

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
 Data File : BG033261.D
 Acq On : 20 Mar 2018 4:30
 Operator : SJ/JU
 Sample : J1954-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 031518-JETT-F-D-M

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	3.501	29	36	46	rBV	152441	314936	7.76%	1.875%
2	3.589	46	51	64	rVB	100566	163282	4.02%	0.972%
3	6.309	508	514	530	rBV	160275	372967	9.19%	2.220%
4	8.001	796	802	818	rBV	89170	260231	6.41%	1.549%
5	8.401	863	870	889	rBV	351522	794499	19.57%	4.729%
6	8.894	947	954	963	rBV2	98677	219920	5.42%	1.309%
7	9.229	1002	1011	1023	rBV	504862	1022389	25.19%	6.086%
8	10.093	1149	1158	1177	rBV	436664	999282	24.62%	5.948%
9	11.779	1437	1445	1463	rBV	145200	339310	8.36%	2.020%
10	14.135	1836	1846	1861	rBV	1408898	2426446	59.78%	14.443%
11	14.929	1969	1981	1990	rBV	52736	96972	2.39%	0.577%
12	15.334	2045	2050	2057	rBV	32958	45868	1.13%	0.273%
13	15.510	2074	2080	2092	rVB2	304882	543728	13.40%	3.236%
14	16.274	2206	2210	2216	rVB	49015	66409	1.64%	0.395%
