110	3115	rBV	54658	73345	3.55%	0.469%
27	22.127	3196	3207	3220	rBV3	87753	240250	11.62%	1.536%
28	22.244	3224	3227	3239	rVB2	19694	43081	2.08%	0.276%
29	22.409	3250	3255	3261	rBV2	15989	27970	1.35%	0.179%
30	22.608	3281	3289	3298	rBV2	417861	814153	39.39%	5.207%
31	22.749	3309	3313	3319	rVB3	18830	27488	1.33%	0.176%
32	23.542	3442	3448	3458	rVB6	13909	32300	1.56%	0.207%
33	24.482	3601	3608	3616	rBV6	14821	41085	1.99%	0.263%
34	26.409	3923	3936	3957	rBV3	195026	758187	36.69%	4.849%

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Misc :
ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
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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:\HPCHEM1\BNA_G\METHODS\8270-BG022118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

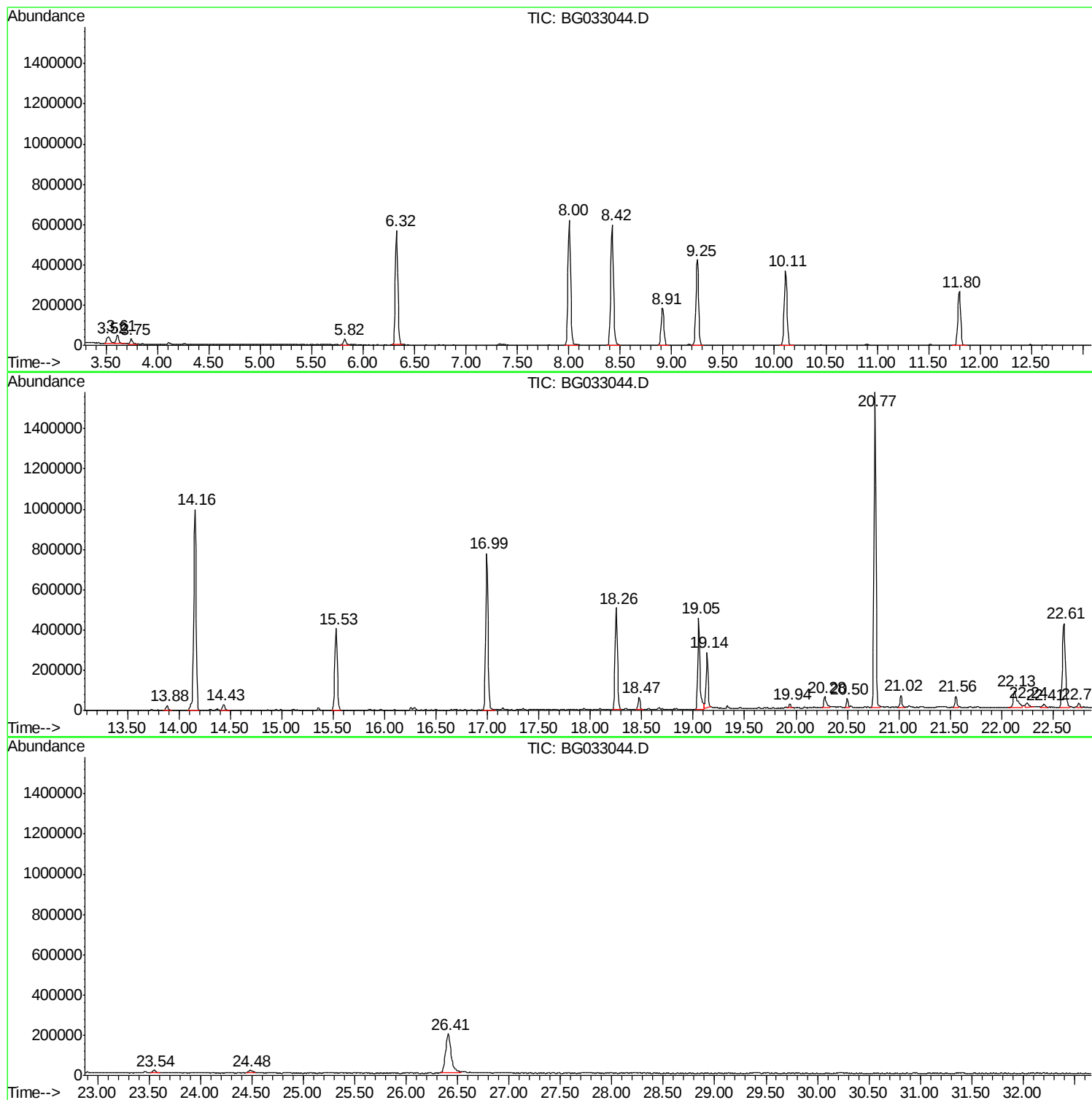
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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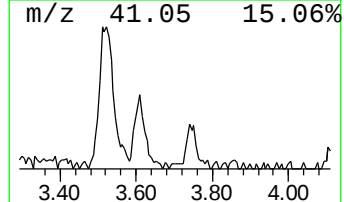
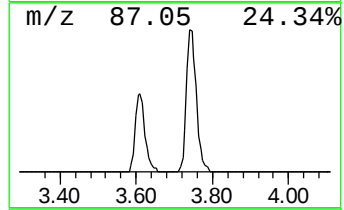
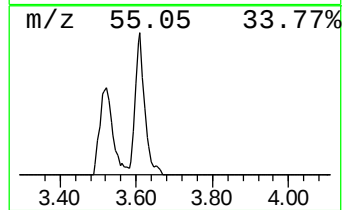
