

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
 Data File : BG033253.D
 Acq On : 19 Mar 2018 23:29
 Operator : SJ/JU
 Sample : J1953-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 031418-TIDO-F-U-S

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-BG031918.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	3.496	29	35	46	rBV	156802	327224	8.42%	1.913%
2	3.590	46	51	62	rVB	106152	172122	4.43%	1.006%
3	6.316	506	515	530	rBV	142792	341231	8.78%	1.995%
4	6.845	599	605	620	rBV	193662	390013	10.04%	2.280%
5	8.003	795	802	818	rBV3	78536	251139	6.46%	1.468%
6	8.402	862	870	892	rBV	344435	788343	20.29%	4.609%
7	8.896	946	954	971	rBV2	98365	242911	6.25%	1.420%
8	9.225	1002	1010	1023	rBV	539066	1105802	28.46%	6.464%
9	10.094	1149	1158	1177	rBV	446115	1035984	26.66%	6.056%
10	11.780	1435	1445	1456	rBV2	153937	339906	8.75%	1.987%
11	14.137	1839	1846	1861	rBV	1484109	2517152	64.78%	14.715%
12	14.930	1973	1981	1991	rBV	33758	63825	1.64%	0.373%
13	15.335	2045	2050	2057	rBV2	29957	44189	1.14%	0.258%
14	15.511	2074	2080	2092	rVB2	318774	553299	14.24%	3.235%