15	16.979	2324	2330	2346	rBV	915601	1571907	38.73%	9.357%
16	17.132	2351	2356	2367	rVB	42819	85332	2.10%	0.508%
17	18.242	2538	2545	2557	rBV	462023	792700	19.53%	4.718%
18	19.036	2675	2680	2689	rBV	188399	301449	7.43%	1.794%
19	20.269	2884	2890	2895	rBV2	51468	83640	2.06%	0.498%
20	20.757	2967	2973	2986	rBV	2876351	4059035	100.00%	24.161%
21	22.108	3197	3203	3217	rBV	222102	429672	10.59%	2.558%
22	22.596	3279	3286	3297	rVB2	428712	855055	21.07%	5.090%
23	24.482	3600	3607	3615	rBV3	55128	127372	3.14%	0.758%
24	26.392	3920	3932	3948	rBV	240769	827516	20.39%	4.926%

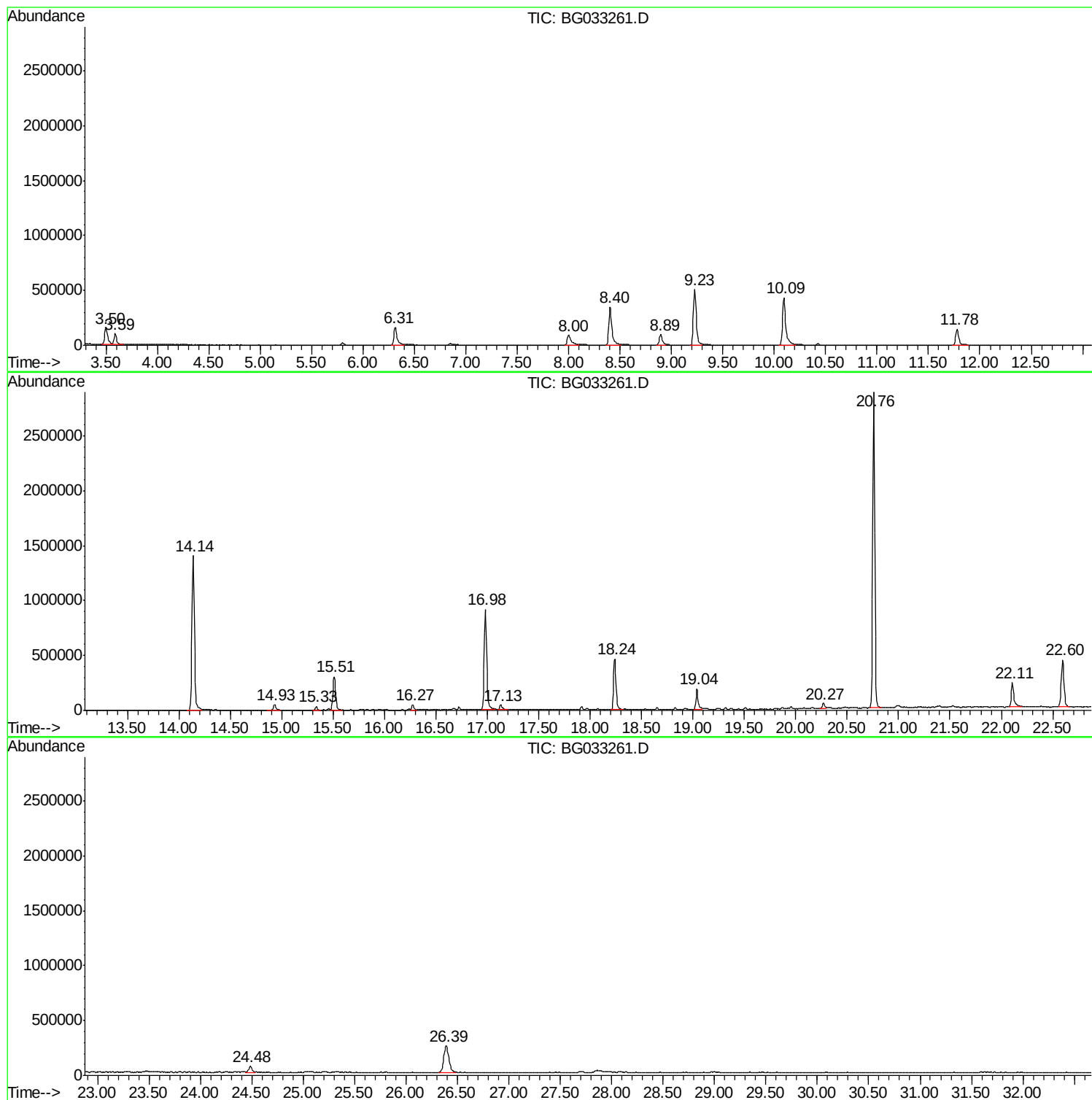
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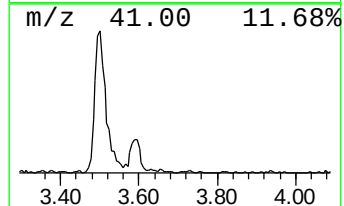
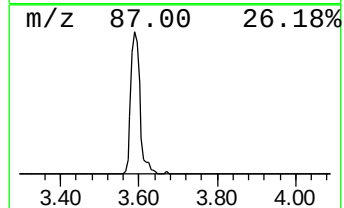
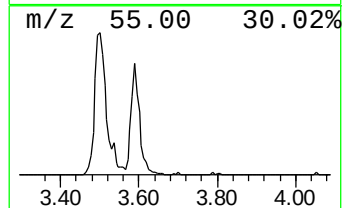
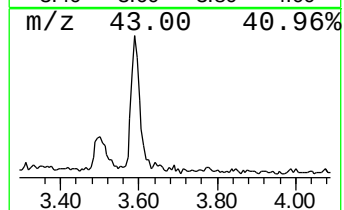
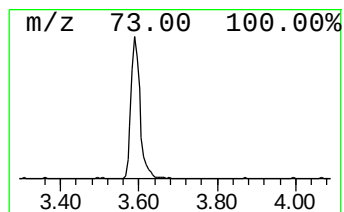
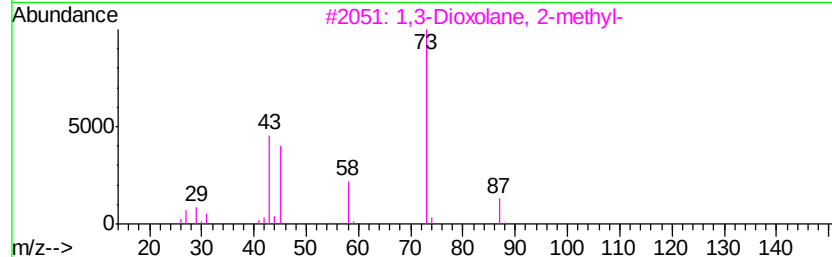
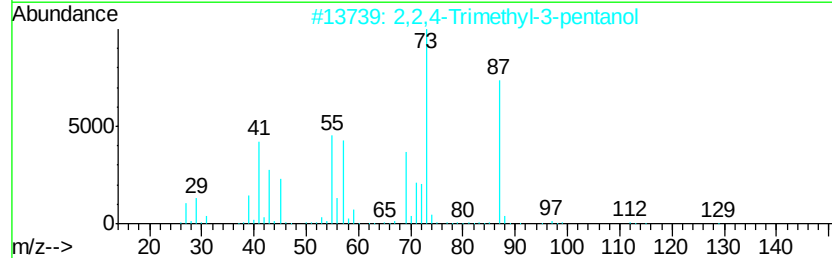
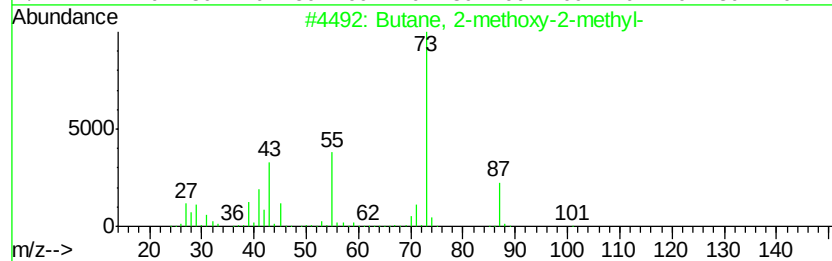
