

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062618\
 Data File : BG035442.D
 Acq On : 27 Jun 2018 12:23
 Operator : JU/SJ
 Sample : J3570-12
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20180375-COMPOSITE-CS-1A-ELU

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.168	313	320	326	rBV2	24693	43124	1.16%	0.220%
2	5.626	391	398	409	rBV	437847	698087	18.83%	3.565%
3	7.212	660	668	678	rBV	358376	667900	18.02%	3.411%
4	7.582	723	731	742	rBV	719578	1255267	33.86%	6.411%
5	8.052	804	811	817	rBV	169578	296336	7.99%	1.513%
6	8.376	857	866	875	rBV	617973	1067596	28.80%	5.452%
7	9.210	1001	1008	1018	rVB	543603	969170	26.14%	4.950%
8	10.855	1281	1288	1296	rBV	235399	402734	10.86%	2.057%
9	13.298	1696	1704	1712	rBV	1503705	2379192	64.17%	12.151%
10	14.121	1836	1844	1853	rBV	330699	504868	13.62%	2.578%
11	14.673	1929	1938	1945	rVB2	398199	645953	17.42%	3.299%
12	15.507	2077	2080	2086	rVB2	31698	45818	1.24%	0.234%
13	15.959	2152	2157	2161	rVB	148350	185544	5.00%	0.948%