15	16.275	2206	2210	2216	rVB3	59874	80832	2.08%	0.473%
16	16.722	2282	2286	2291	rVB2	27143	40513	1.04%	0.237%
17	16.980	2322	2330	2347	rBV	906332	1585297	40.80%	9.267%
18	17.127	2351	2355	2364	rVB	64478	108978	2.80%	0.637%
19	17.920	2486	2490	2494	rBV2	39753	49975	1.29%	0.292%
20	18.238	2534	2544	2556	rBV2	465147	843991	21.72%	4.934%
21	19.037	2675	2680	2691	rBV2	129917	207606	5.34%	1.214%
22	20.270	2884	2890	2894	rBV5	33217	54757	1.41%	0.320%
23	20.758	2967	2973	2983	rBV	2871324	3885697	100.00%	22.715%
24	22.104	3197	3202	3214	rBV2	101437	203193	5.23%	1.188%
25	22.591	3278	3285	3298	rVB	440899	918421	23.64%	5.369%
26	24.483	3601	3607	3616	rVB3	38981	92373	2.38%	0.540%
27	26.387	3920	3931	3948	rBV	243865	861393	22.17%	5.036%

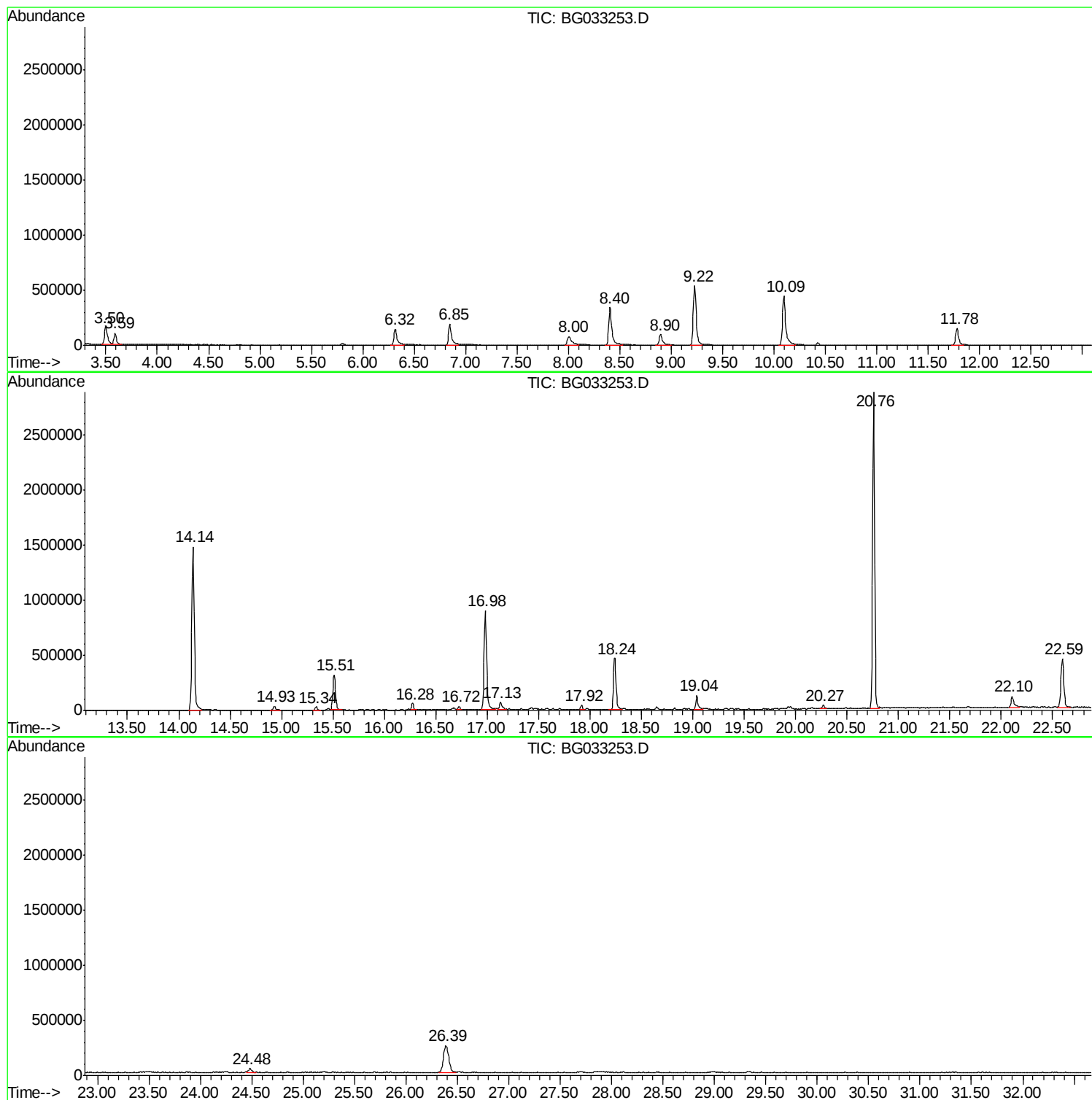
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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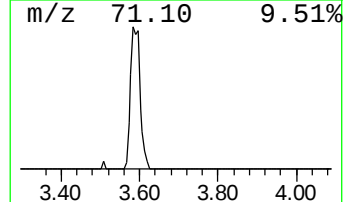
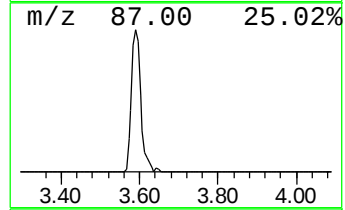
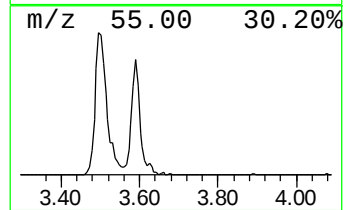
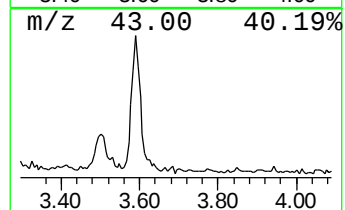
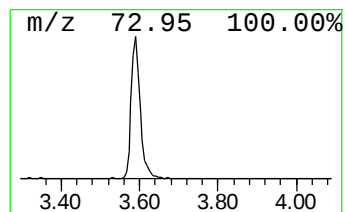