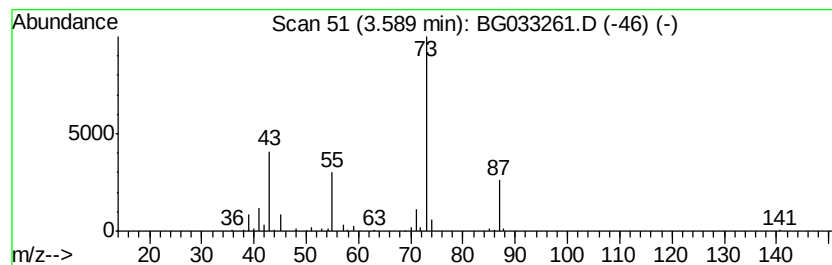
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	14.85 ng	163282	1,4-Dichlorobenzene-d4	8.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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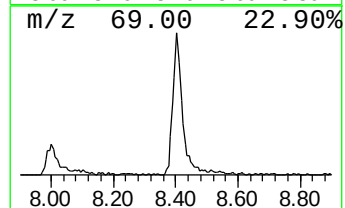
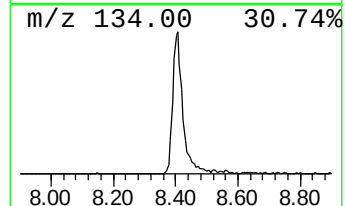
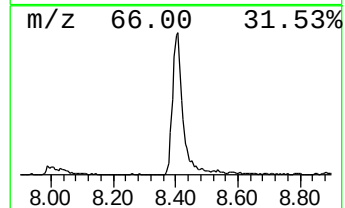
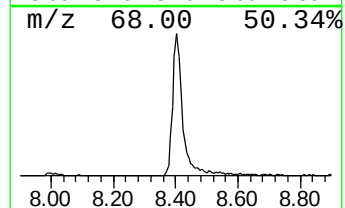
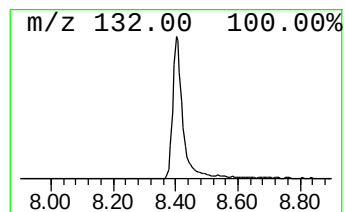
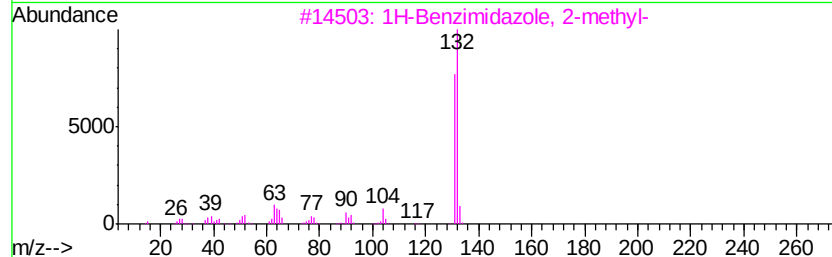
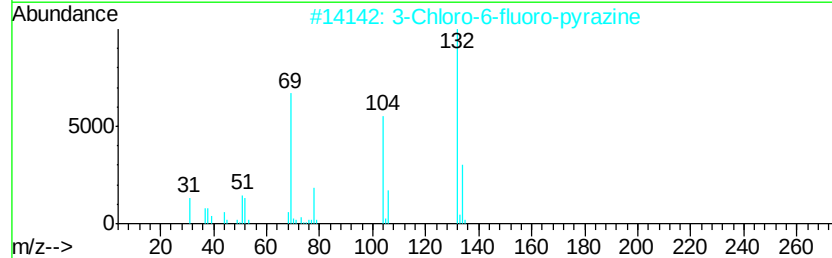
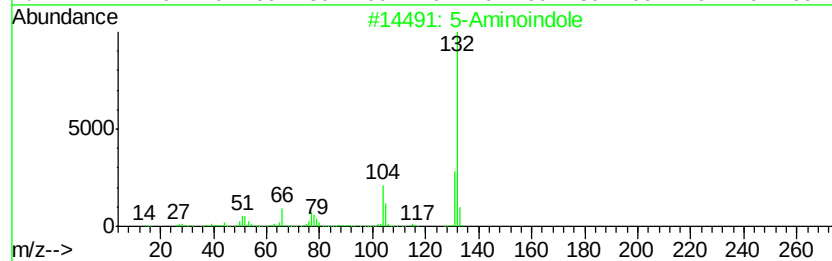
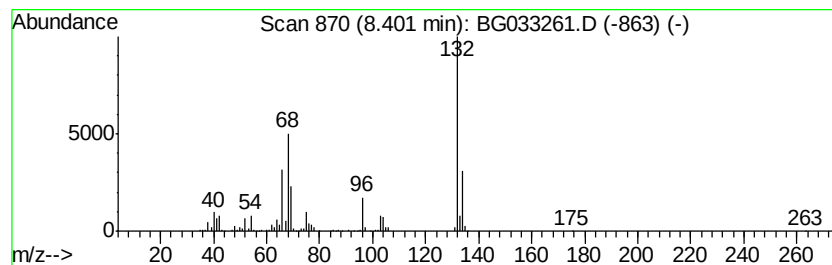
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Peak Number 3 unknown8.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	72.25 ng	794499	1,4-Dichlorobenzene-d4	8.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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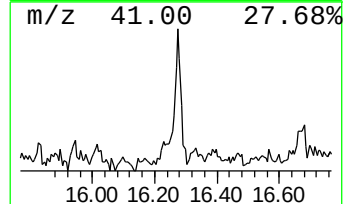
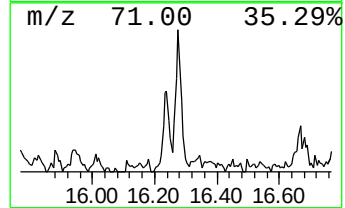