14	16.024	2162	2168	2173	rBV	96832	133892	3.61%	0.684%
15	16.159	2183	2191	2200	rBV	1268477	1981611	53.45%	10.121%
16	16.371	2223	2227	2230	rBV2	36213	51429	1.39%	0.263%
17	16.553	2251	2258	2262	rVV9	19579	39007	1.05%	0.199%
18	16.805	2298	2301	2308	rVB7	23213	47218	1.27%	0.241%
19	17.164	2357	2362	2366	rBV6	26801	40096	1.08%	0.205%
20	17.211	2366	2370	2375	rVB8	21145	37439	1.01%	0.191%
21	17.416	2396	2405	2413	rBV2	550919	887338	23.93%	4.532%
22	17.686	2447	2451	2456	rBV	40908	53682	1.45%	0.274%
23	18.109	2520	2523	2529	rBV7	18508	41084	1.11%	0.210%
24	18.297	2550	2555	2564	rBV	353713	525263	14.17%	2.683%
25	19.566	2767	2771	2776	rBV2	153140	207276	5.59%	1.059%
26	19.836	2813	2817	2824	rVB2	32021	52884	1.43%	0.270%
27	20.024	2842	2849	2857	rBV	2706251	3707406	100.00%	18.935%
28	21.323	3066	3070	3084	rVB2	150513	293011	7.90%	1.496%
29	21.681	3124	3131	3139	rBV	600882	973833	26.27%	4.974%
30	22.527	3273	3275	3282	rVB8	27094	38711	1.04%	0.198%