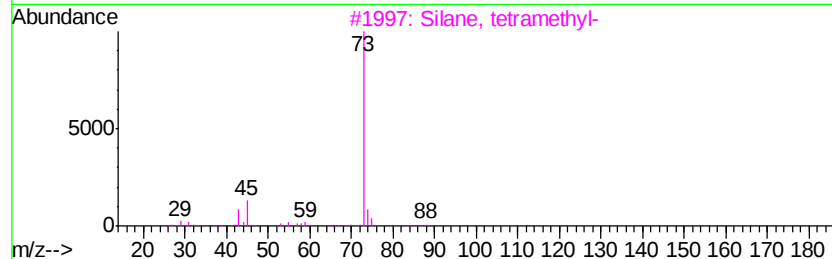
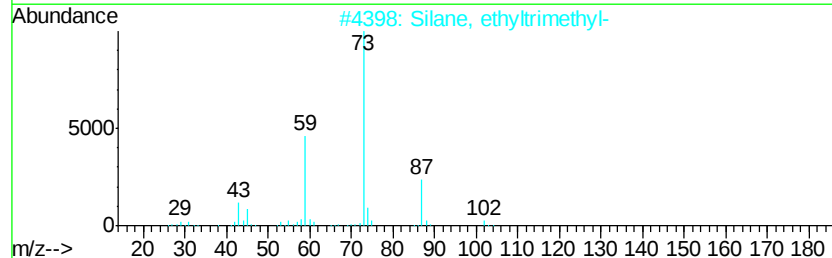
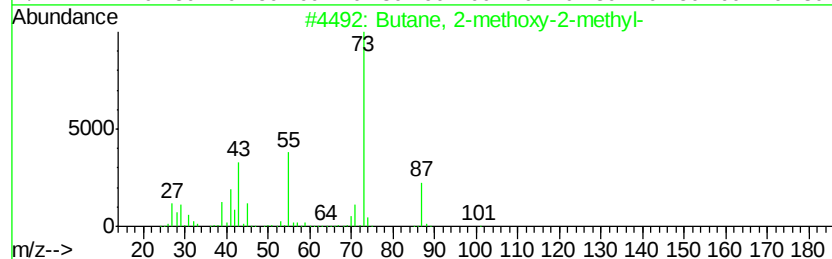
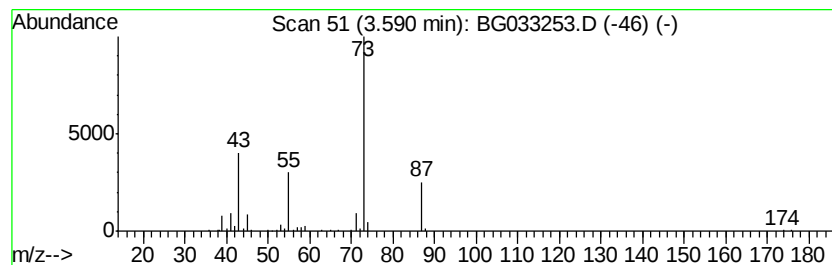
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	14.17 ng	172122	1,4-Dichlorobenzene-d4	8.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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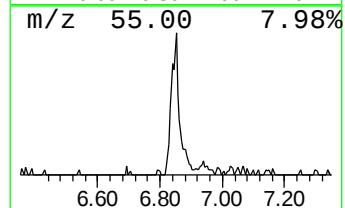
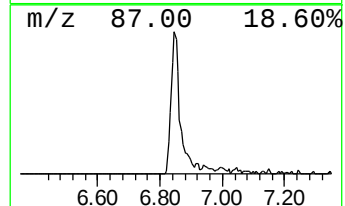
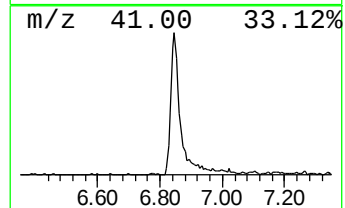
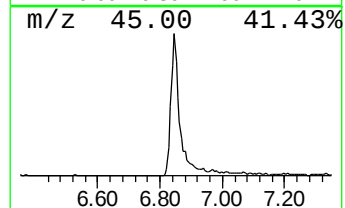
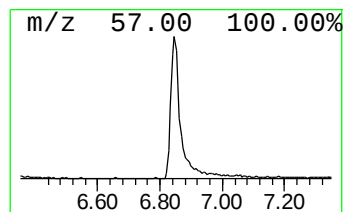
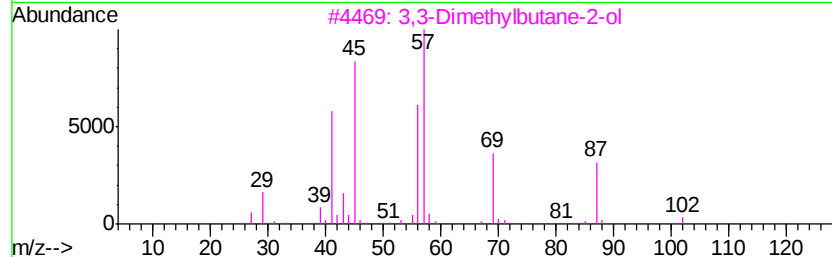
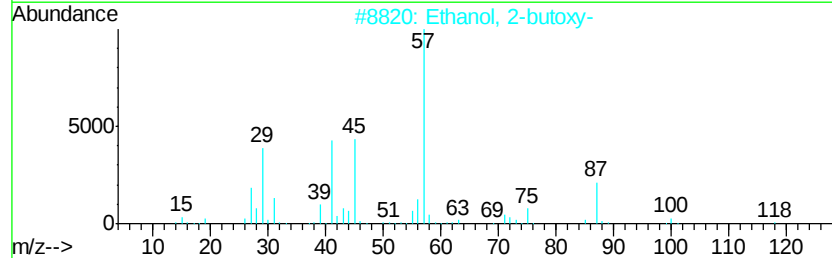
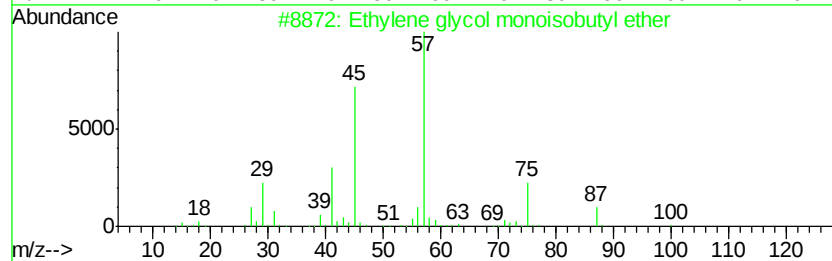
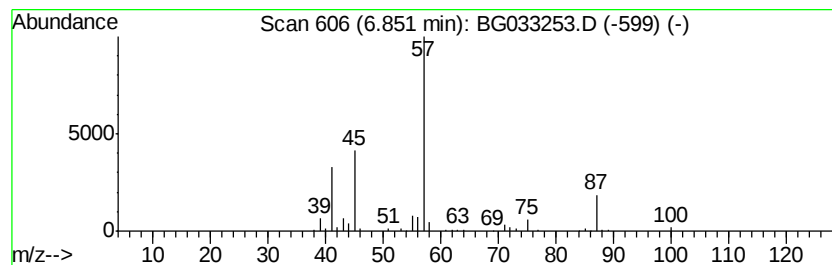
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Peak Number 3 Ethylene glycol monoisobuty... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.85	32.11 ng	390013	1,4-Dichlorobenzene-d4	8.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
2		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	49