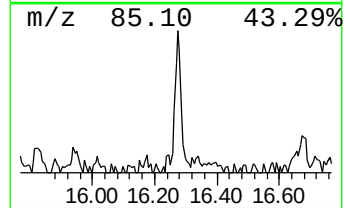
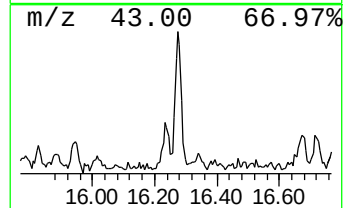
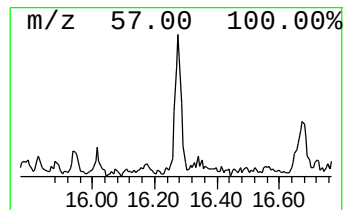
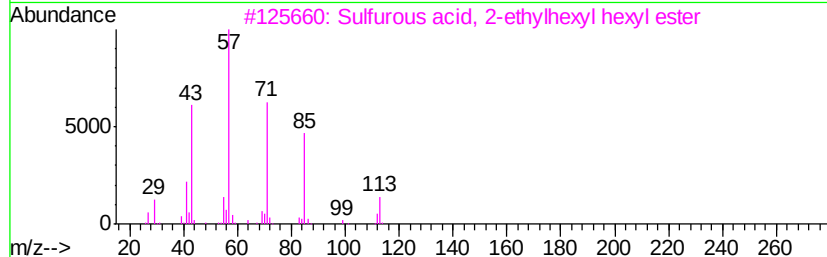
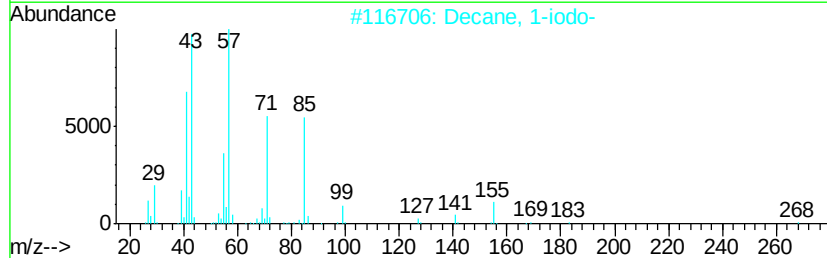
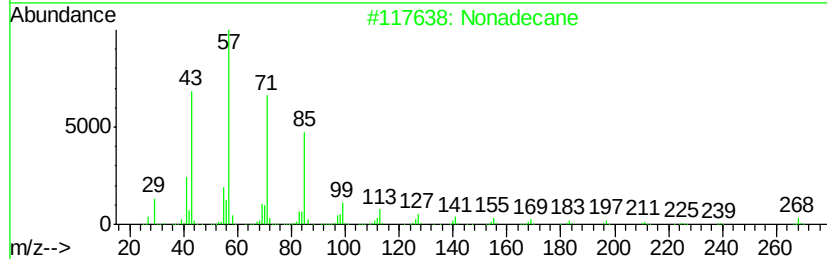
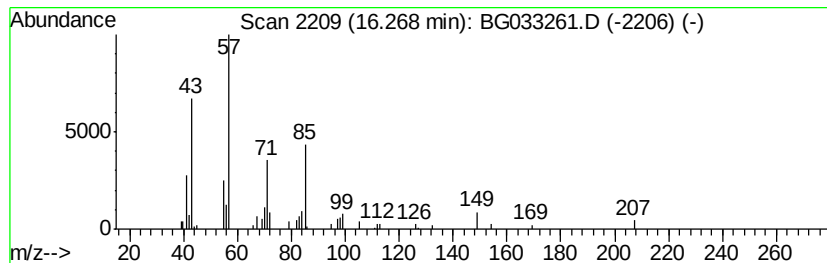
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Peak Number 5 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	2.44 ng	66409	Acenaphthene-d10	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	80
2	Decane, 1-iodo-		268	C10H21I	002050-77-3	72
3	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	59
4	Undecane		156	C11H24	001120-21-4	59
5	Oxalic acid, heptadecyl hexyl ester		412	C25H48O4	1000309-25-1	53



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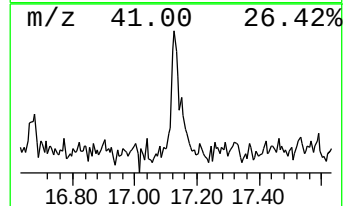
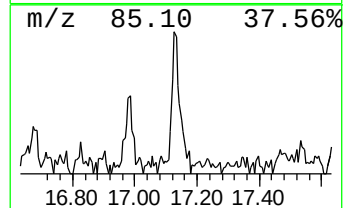
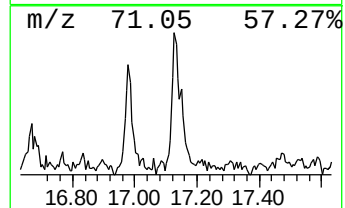
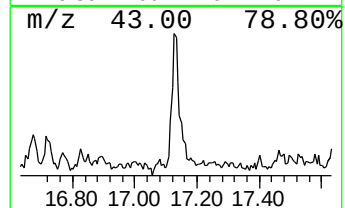
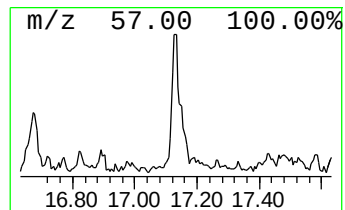
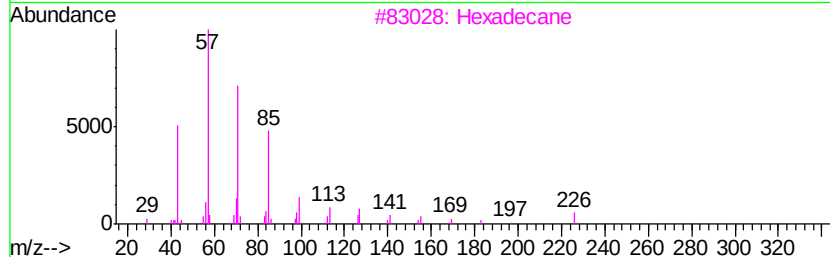