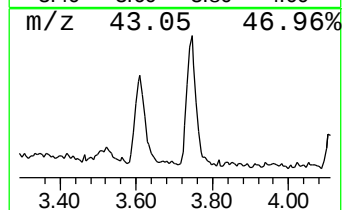
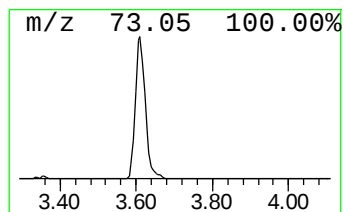
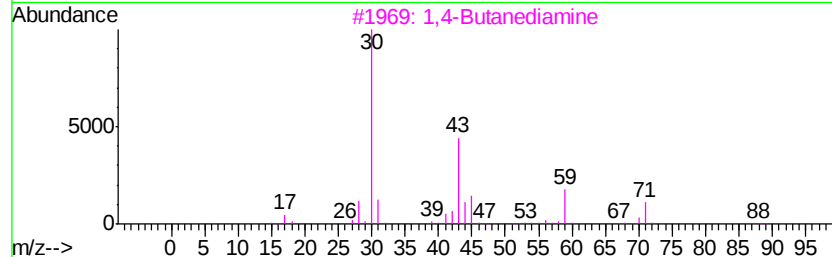
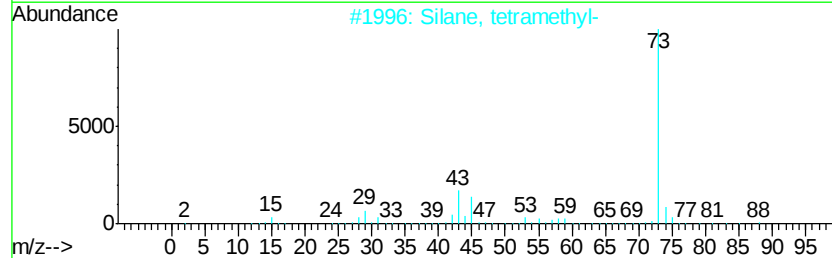
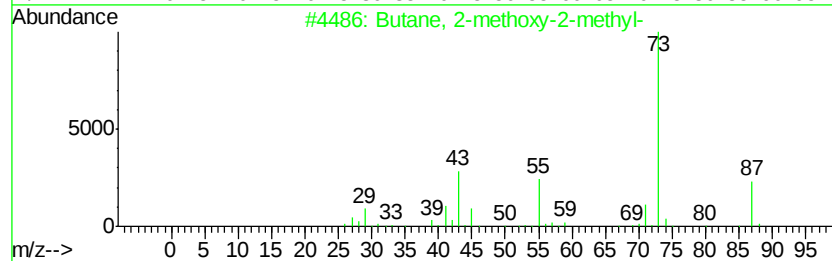
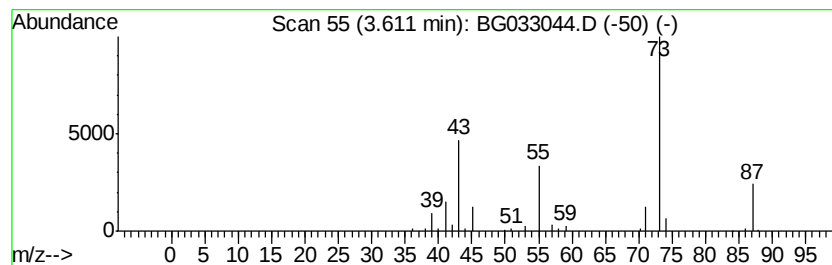
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	4.97 ng	83025	1,4-Dichlorobenzene-d4	8.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3		1,4-Butanediamine	88	C4H12N2	000110-60-1	9
4		1-Propene-1-thiol	74	C3H6S	000925-89-3	9
5		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9



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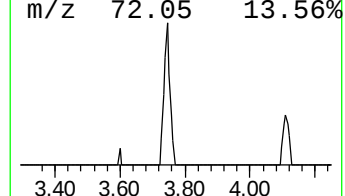
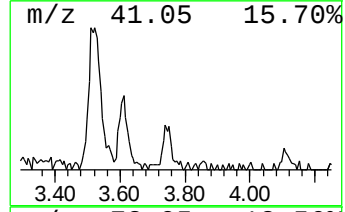
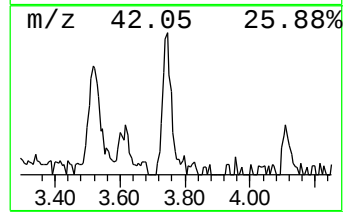
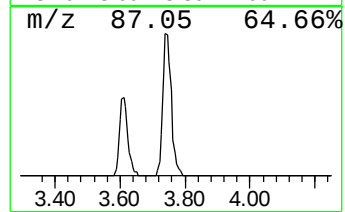
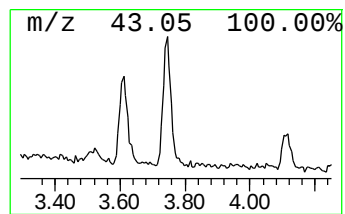
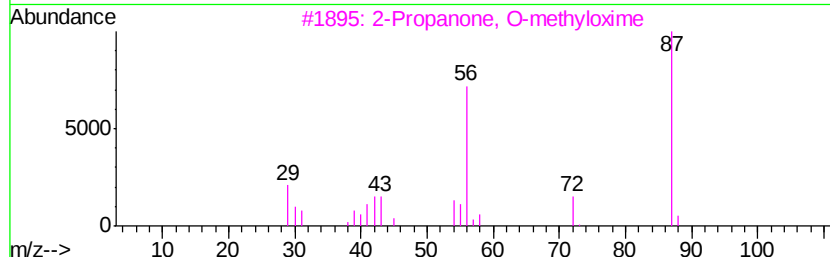
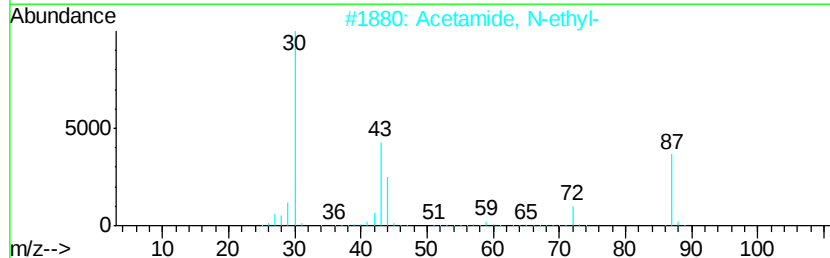
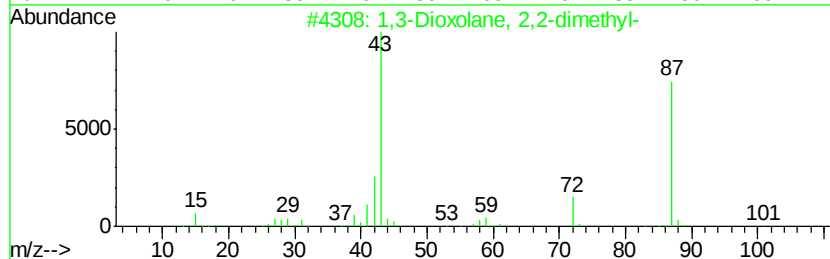
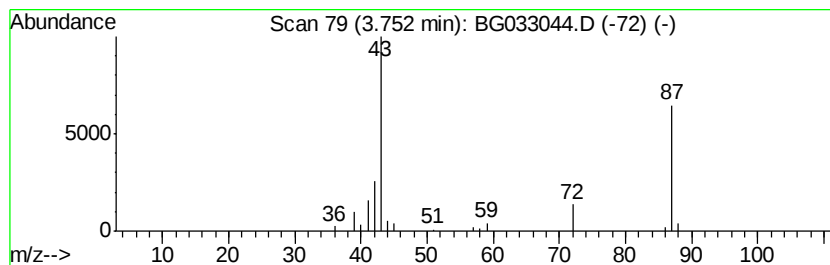
