

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
 Data File : BG033254.D
 Acq On : 20 Mar 2018 00:06
 Operator : SJ/JU
 Sample : J1953-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 031418-JETT-E-D-B

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-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	3.498	30	36	47	rBV	108864	225924	7.60%	1.543%
2	3.587	47	51	59	rVB	66436	97870	3.29%	0.668%
3	5.802	422	428	439	rVB2	27677	50971	1.71%	0.348%
4	6.313	506	515	523	rBV	126529	264971	8.91%	1.810%
5	6.848	600	606	619	rBV	77730	177853	5.98%	1.215%
6	7.999	796	802	819	rBV3	81594	286995	9.65%	1.960%
7	8.405	863	871	891	rBV	264907	614517	20.67%	4.197%
8	8.892	946	954	966	rBV	97599	234030	7.87%	1.599%
9	9.227	1003	1011	1022	rBV	395646	805397	27.09%	5.501%
10	10.091	1151	1158	1173	rBV	304928	728876	24.51%	4.979%
11	11.777	1436	1445	1462	rBV	149679	340067	11.44%	2.323%
12	14.139	1840	1847	1860	rBV	1050463	1827157	61.45%	12.480%
13	14.932	1972	1982	1997	rVB	63819	121389	4.08%	0.829%
14	15.338	2045	2051	2057	rBV2	42423	63879	2.15%	0.436%
15	15.508	2074	2080	2091	rBV2	309145	539364	18.14%	3.684%
16	16.272	2206	2210	2215	rVB	76059	100025	3.36%	0.683%
17	16.671	2271	2278	2283	rBV5	20622	42184	1.42%	0.288%
18	16.724	2283	2287	2291	rVB	68793	85693	2.88%	0.585%
19	16.983	2324	2331	2344	rBV	652572	1154993	38.84%	7.889%
20	17.130	2351	2356	2365	rVB	66867	126312	4.25%	0.863%
21	17.429	2402	2407	2411	rBV2	21069	32223	1.08%	0.220%
22	17.576	2426	2432	2437	rVB4	15569	34086	1.15%	0.233%
23	17.917	2486	2490	2495	rBV2	42885	57321	1.93%	0.392%
24	18.240	2538	2545	2556	rBV	466118	800724	26.93%	5.469%
25	18.328	2557	2560	2568	rVB7	15238	30897	1.04%	0.211%
26	18.916	2653	2660	2664	rBV5	43433	68587	2.31%	0.468%
27	19.039	2675	2681	2691	rBV	231918	364731	12.27%	2.491%
28	20.155	2865	2871	2876	rBV9	27561	56265	1.89%	0.384%
29	20.267	2886	2890	2894	rBV2	39888	52307	1.76%	0.357%
30	20.761	2967	2974	2984	rBV	2160118	2973385	100.00%	20.310%
31	22.106	3197	3203	3217	rBV2	149674	285100	9.59%	1.947%
32	22.594	3278	3286	3302	rVB	470280	900147	30.27%	6.148%
33	24.486	3600	3608	3617	rBV	115007	251703	8.47%	1.719%
34	26.389	3921	3932	3947	rBV3	245432	844323	28.40%	5.767%

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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

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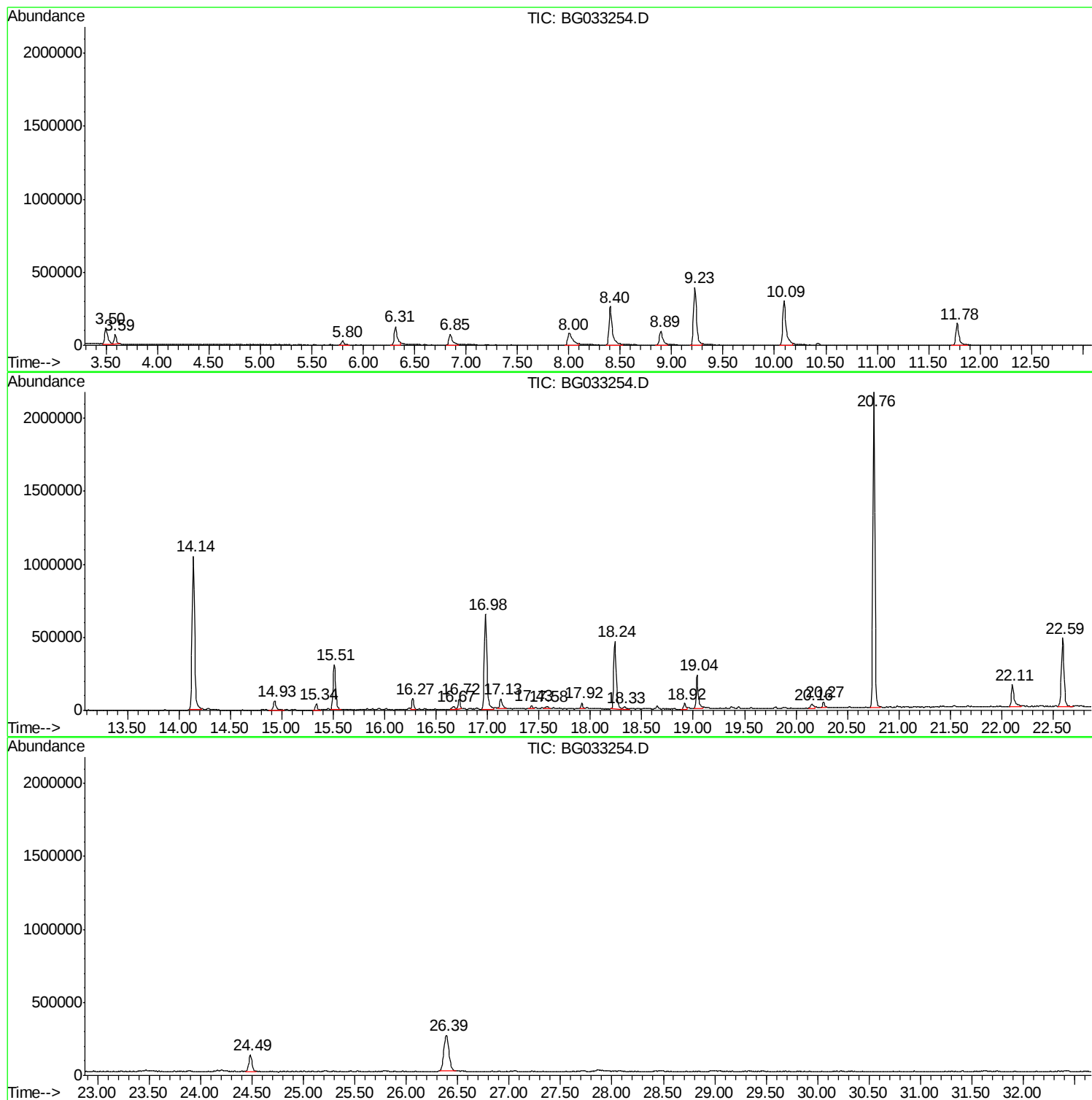
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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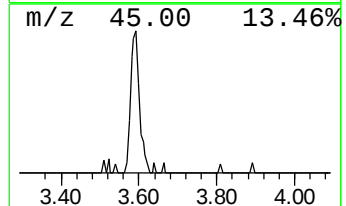
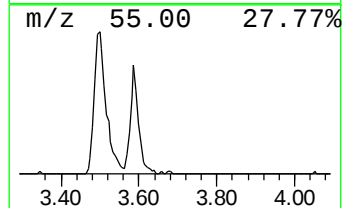
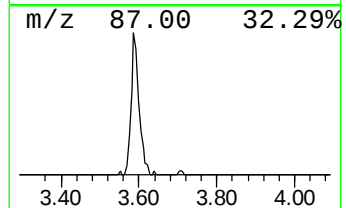
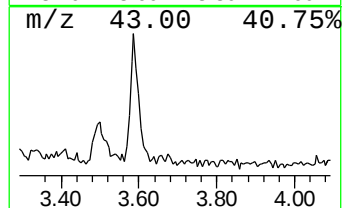
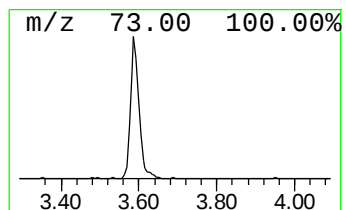
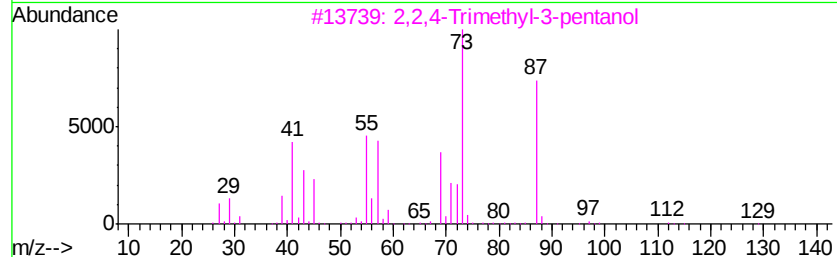
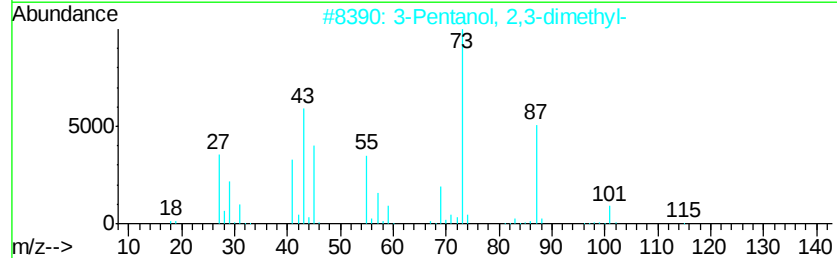
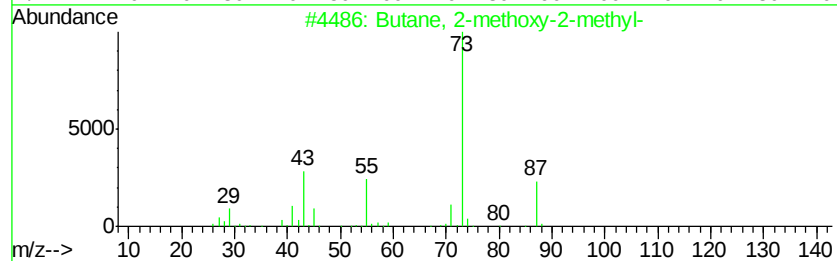
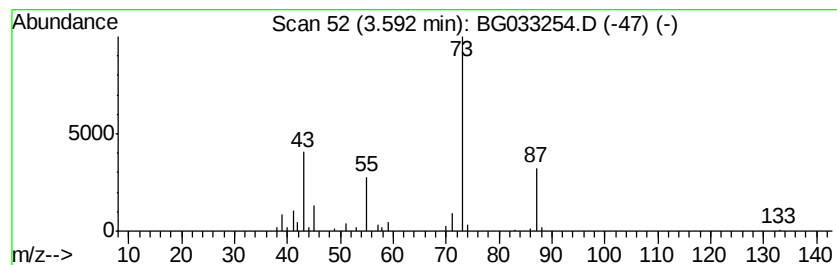
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	8.36 ng	97870	1,4-Dichlorobenzene-d4	8.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	42
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32