3		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	36
4		Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	36
5		Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	17



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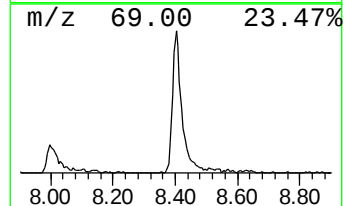
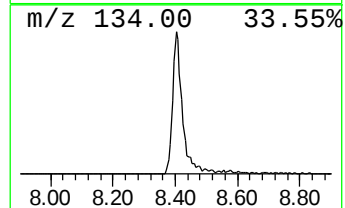
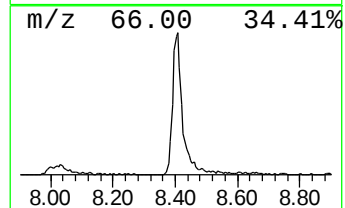
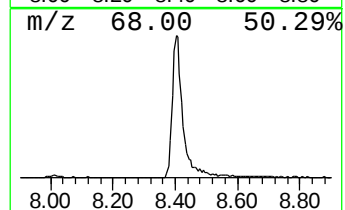
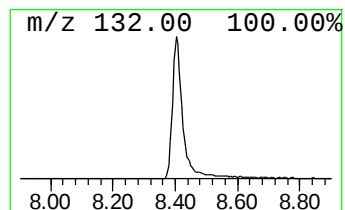
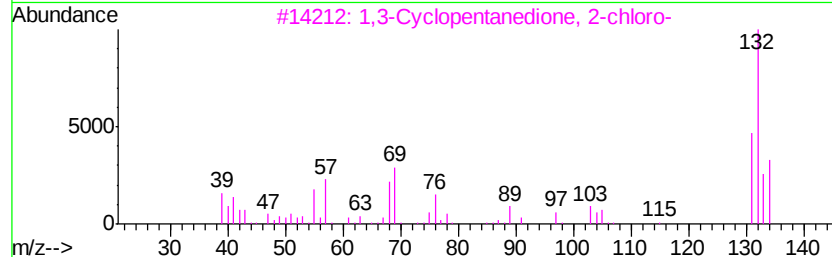
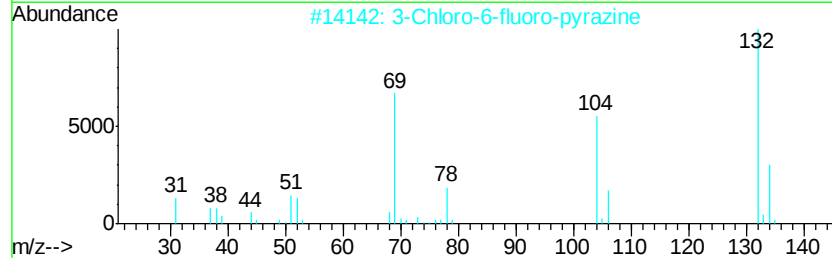
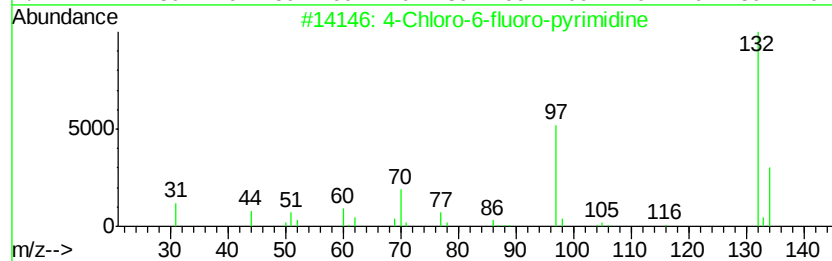
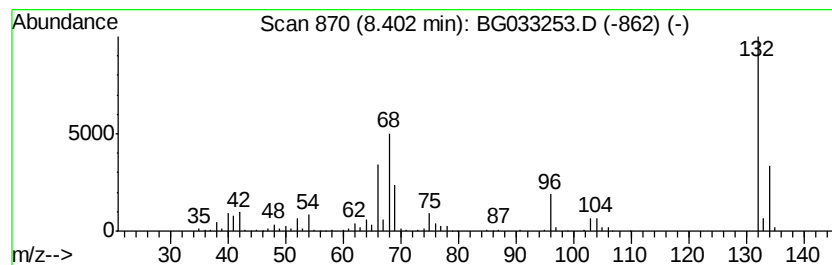
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Peak Number 4 unknown8.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	64.91 ng	788343	1,4-Dichlorobenzene-d4	8.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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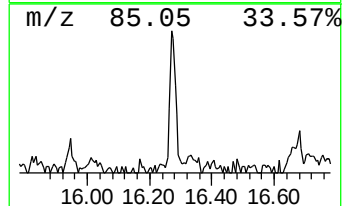
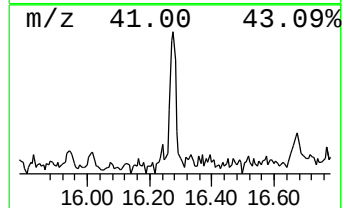
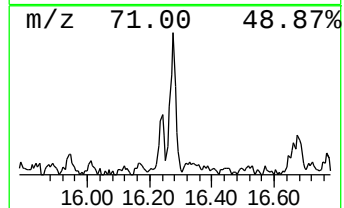
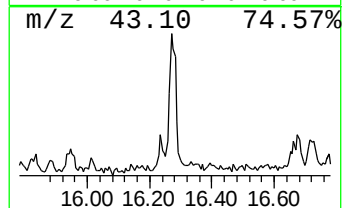
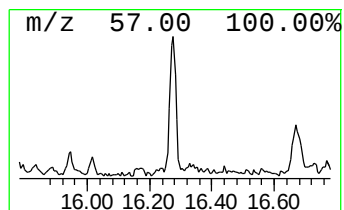