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,3-Dioxolane, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.75	2.67 ng	44641	1,4-Dichlorobenzene-d4	8.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2-dimethyl-	102	C5H10O2	002916-31-6	83
2			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	64
3			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	43
4			Morpholine	87	C4H9NO	000110-91-8	9
5			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	9



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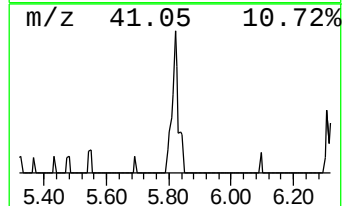
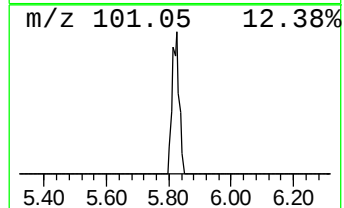
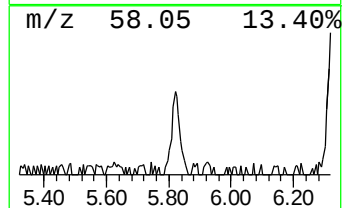
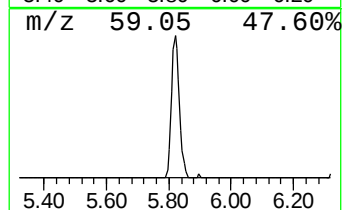
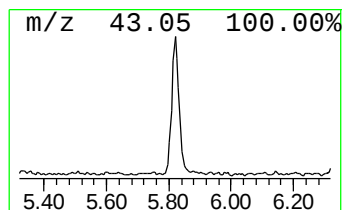
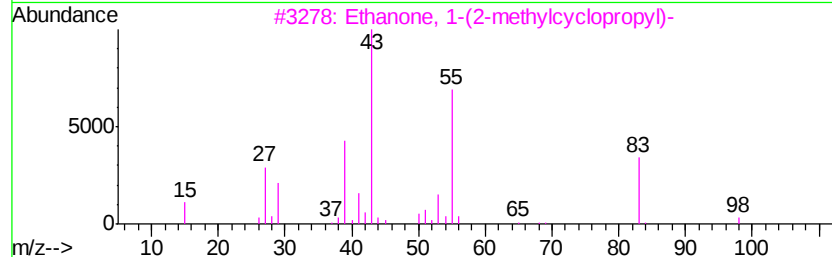
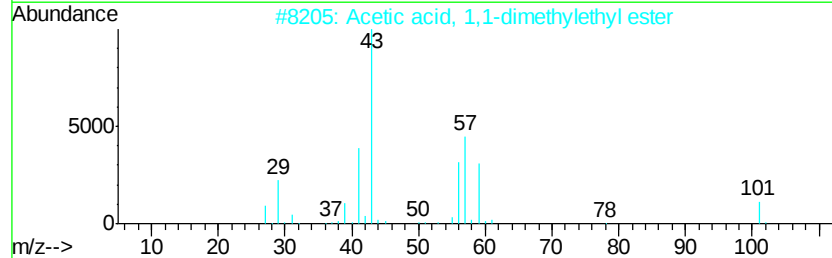
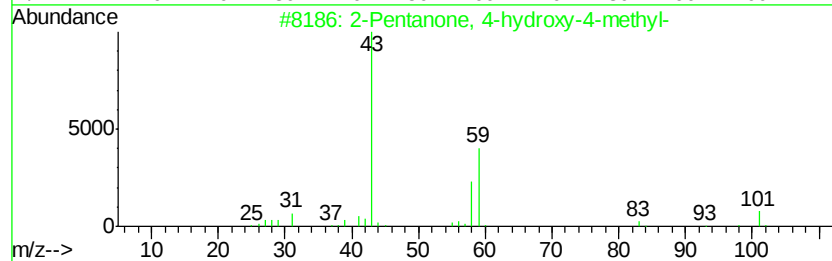
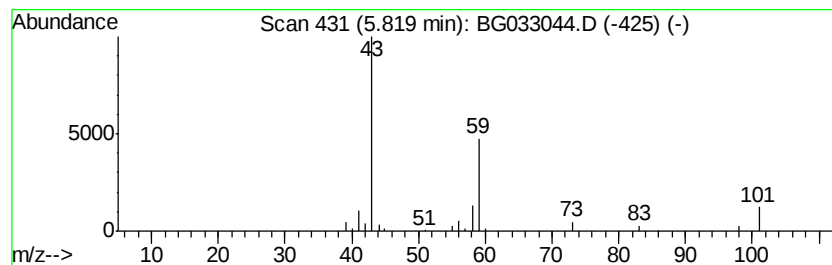
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	3.15 ng	52503	1,4-Dichlorobenzene-d4	8.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25	
3	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9	
4	Diacetamide	101	C4H7NO2	000625-77-4	9	