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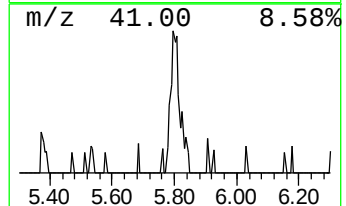
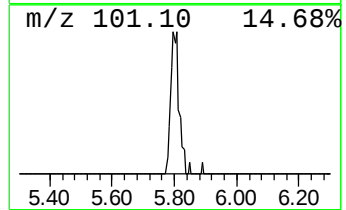
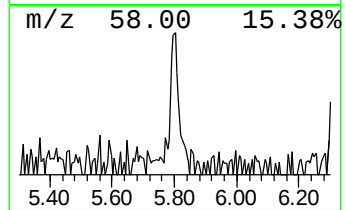
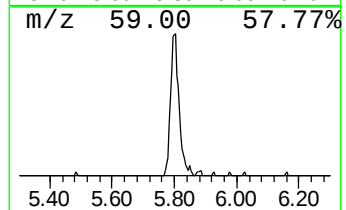
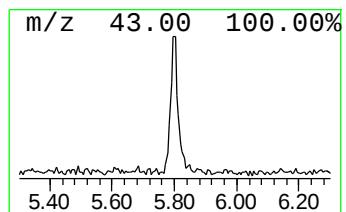
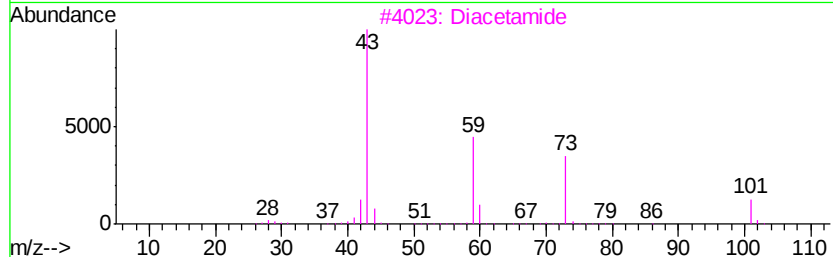
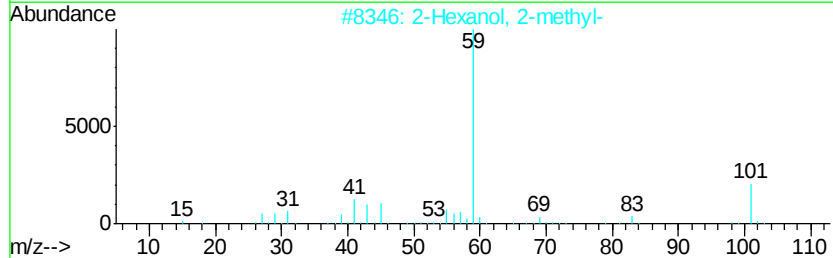
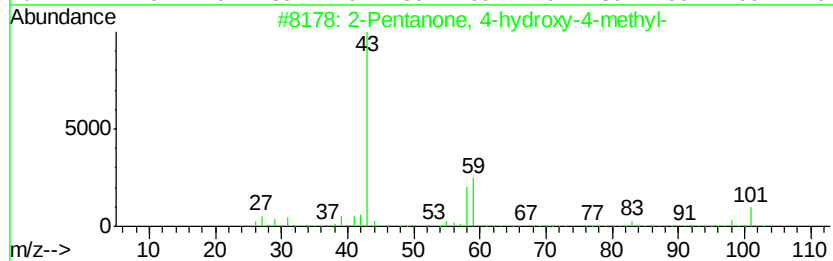
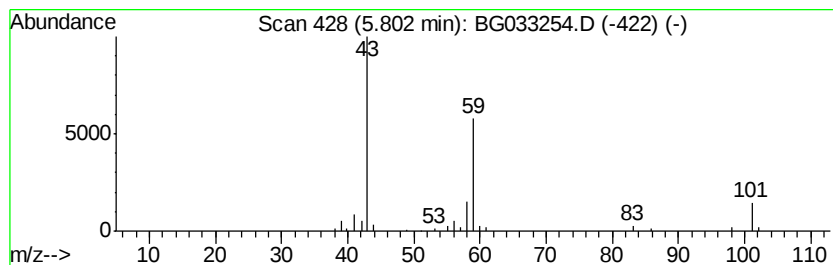
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.80	4.36 ng	50971	1,4-Dichlorobenzene-d4	8.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3		Diacetamide	101	C4H7NO2	000625-77-4	38
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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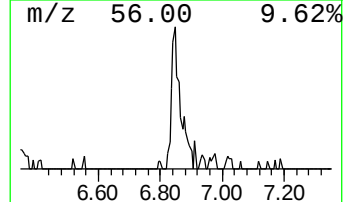
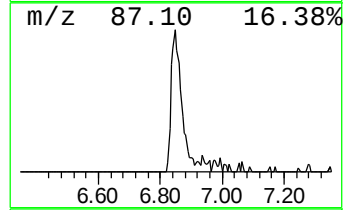
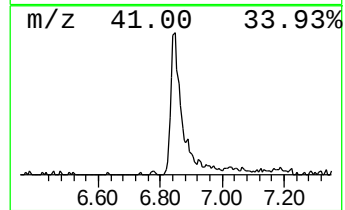
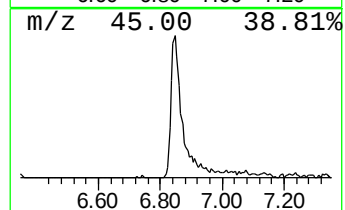
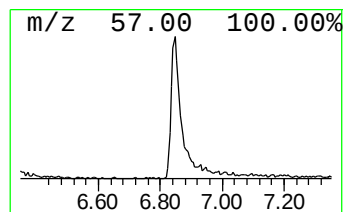
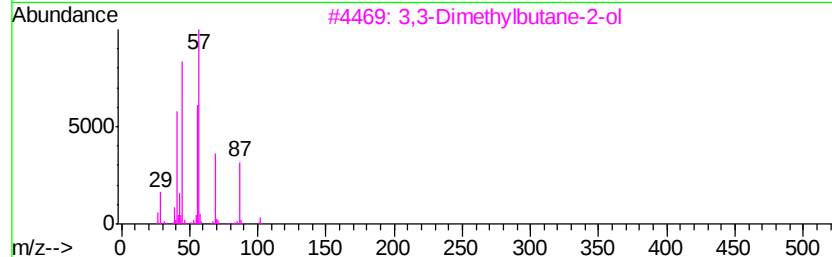
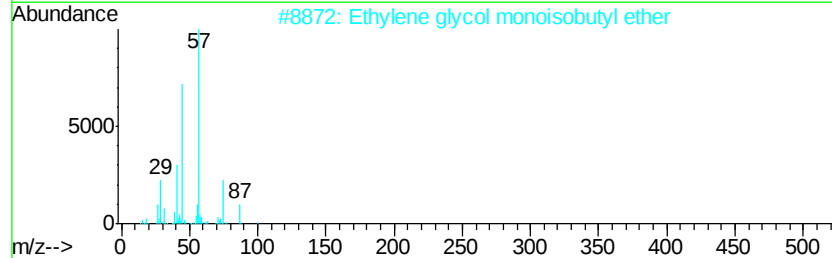
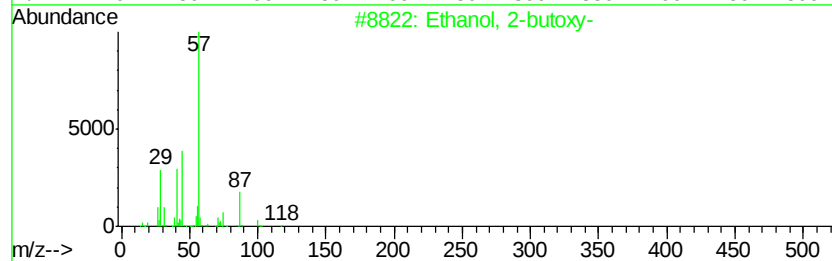
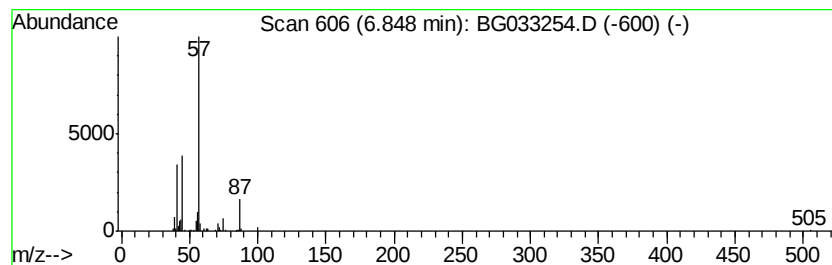
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Peak Number 4 Ethanol, 2-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.85	15.20 ng	177853	1,4-Dichlorobenzene-d4	8.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	28
4		Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	22
5		1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	17