31	23.361	3411	3417	3426	rVB	133496	256529	6.92%	1.310%
32	23.966	3516	3520	3528	rBV	16794	39204	1.06%	0.200%
33	24.894	3668	3678	3693	rVB2	322252	966279	26.06%	4.935%
34	26.046	3868	3874	3882	rVB2	15496	45367	1.22%	0.232%

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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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

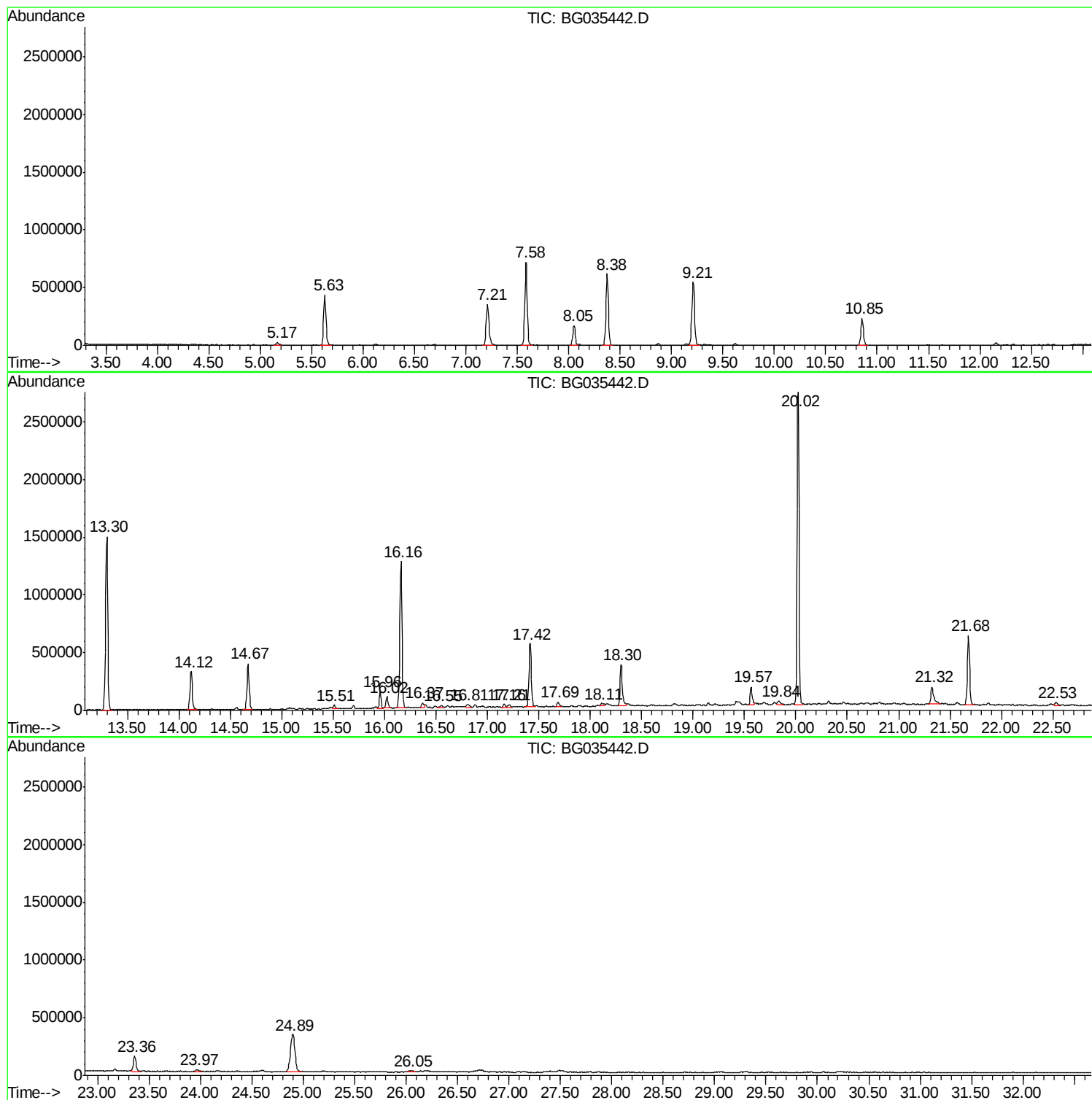
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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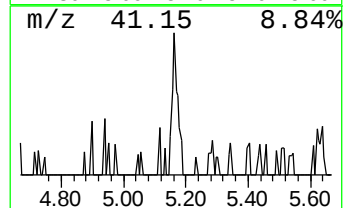
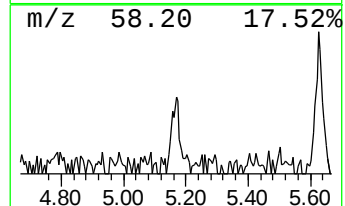
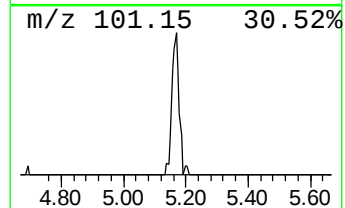
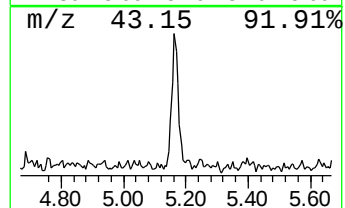
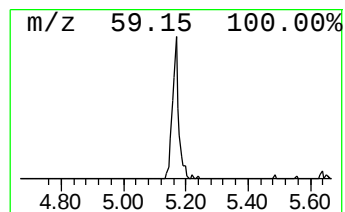
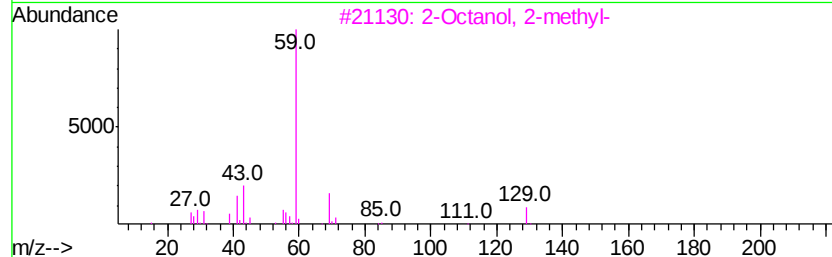
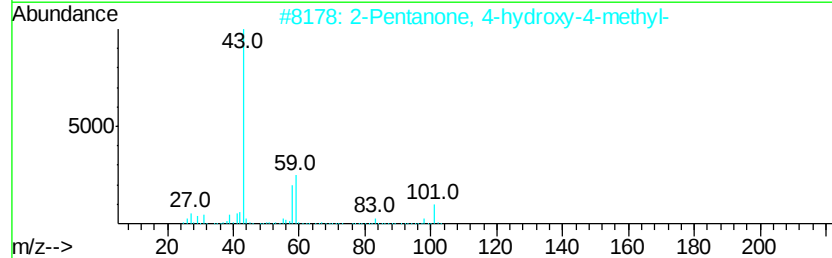
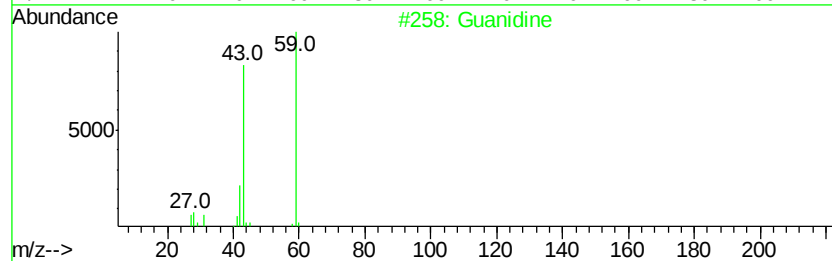
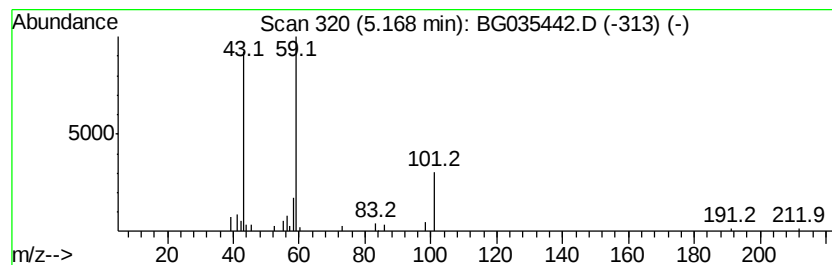
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	2.91 ng	43124	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Guanidine	59	CH5N3	000113-00-8	40