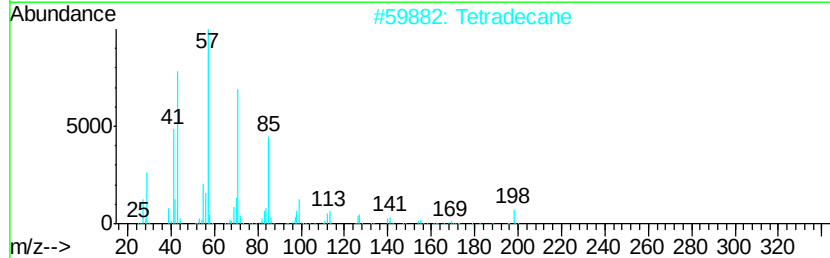
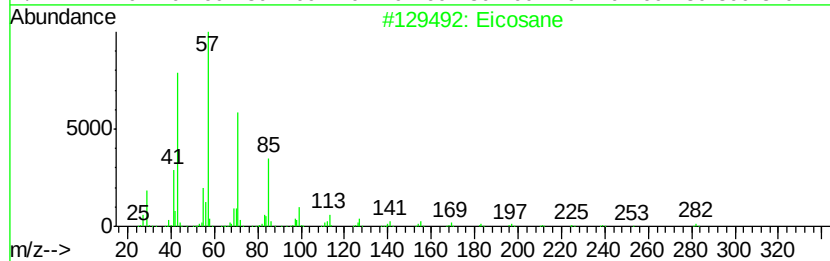
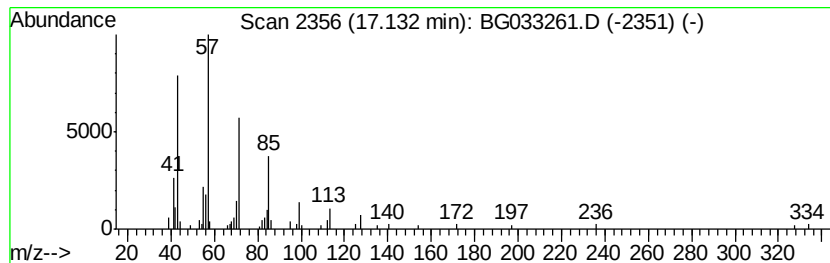
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Peak Number 6 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.		
17.13	2.15 ng	85332	Phenanthrene-d10		18.24		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	86
2	Tetradecane			198	C14H30	000629-59-4	86
3	Hexadecane			226	C16H34	000544-76-3	78
4	Heptadecane			240	C17H36	000629-78-7	78
5	Dodecane			170	C12H26	000112-40-3	78



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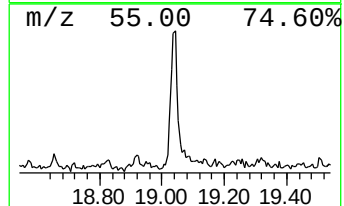
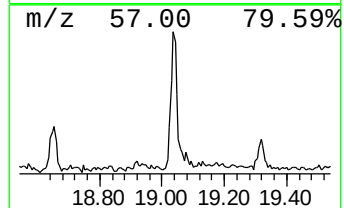
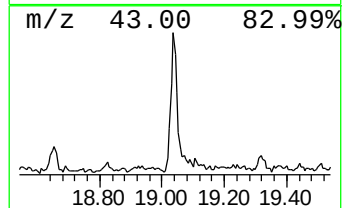
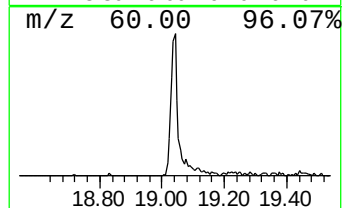
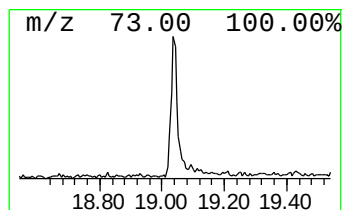
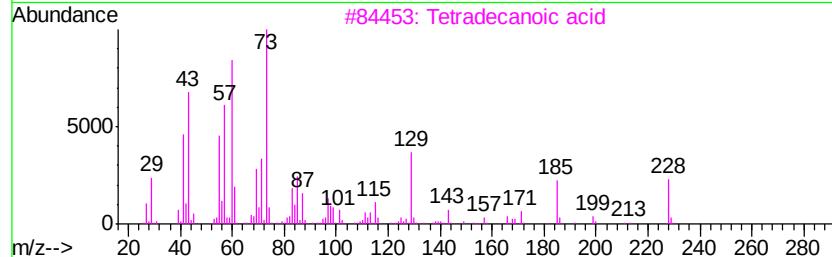
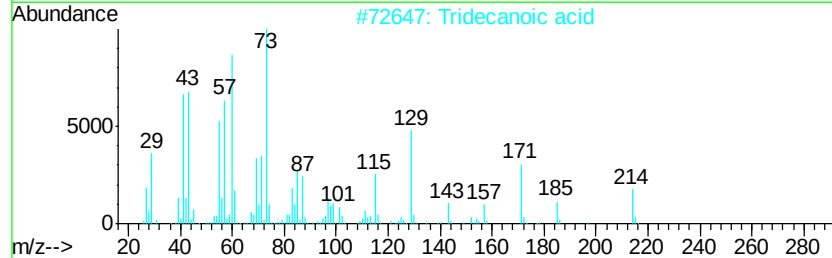
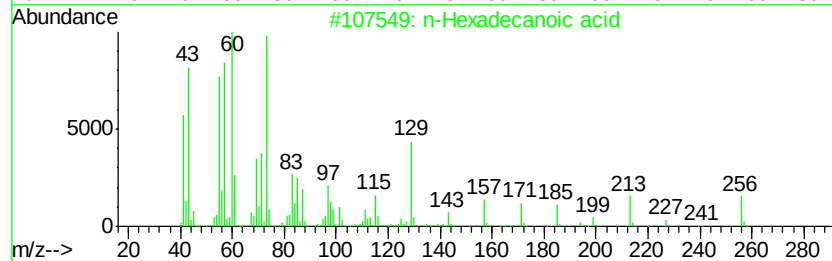
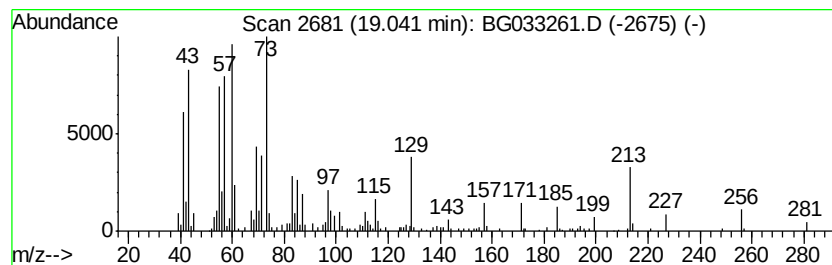