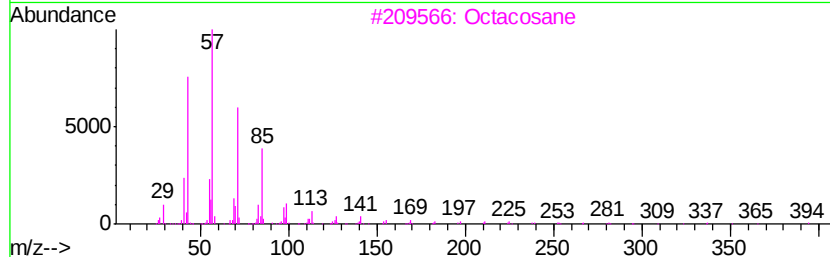
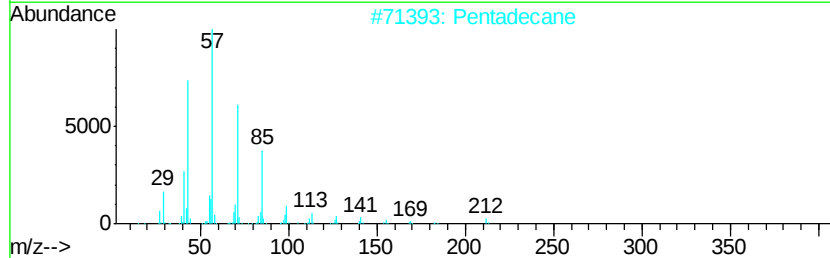
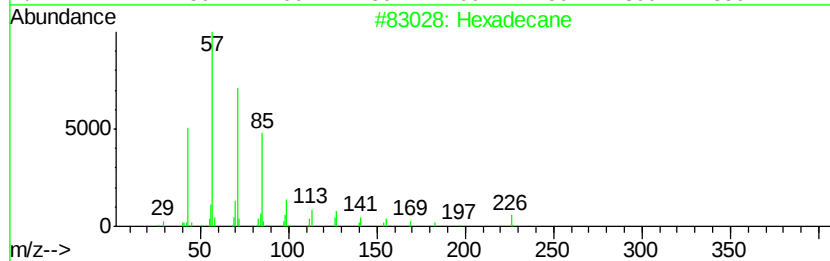
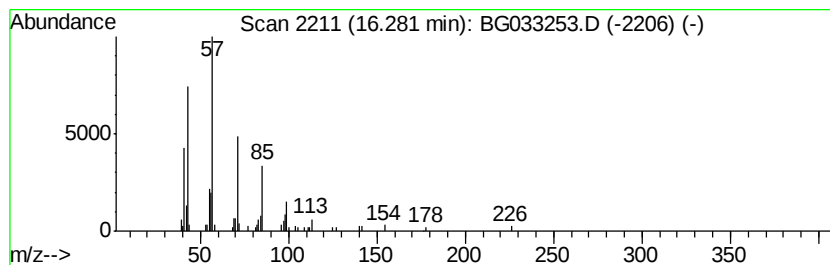
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Peak Number 6 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.28	2.92 ng	80832	Acenaphthene-d10	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	95
2		Pentadecane	212	C15H32	000629-62-9	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Heneicosane	296	C21H44	000629-94-7	86
5		Tetracosane	338	C24H50	000646-31-1	78



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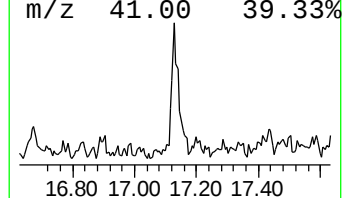
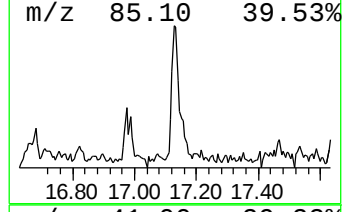
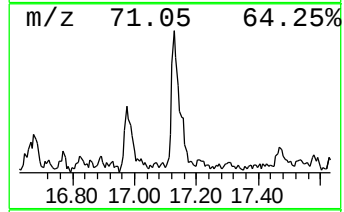
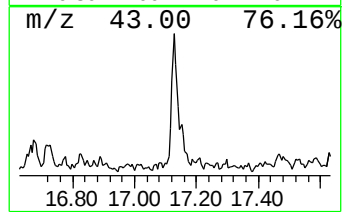
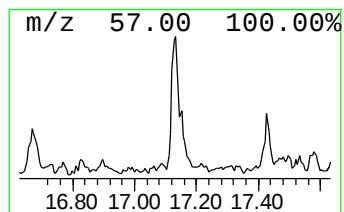
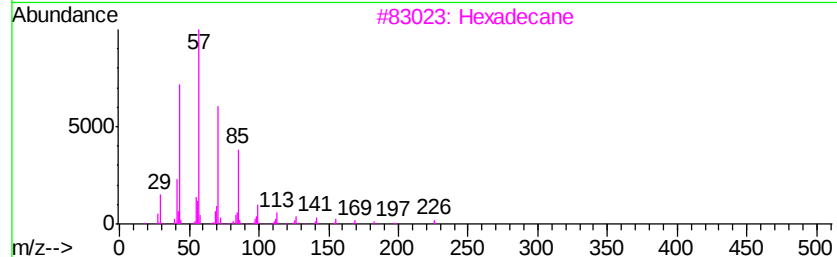
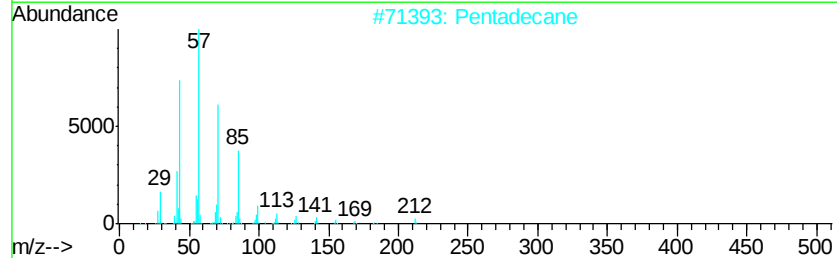
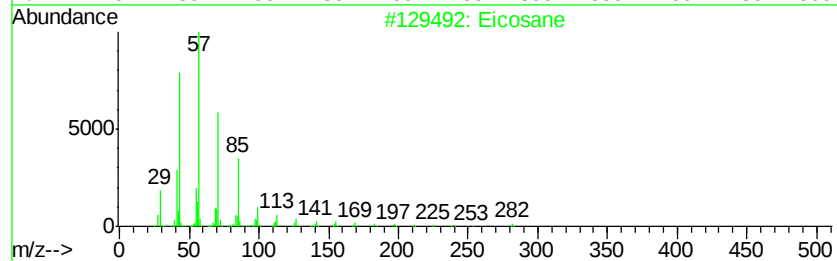
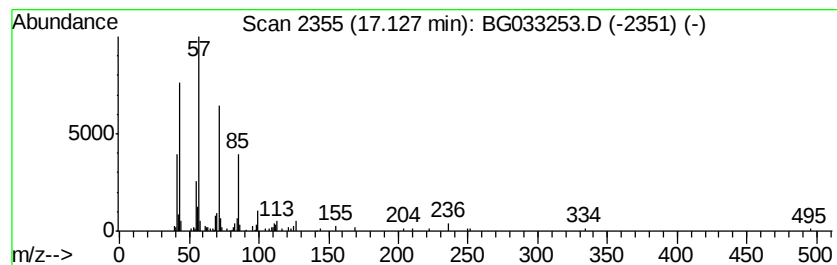
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Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	2.58 ng	108978	Phenanthrene-d10	18.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	80