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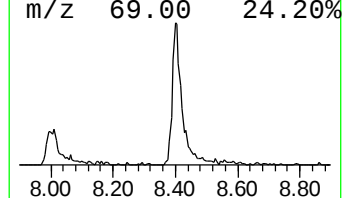
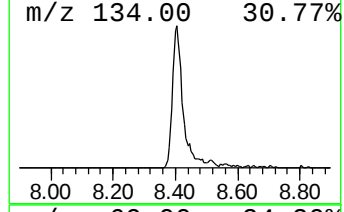
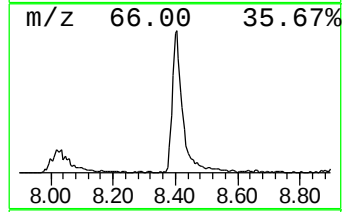
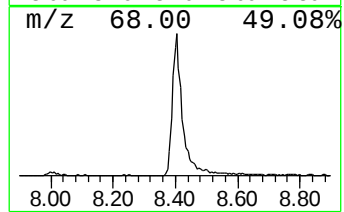
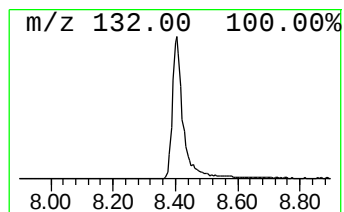
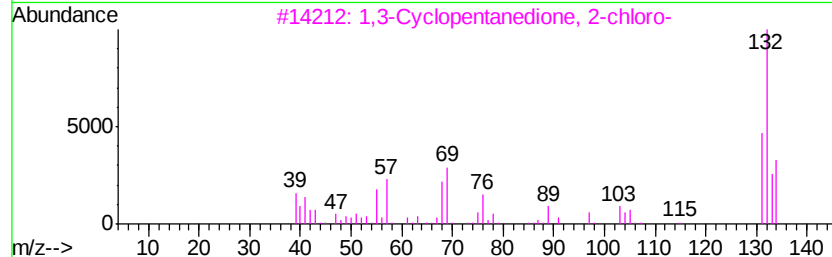
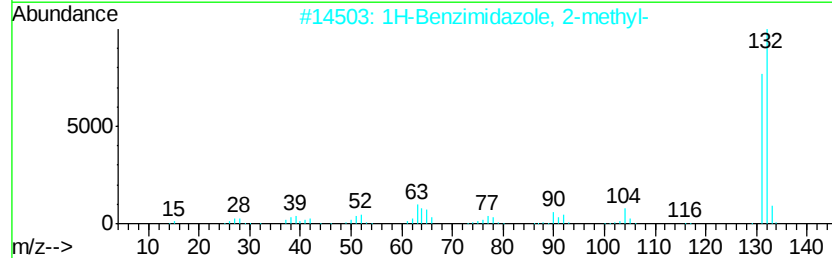
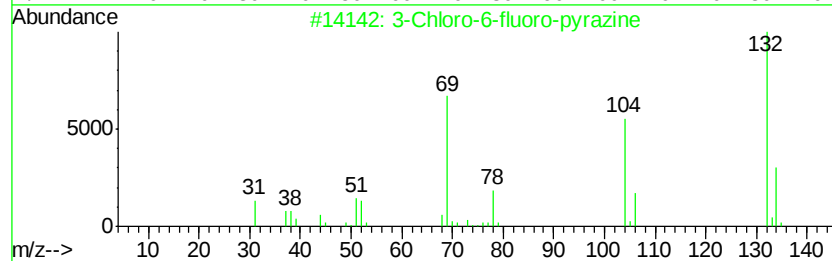
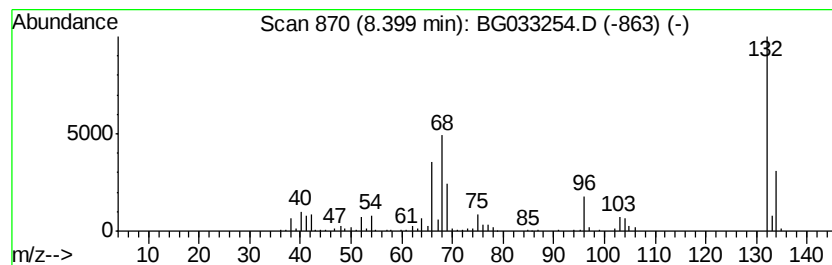
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Peak Number 5 unknown8.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	52.52 ng	614517	1,4-Dichlorobenzene-d4	8.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	22
3	1,3-Cyclopentanedione, 2-chloro-			132	C5H5ClO2	014203-19-1	13
4	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	12
5	2-Cyclohexen-1-one			96	C6H8O	000930-68-7	10