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	7.61 ng	301449	Phenanthrene-d10	18.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	97
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5		Undecanoic acid	186	C11H22O2	000112-37-8	59



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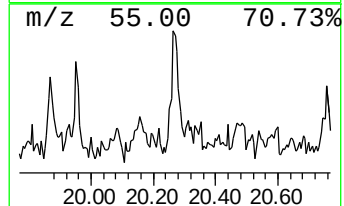
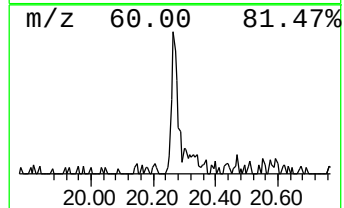
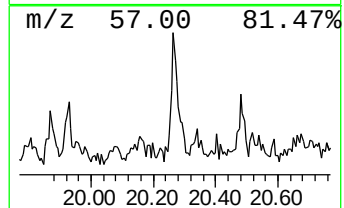
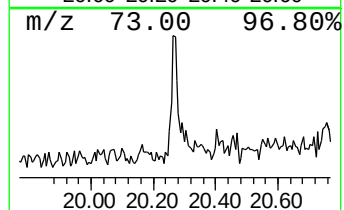
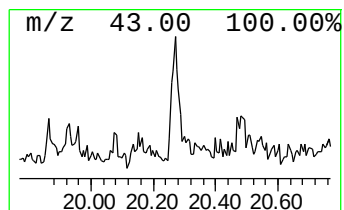
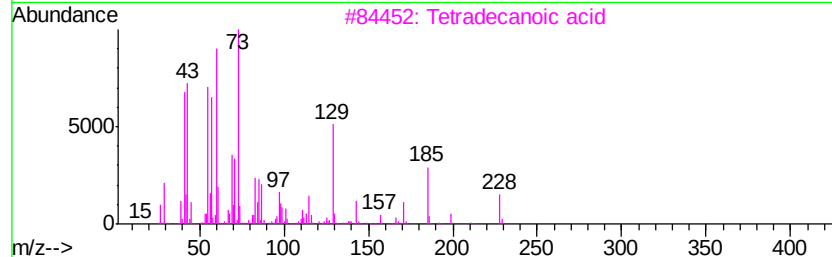
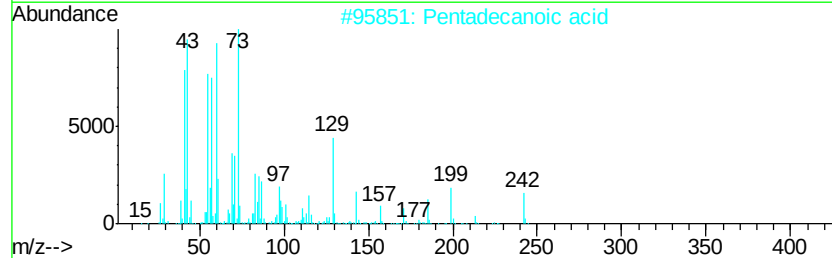
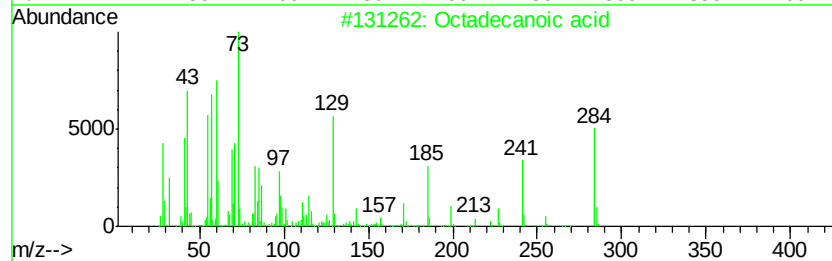
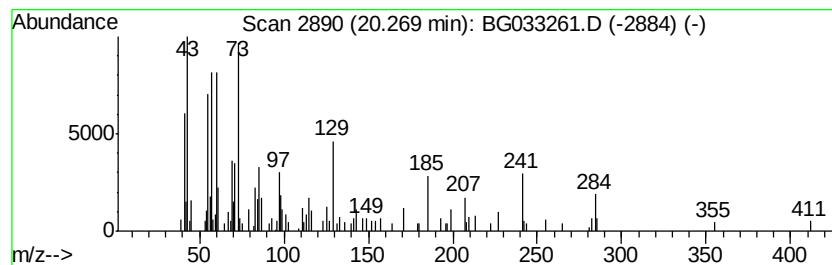
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.27	2.11 ng	83640	Phenanthrene-d10	18.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	96
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	58



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033261.D
Acq On : 20 Mar 2018 4:30
Operator : SJ/JU
Sample : J1954-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