2	Pentadecane		212	C15H32	000629-62-9	80
3	Hexadecane		226	C16H34	000544-76-3	80
4	Tetracosane		338	C24H50	000646-31-1	80
5	Heptadecane		240	C17H36	000629-78-7	72



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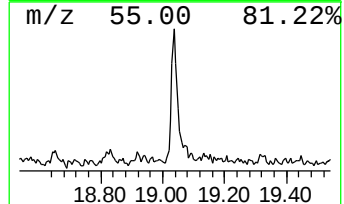
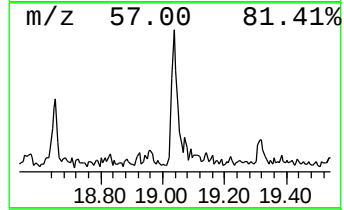
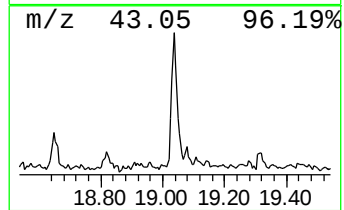
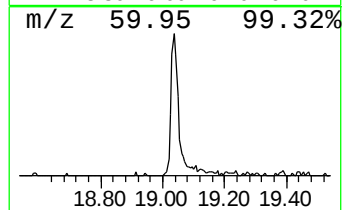
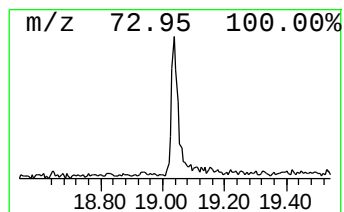
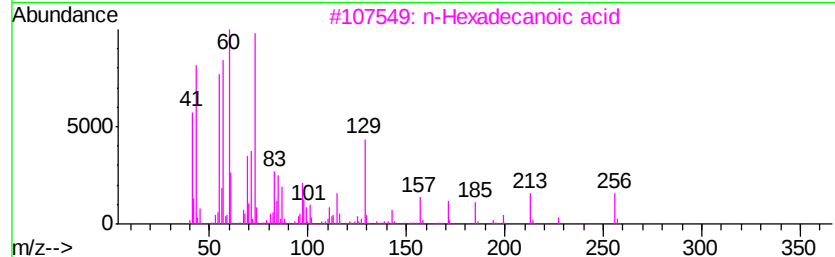
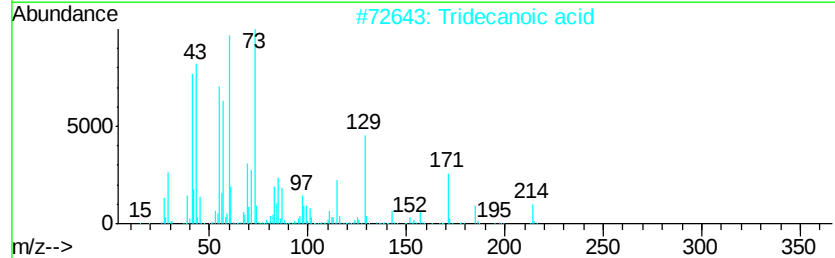
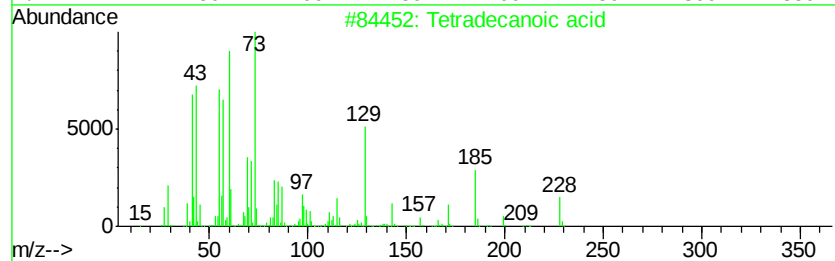
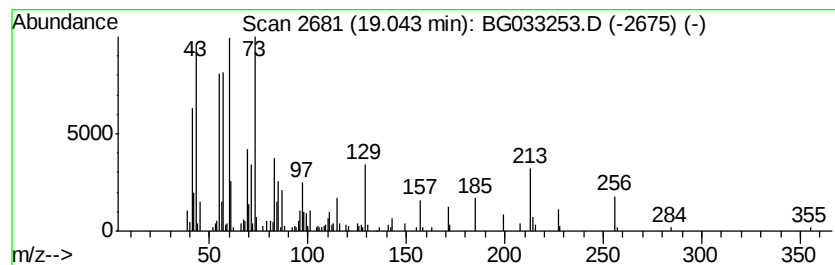
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	4.92 ng	207606	Phenanthrene-d10	18.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033253.D
Acq On : 19 Mar 2018 23:29
Operator : SJ/JU
Sample : J1953-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
031418-TIDO-F-U-S

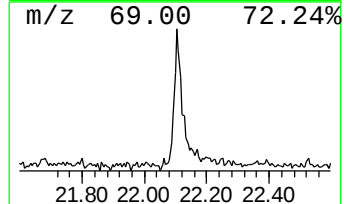
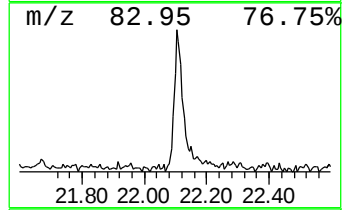
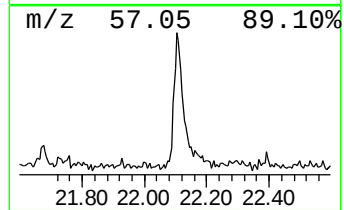