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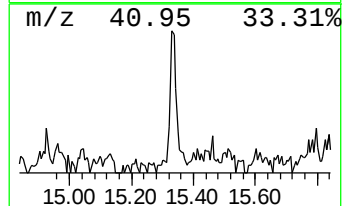
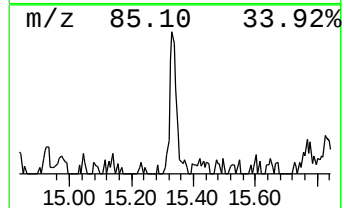
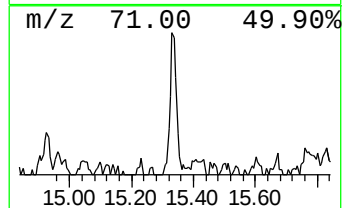
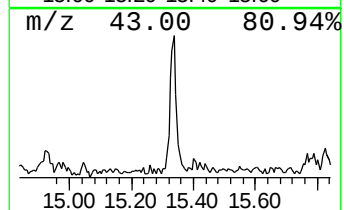
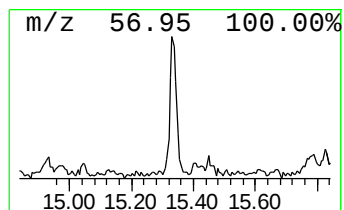
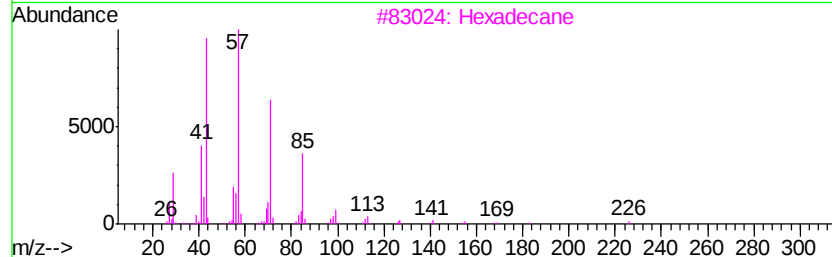
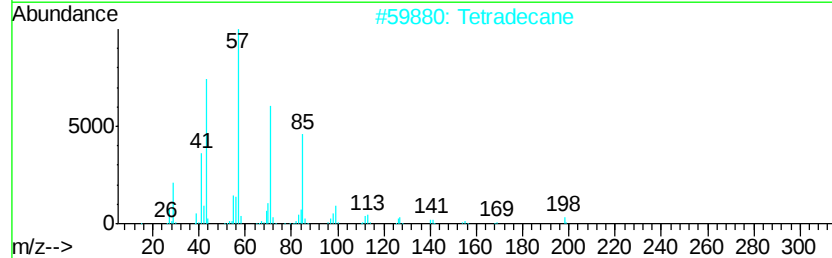
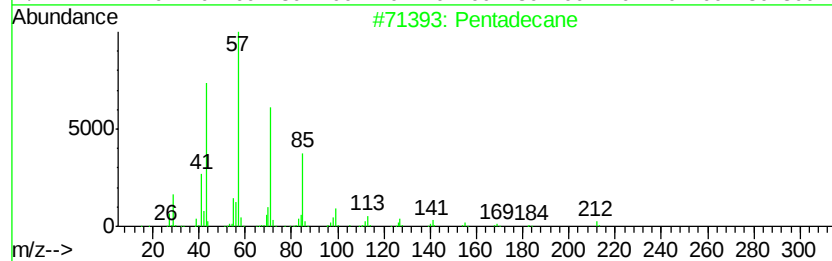
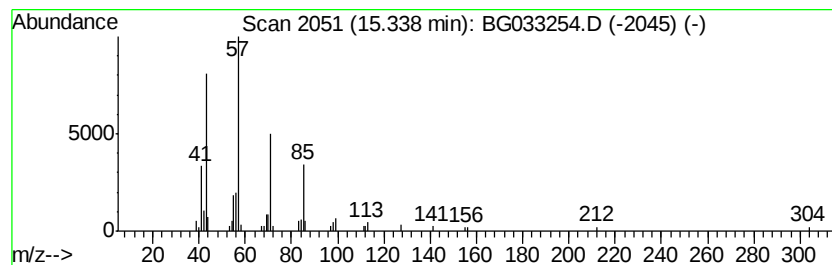
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Peak Number 7 Pentadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	2.37 ng	63879	Acenaphthene-d10	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	93
2		Tetradecane	198	C14H30	000629-59-4	80
3		Hexadecane	226	C16H34	000544-76-3	80
4		Tridecane	184	C13H28	000629-50-5	80
5		Dodecane	170	C12H26	000112-40-3	80