031518-JETT-F-D-M

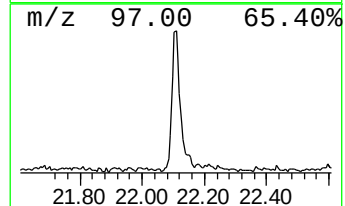
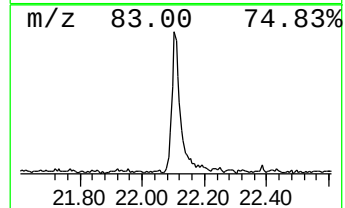
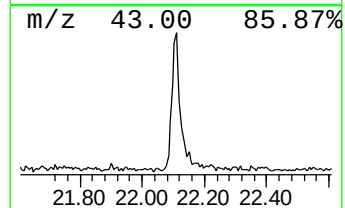
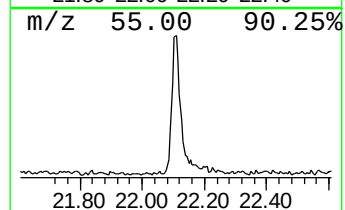
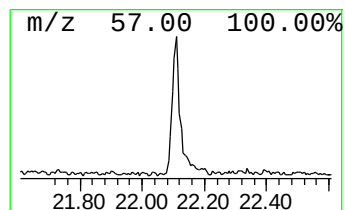
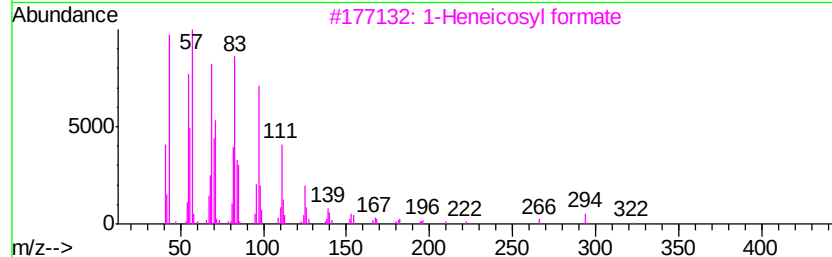
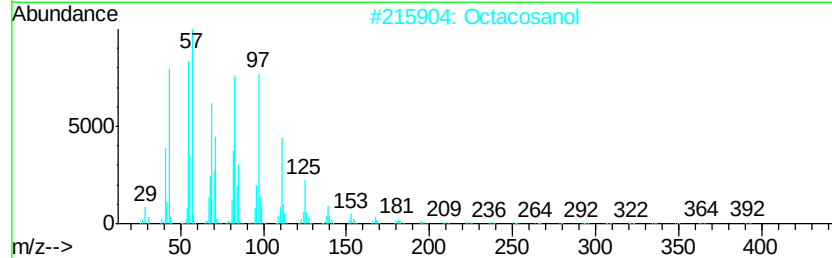
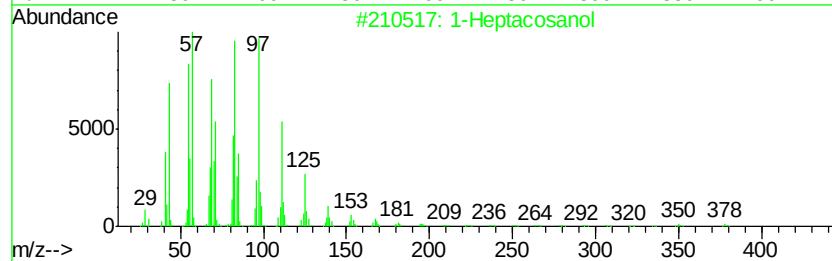
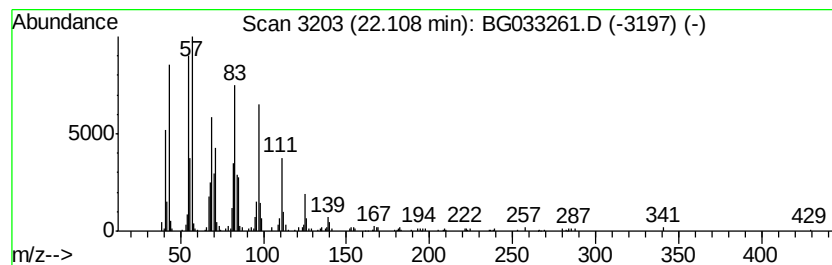
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 9 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	10.05 ng	429672	Chrysene-d12	22.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	94
2		Octacosanol	410	C28H58O	000557-61-9	94
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
5		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94



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Sample : J1954-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
031518-JETT-F-D-M

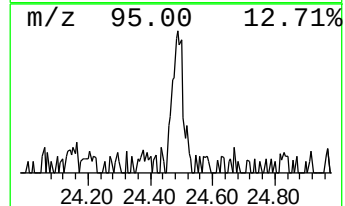
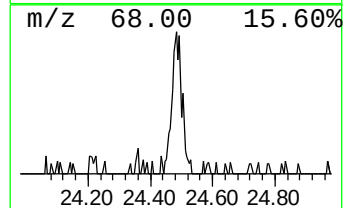
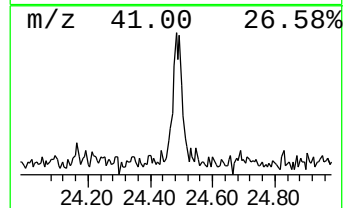