5	2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	9	



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FK-BPM-01-C0-C0a-D0-D0a

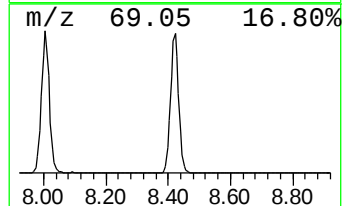
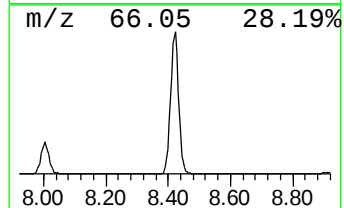
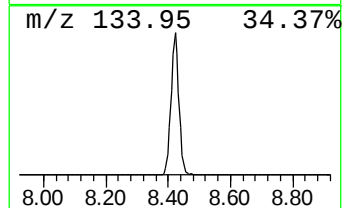
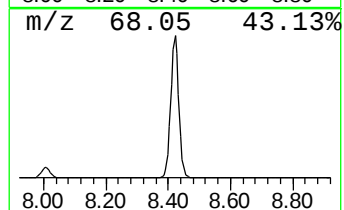
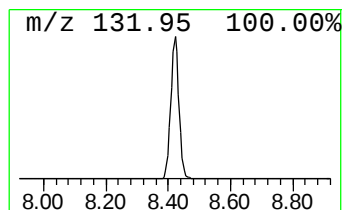
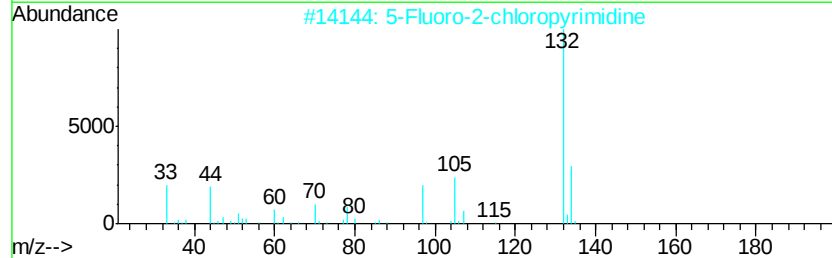
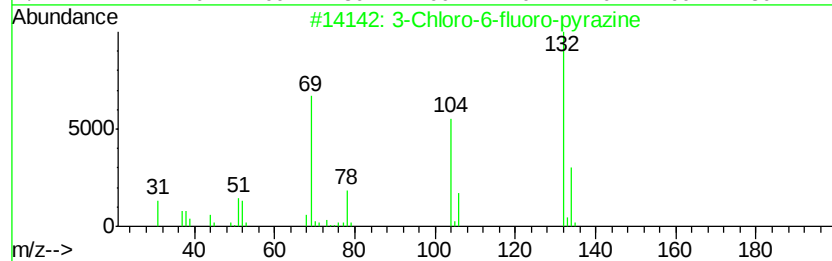
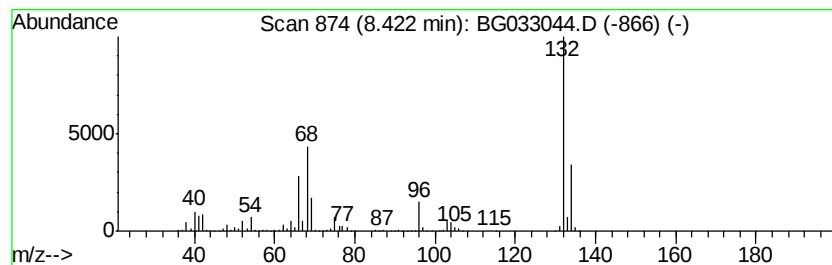
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown8.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	65.42 ng	1092050	1,4-Dichlorobenzene-d4	8.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
3	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10	
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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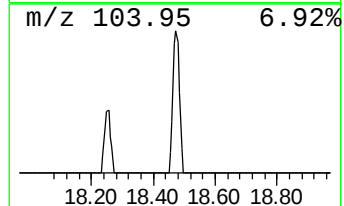
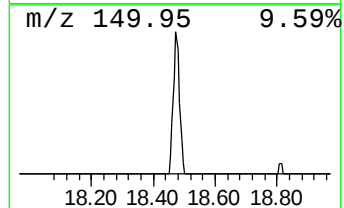
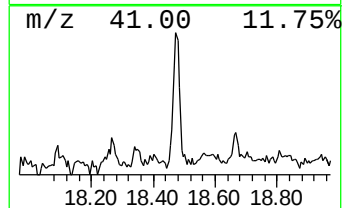
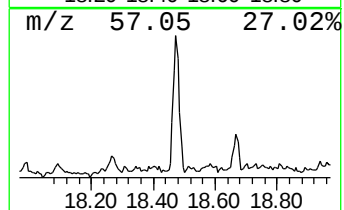
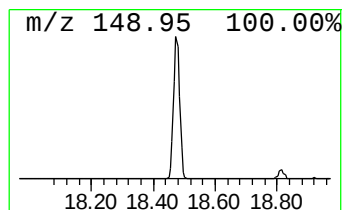
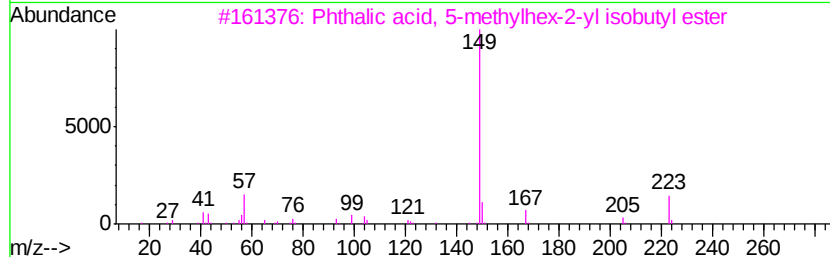