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
031418-JETT-E-D-B

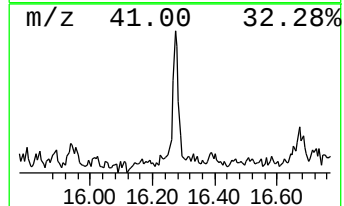
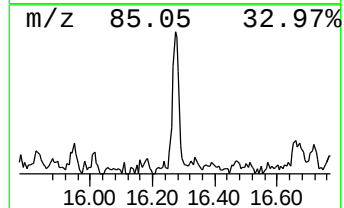
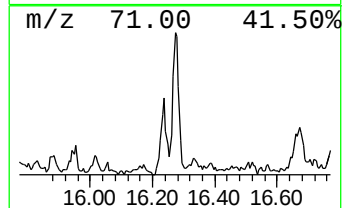
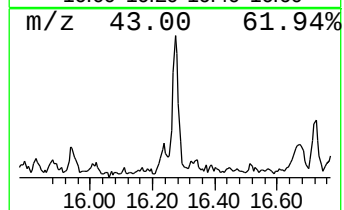
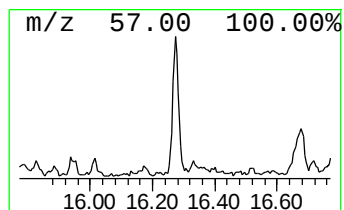
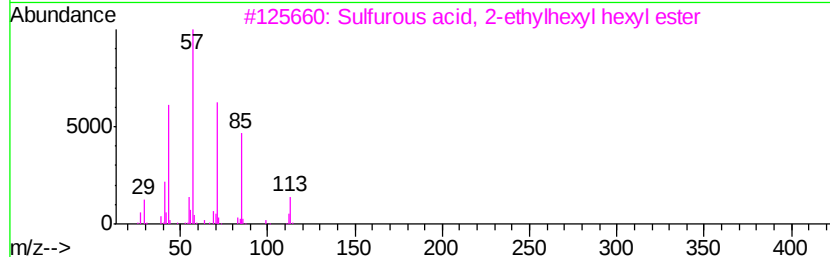
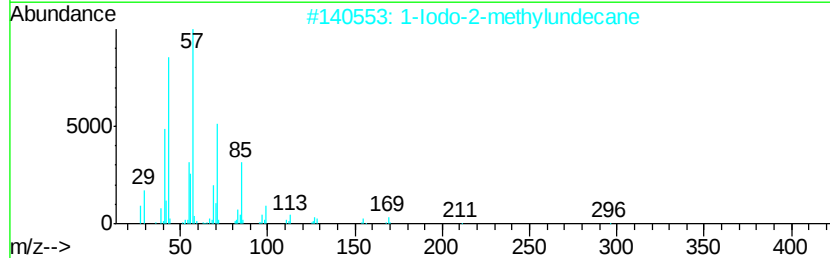
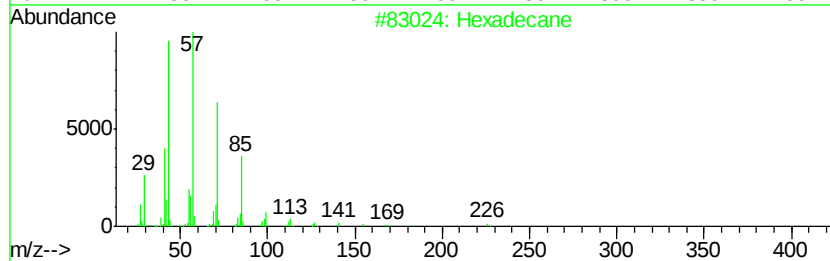
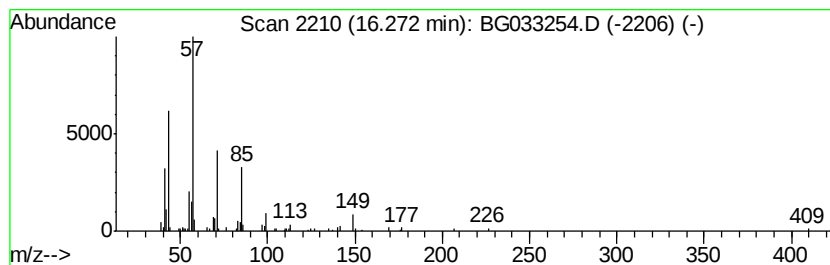
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	3.71 ng	100025	Acenaphthene-d10	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	81
2	1-Iodo-2-methylundecane		296	C12H25I	073105-67-6	72
3	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	64
4	Tetradecane		198	C14H30	000629-59-4	64
5	Eicosane		282	C20H42	000112-95-8	64



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033254.D
Acq On : 20 Mar 2018 00:06
Operator : SJ/JU
Sample : J1953-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
031418-JETT-E-D-B