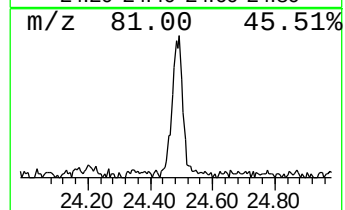
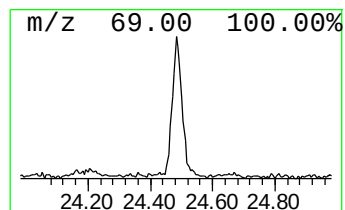
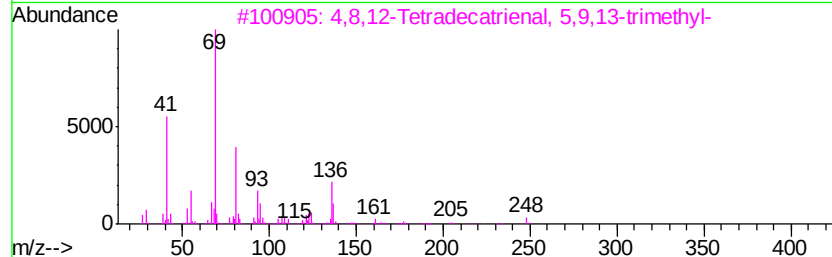
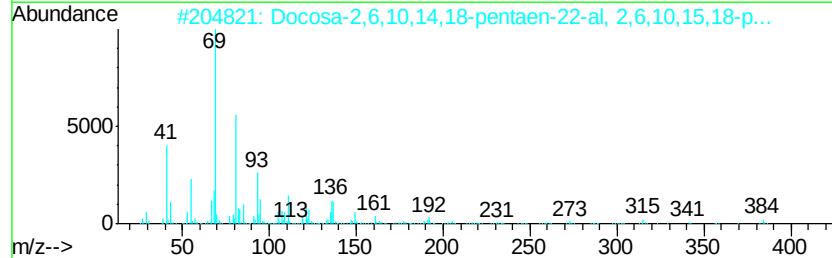
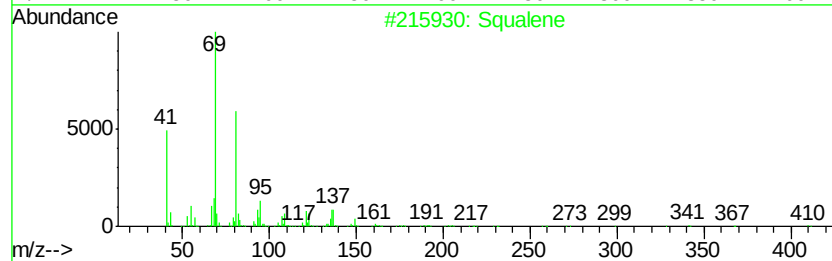
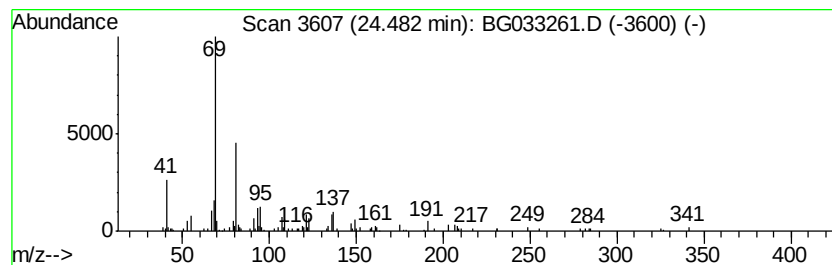
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.48	2.98 ng	127372	Chrysene-d12	22.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	80
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4		3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
031518-JETT-F-D-M

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	14.9	ng	163282	1	8.89	219920	20.0
unknown8.40	8.40	72.3	ng	794499	1	8.89	219920	20.0
Nonadecane	16.27	2.4	ng	66409	3	15.51	543728	20.0
Eicosane	17.13	2.1	ng	85332	4	18.24	792700	20.0
n-Hexadecanoic acid	19.04	7.6	ng	301449	4	18.24	792700	20.0
Octadecanoic acid	20.27	2.1	ng	83640	4	18.24	792700	20.0
1-Heptacosanol	22.11	10.1	ng	429672	5	22.60	855055	20.0
Squalene	24.48	3.0	ng	127372	5	22.60	855055	20.0