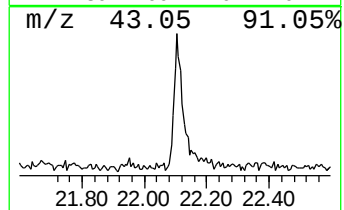
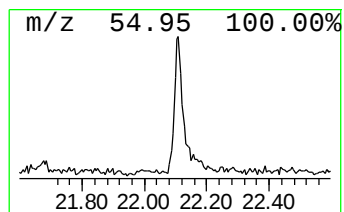
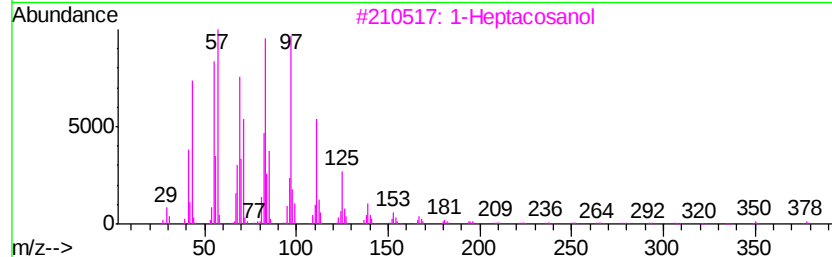
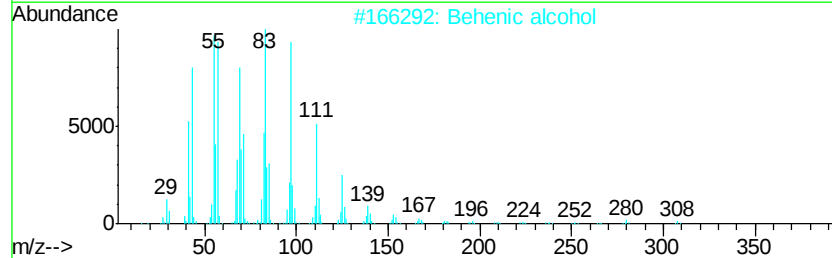
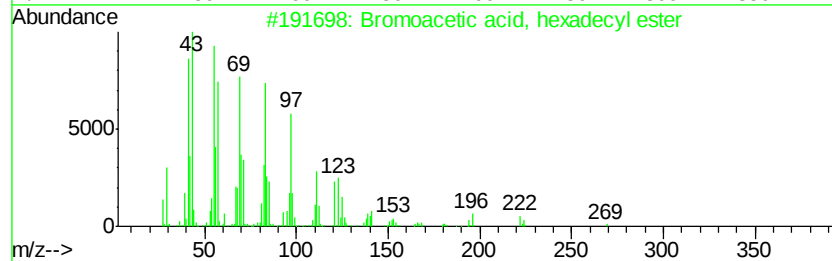
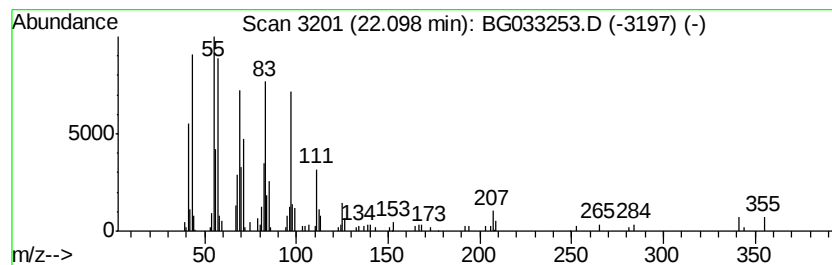
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bromoacetic acid, hexadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.10	4.42 ng	203193	Chrysene-d12	22.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	93
2		Behenic alcohol	326	C22H46O	000661-19-8	91
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033253.D
Acq On : 19 Mar 2018 23:29
Operator : SJ/JU
Sample : J1953-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
031418-TIDO-F-U-S

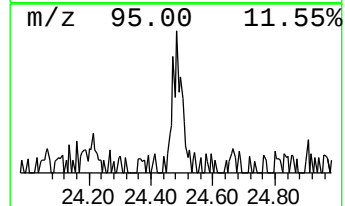
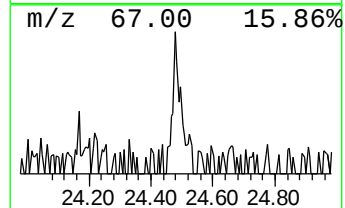
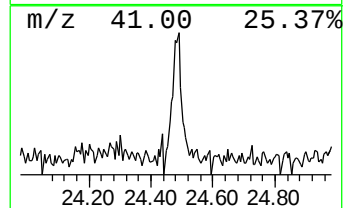
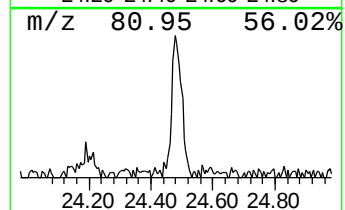
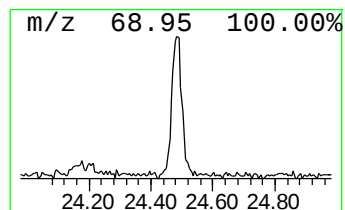
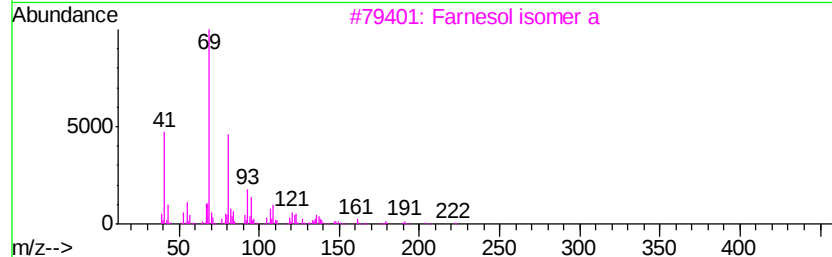
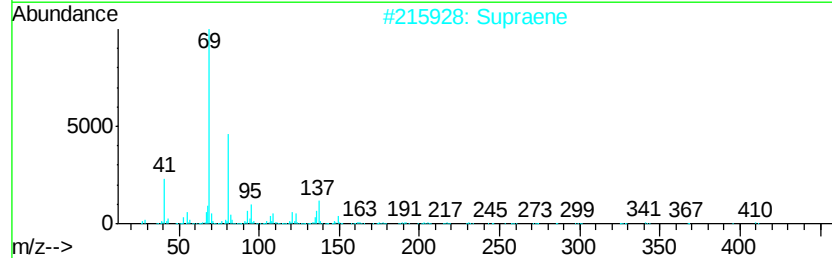
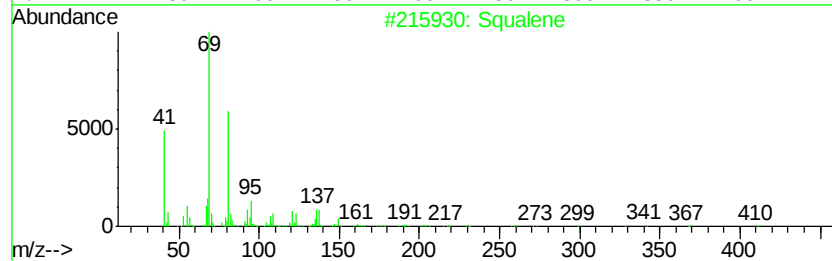
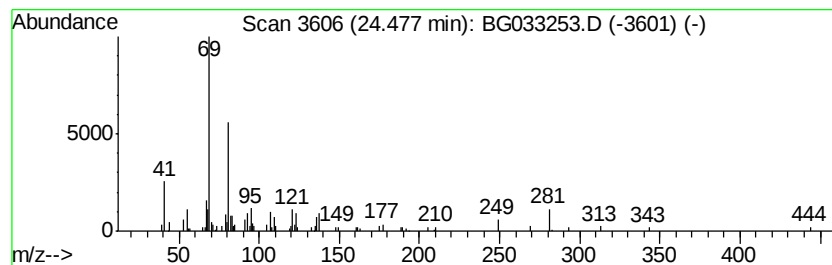
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.48	2.01 ng	92373	Chrysene-d12	22.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	68
2		Supraene	410	C30H50	007683-64-9	64
3		Farnesol isomer a	222	C15H26O	1000108-92-4	59
4		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	59
5		trans-Farnesol	222	C15H26O	000106-28-5	53



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG031918\
Data File : BG033253.D
Acq On : 19 Mar 2018 23:29
Operator : SJ/JU
Sample : J1953-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
031418-TIDO-F-U-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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...	3.59	14.2	ng	172122	1	8.90	242911	20.0
Ethylene glycol m...	6.85	32.1	ng	390013	1	8.90	242911	20.0
unknown8.40	8.40	64.9	ng	788343	1	8.90	242911	20.0
Hexadecane	16.28	2.9	ng	80832	3	15.51	553299	20.0
Eicosane	17.13	2.6	ng	108978	4	18.24	843991	20.0
Tetradecanoic acid	19.04	4.9	ng	207606	4	18.24	843991	20.0
Bromoacetic acid,...	22.10	4.4	ng	203193	5	22.60	918421	20.0
Squalene	24.48	2.0	ng	92373	5	22.60	918421	20.0