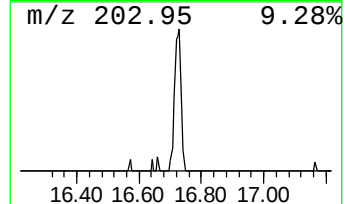
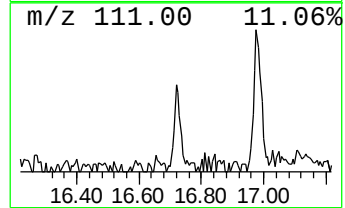
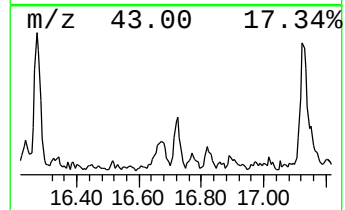
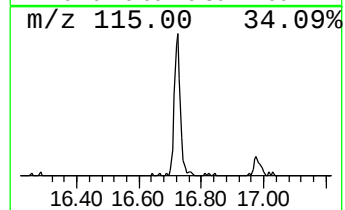
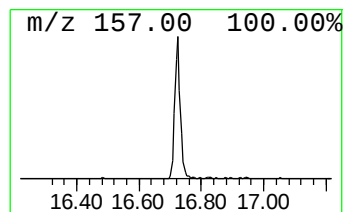
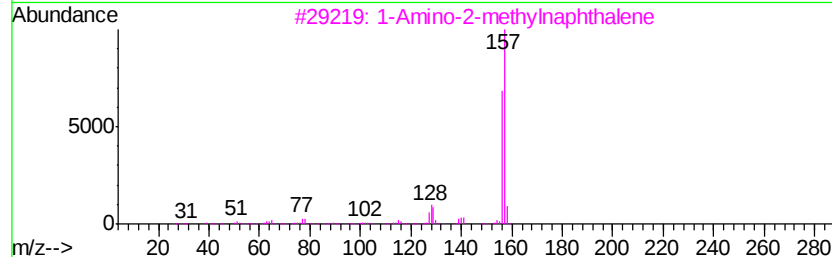
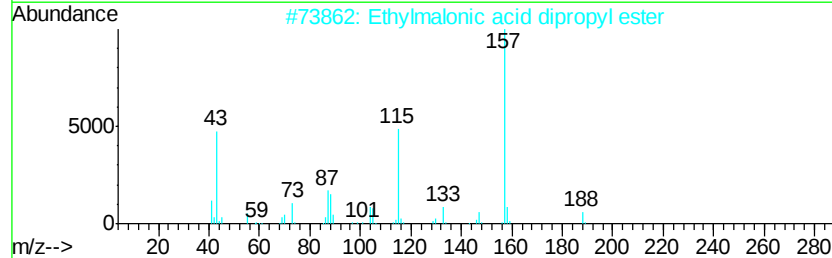
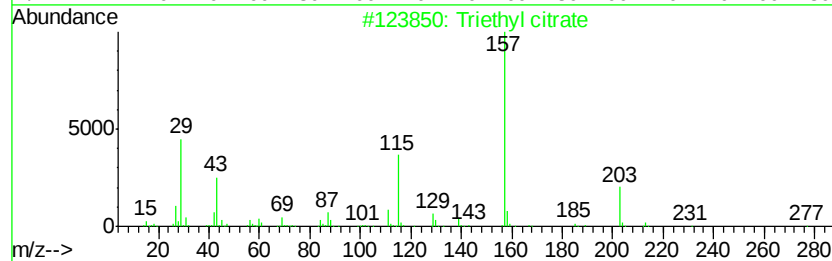
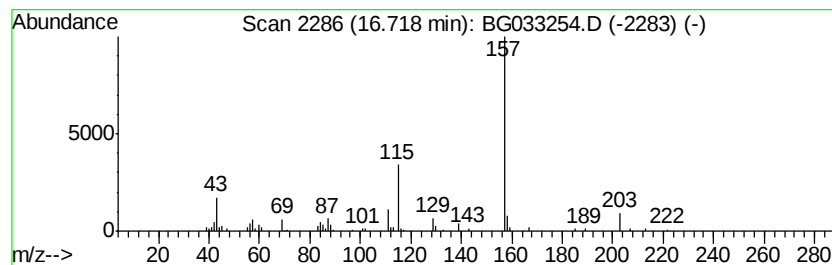
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triethyl citrate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	3.18 ng	85693	Acenaphthene-d10	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triethyl citrate	276	C12H20O7	000077-93-0	86
2		Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3		1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	53
4		3-Chloro2-fluorobenzoic acid, 3-...	342	C19H28ClF02	1000338-63-8	38
5		3-Chloro2-fluorobenzoic acid, 4-...	356	C20H30ClF02	1000338-64-4	38



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033254.D
Acq On : 20 Mar 2018 00:06
Operator : SJ/JU
Sample : J1953-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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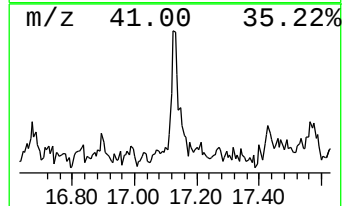
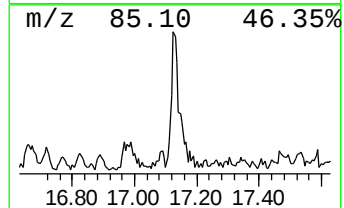
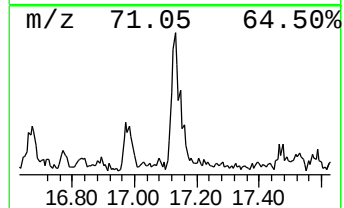
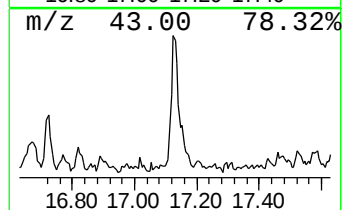
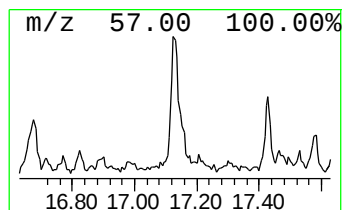
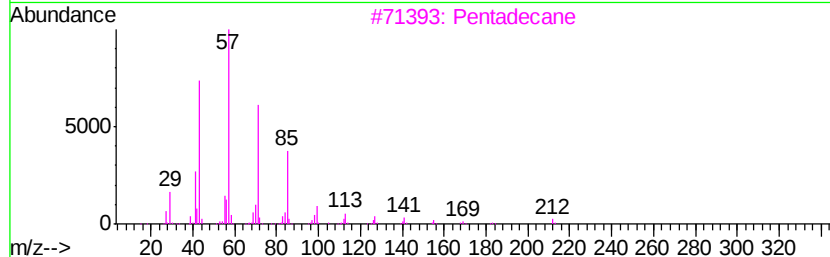
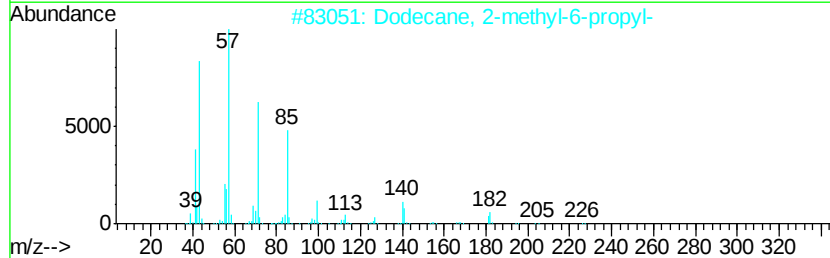
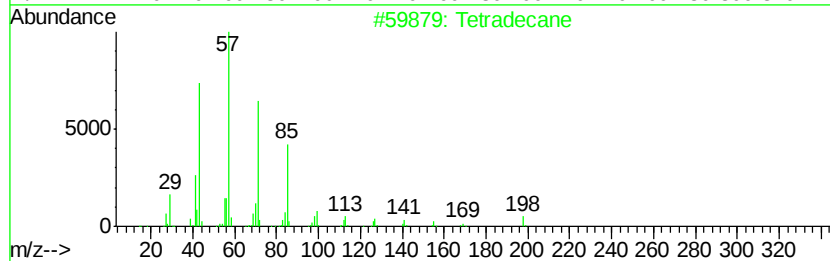
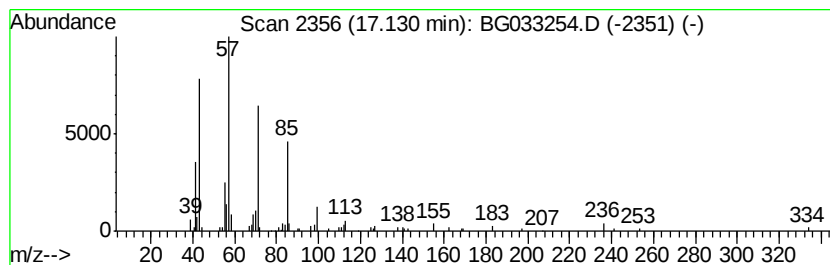
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetradecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	3.15 ng	126312	Phenanthrene-d10	18.24

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	86
2			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72
3			Pentadecane	212	C15H32	000629-62-9	72
4			Hexadecane	226	C16H34	000544-76-3	53
5			Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	53