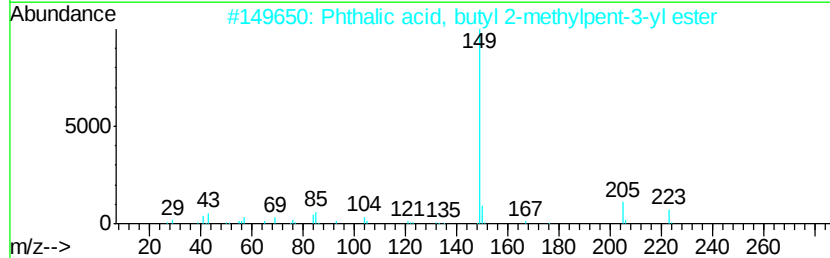
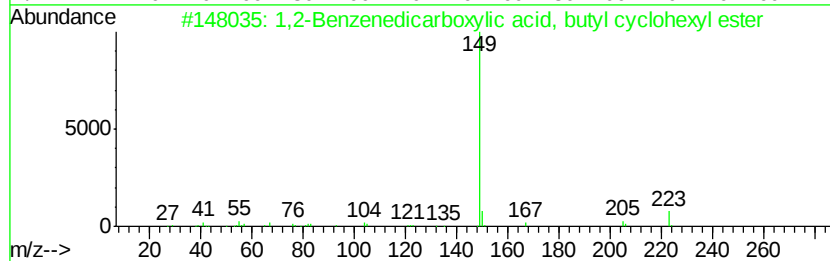
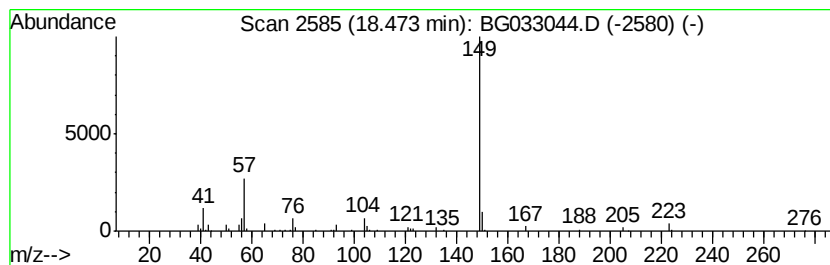
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 1,2-Benzenedicarboxylic aci... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.06 ng	84420	Phenanthrene-d10	18.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	83
2		Phthalic acid, butyl 2-methylpen...	306	C18H26O4	1000356-90-8	78
3		Phthalic acid, 5-methylhex-2-yl ...	320	C19H28O4	1000371-09-1	78
4		Phthalic acid, hex-3-yl isobutyl...	306	C18H26O4	1000356-95-4	72
5		Phthalic acid, hexadecyl propyl ...	432	C27H44O4	1000309-06-5	72



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Misc :
ALS Vial : 8 Sample Multiplier: 1

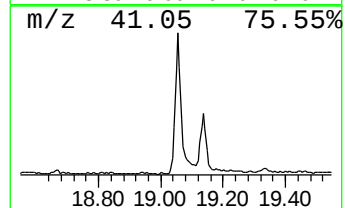
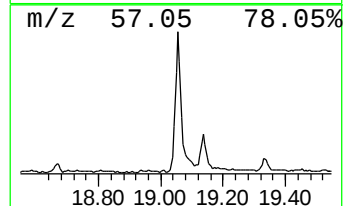
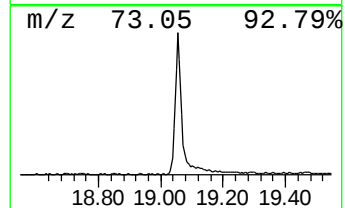
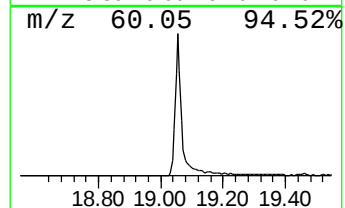
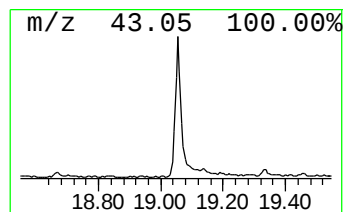
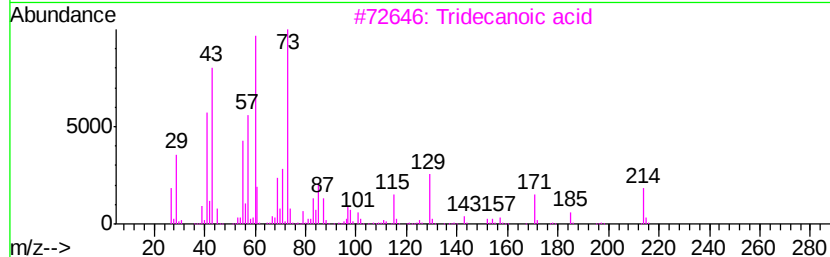
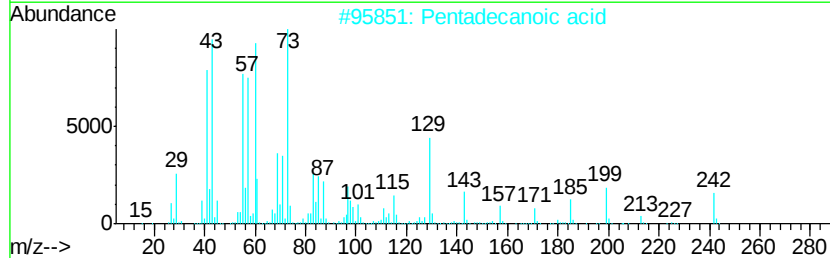
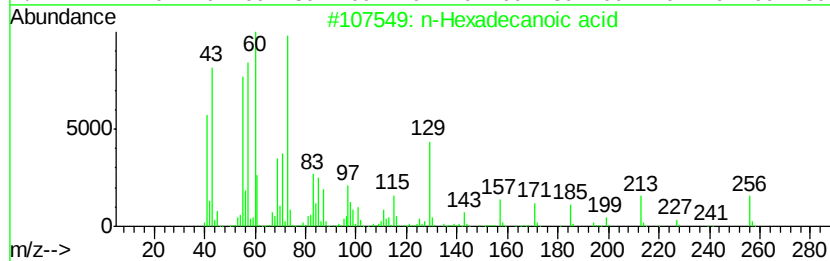