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033254.D
Acq On : 20 Mar 2018 00:06
Operator : SJ/JU
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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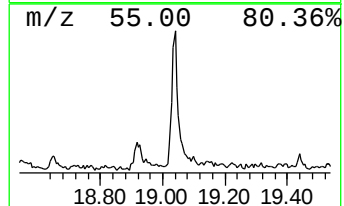
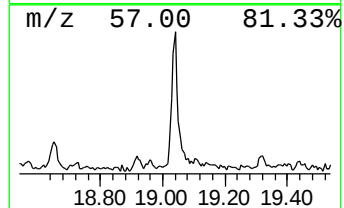
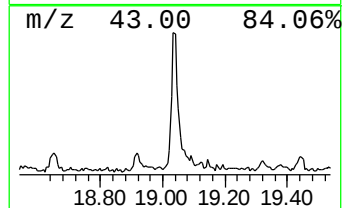
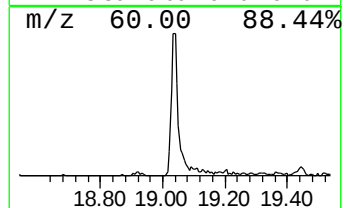
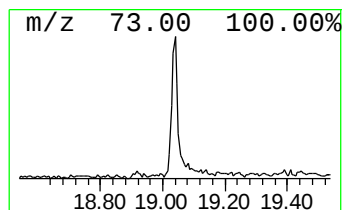
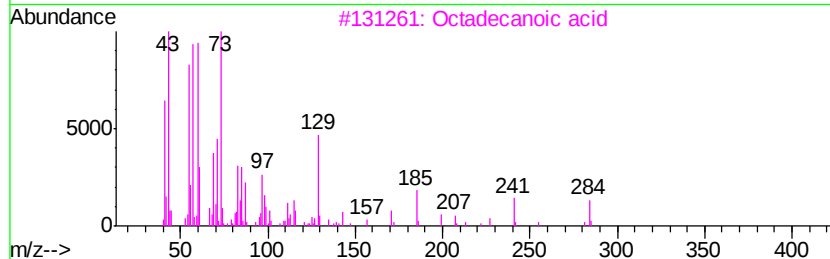
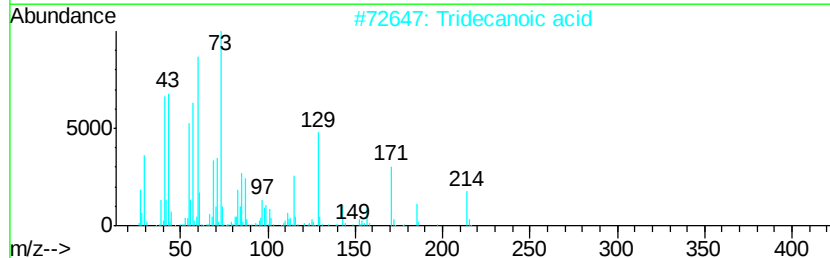
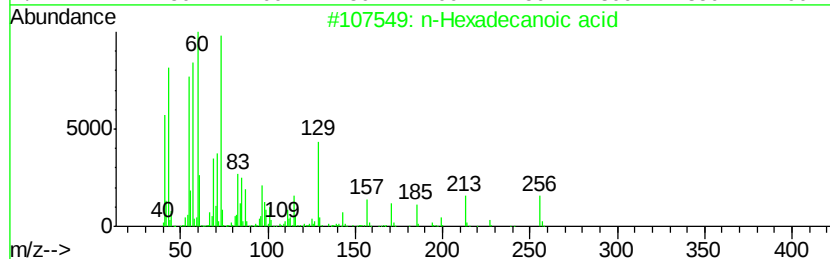
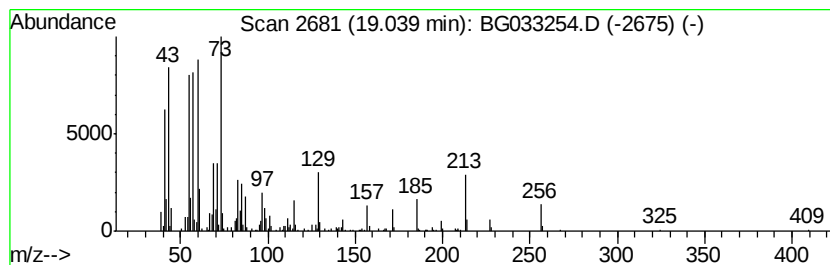
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	9.11 ng	364731	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	96
3		Octadecanoic acid	284	C18H36O2	000057-11-4	81
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
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Acq On : 20 Mar 2018 00:06
Operator : SJ/JU
Sample : J1953-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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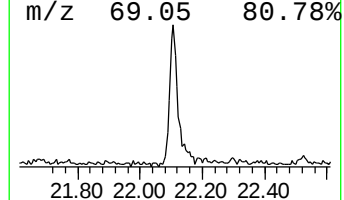
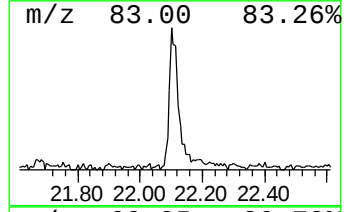
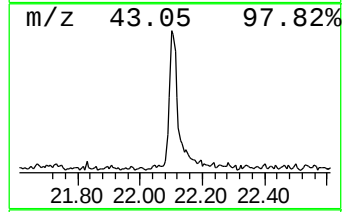
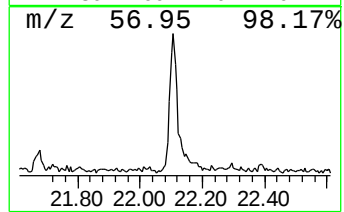
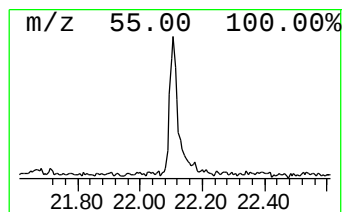
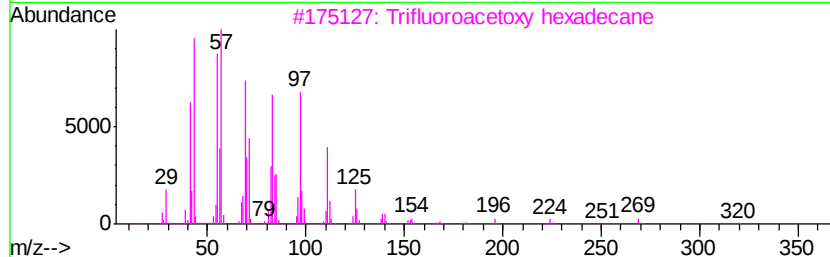
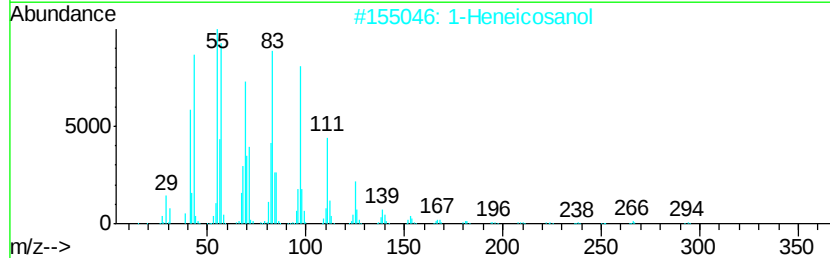
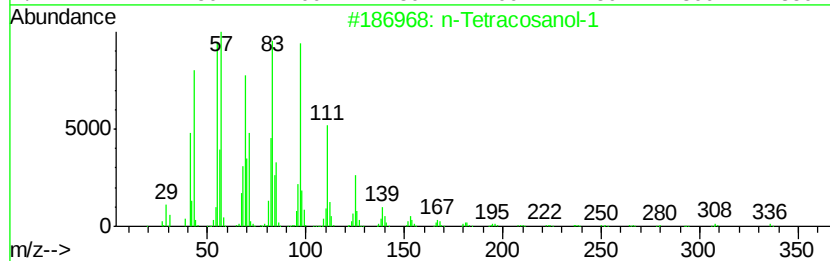
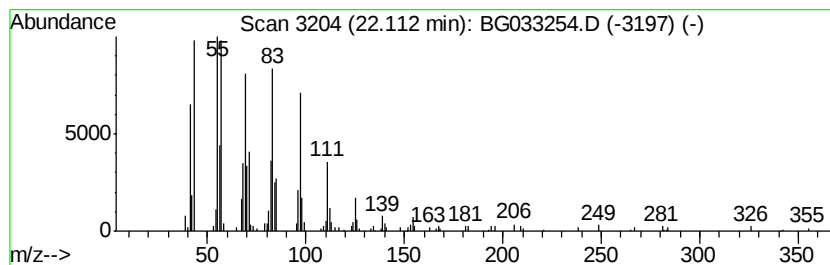
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	6.33 ng	285100	Chrysene-d12	22.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
5		1-Octadecanol	270	C18H38O	000112-92-5	87