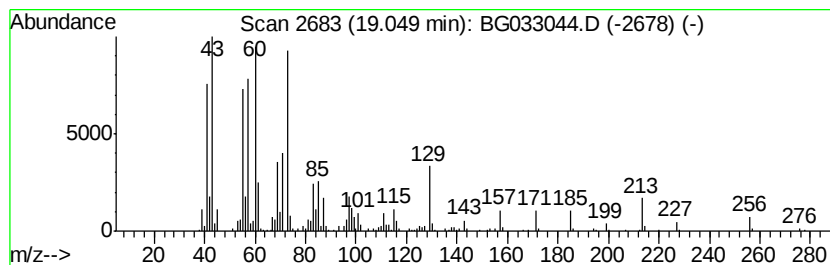
Instrument :
BNA_G
ClientSampleId :
FK-BPM-01-C0-C0a-D0-D0a

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022118.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 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.05	16.02 ng	656466	Phenanthrene-d10	18.25		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\HPCHEM1\BNA G\DATA\BG030818\
Data File : BG033044.D
Acq On : 8 Mar 2018 17:15
Operator : SJ/JU
Sample : J1825-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

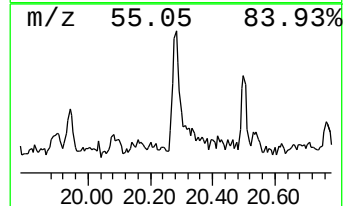
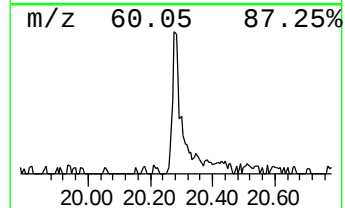
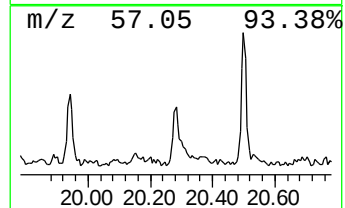
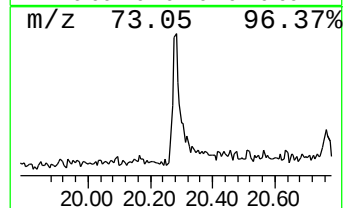
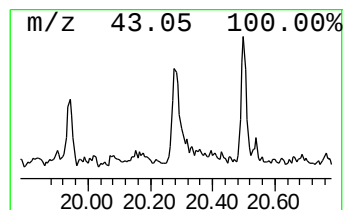
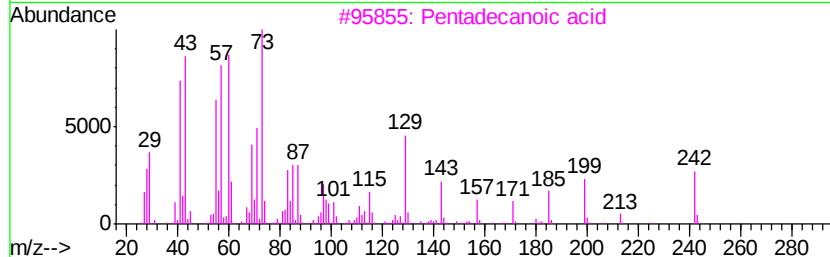
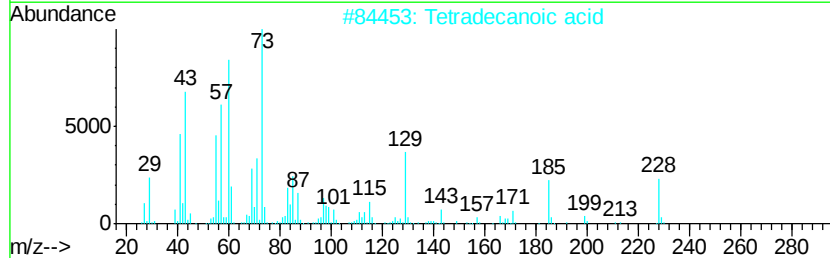
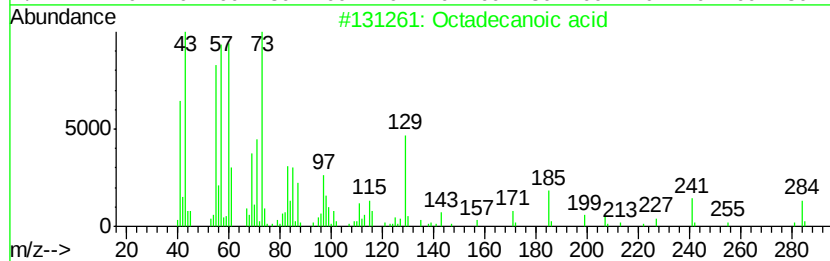
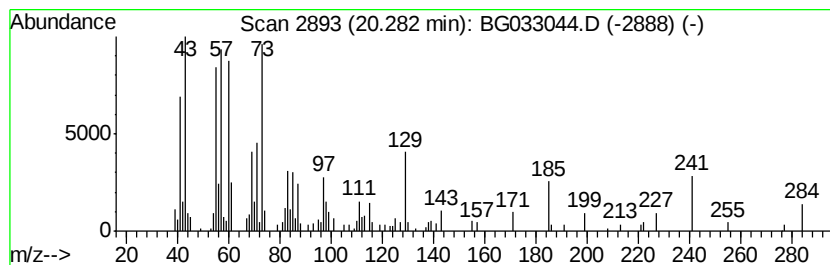
Instrument :
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ClientSampleId :
FK-BPM-01-C0-C0a-D0-D0a

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022118.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 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.28	2.51 ng	102853	Phenanthrene-d10	18.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG030818\
Data File : BG033044.D
Acq On : 8 Mar 2018 17:15
Operator : SJ/JU
Sample : J1825-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

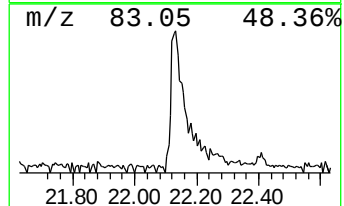
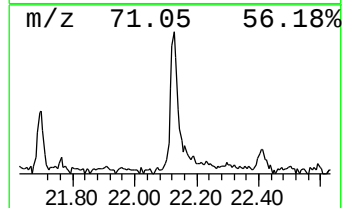
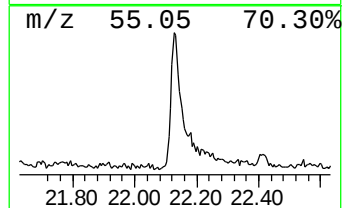
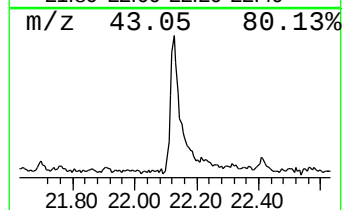
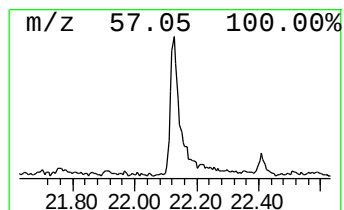
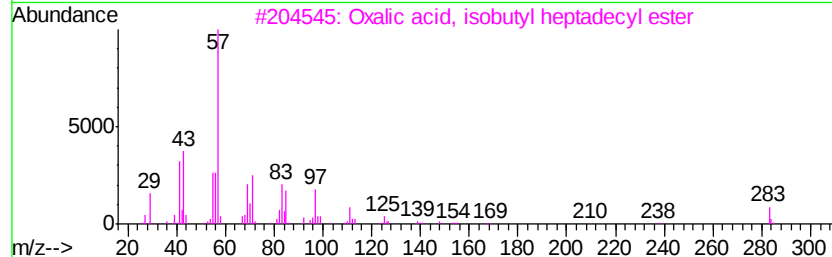
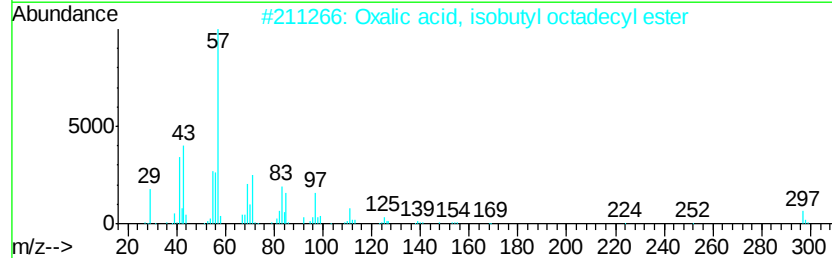
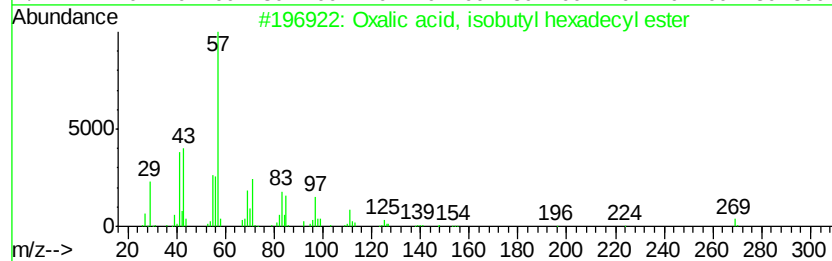
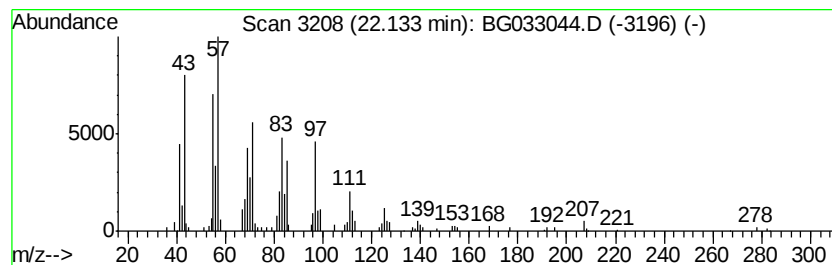
Instrument :
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ClientSampleId :
FK-BPM-01-C0-C0a-D0-D0a

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxalic acid, isobutyl hexadec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
22.13	5.90 ng	240250	Chrysene-d12	22.61		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid,	isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Oxalic acid,	isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
3	Oxalic acid,	isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
4	Oxalic acid,	cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	91
5	Oxalic acid,	cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030818\
Data File : BG033044.D
Acq On : 8 Mar 2018 17:15
Operator : SJ/JU
Sample : J1825-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-BPM-01-C0-C0a-D0-D0a

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.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
Butane, 2-methoxy...	3.61	5.0	ng	83025	1	8.91	333839	20.0
1,3-Dioxolane, 2,...	3.75	2.7	ng	44641	1	8.91	333839	20.0
2-Pentanone, 4-hy...	5.82	3.1	ng	52503	1	8.91	333839	20.0
unknown8.42	8.42	65.4	ng	1092050	1	8.91	333839	20.0
1,2-Benzenedicarb...	18.47	2.1	ng	84420	4	18.25	819390	20.0
n-Hexadecanoic acid	19.05	16.0	ng	656466	4	18.25	819390	20.0
Octadecanoic acid	20.28	2.5	ng	102853	4	18.25	819390	20.0
Oxalic acid, isob...	22.13	5.9	ng	240250	5	22.61	814153	20.0