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
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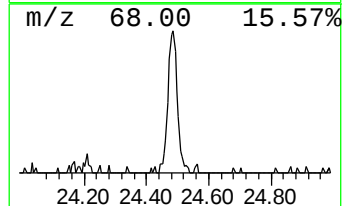
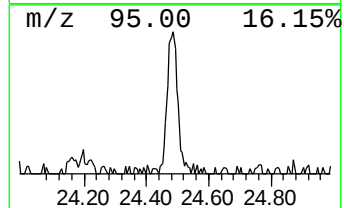
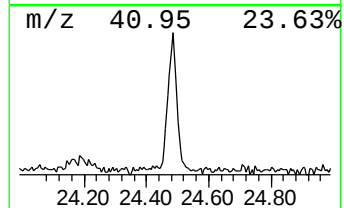
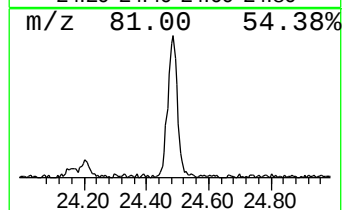
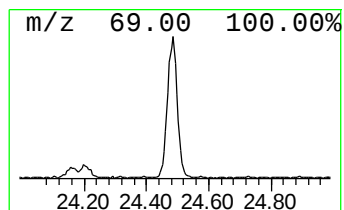
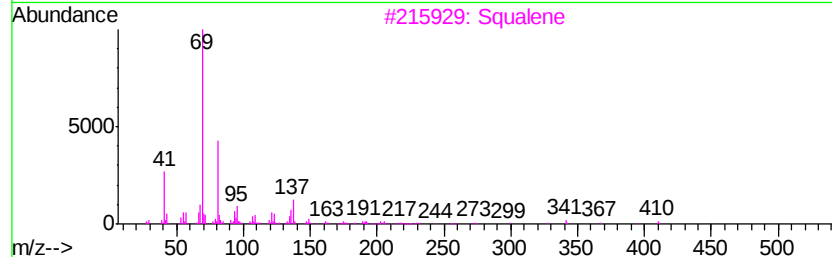
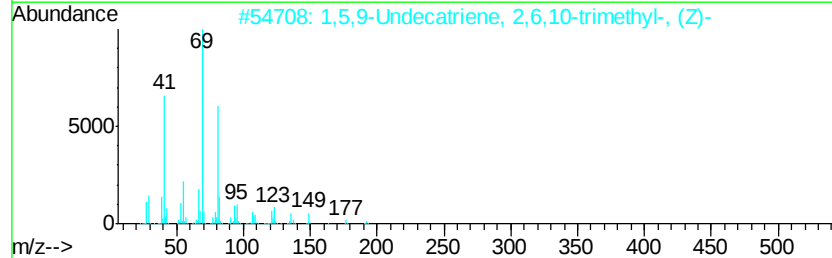
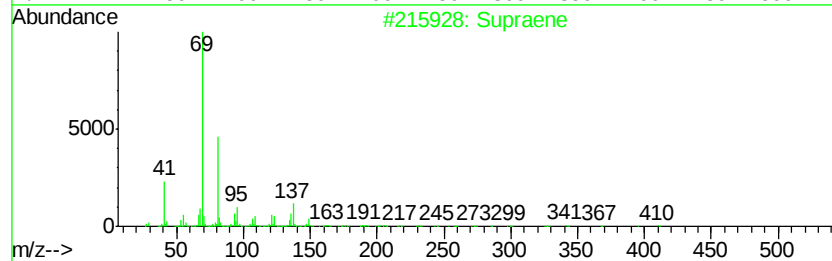
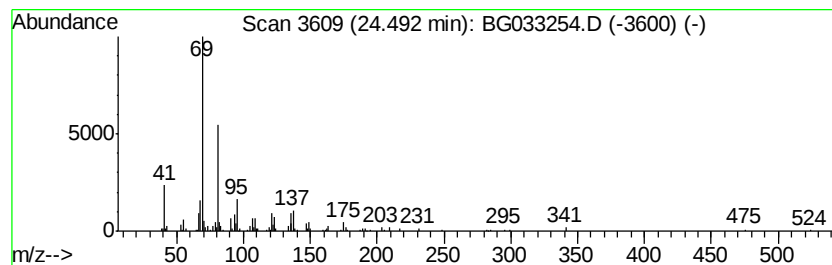
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.49	5.59 ng	251703	Chrysene-d12	22.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
3			Squalene	410	C30H50	000111-02-4	86
4			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
5			3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	59



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG031918\
 Data File : BG033254.D
 Acq On : 20 Mar 2018 00:06
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 Sample : J1953-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.59	8.4	ng	97870	1	8.89	234030	20.0
2-Pentanone, 4-hy...	5.80	4.4	ng	50971	1	8.89	234030	20.0
Ethanol, 2-butoxy-	6.85	15.2	ng	177853	1	8.89	234030	20.0
unknown8.40	8.40	52.5	ng	614517	1	8.89	234030	20.0
Pentadecane	15.34	2.4	ng	63879	3	15.51	539364	20.0
Hexadecane	16.27	3.7	ng	100025	3	15.51	539364	20.0
Triethyl citrate	16.72	3.2	ng	85693	3	15.51	539364	20.0
Tetradecane	17.13	3.1	ng	126312	4	18.24	800724	20.0
n-Hexadecanoic acid	19.04	9.1	ng	364731	4	18.24	800724	20.0
n-Tetracosanol-1	22.11	6.3	ng	285100	5	22.59	900147	20.0
Supraene	24.49	5.6	ng	251703	5	22.59	900147	20.0