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32
3		2-Octanol, 2-methyl-	144	C9H20O	000628-44-4	32
4		Pentanamide	101	C5H11NO	000626-97-1	25
5		Hexanamide	115	C6H13NO	000628-02-4	25



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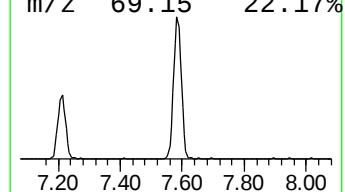
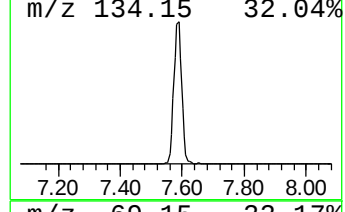
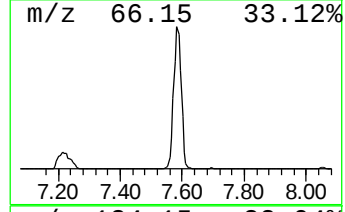
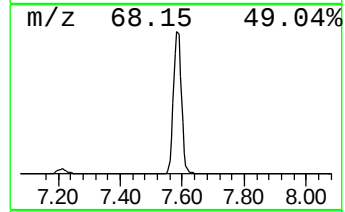
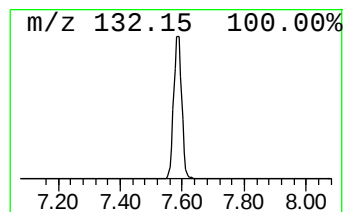
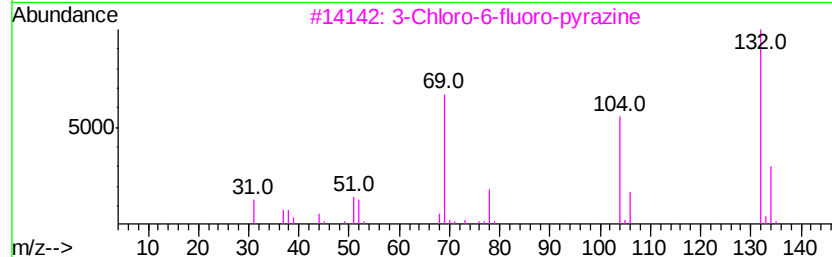
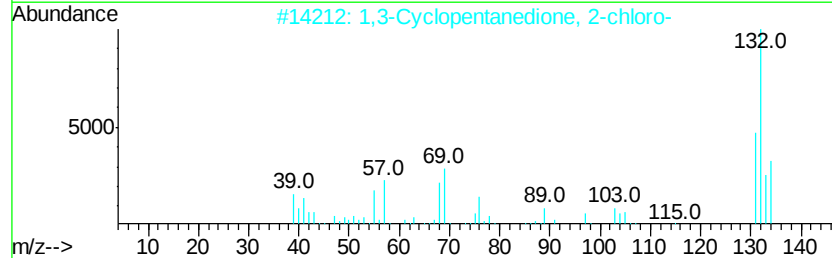
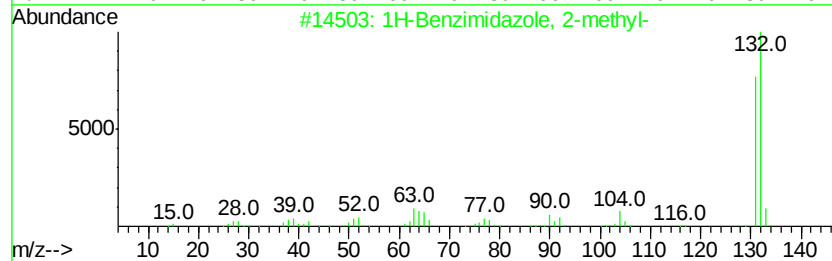
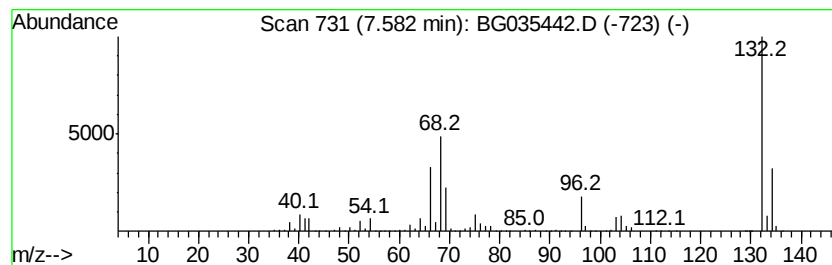
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Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	84.72 ng	1255270	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		1H-Indazole, 3-methyl-	132	C8H8N2	1000316-00-2	12



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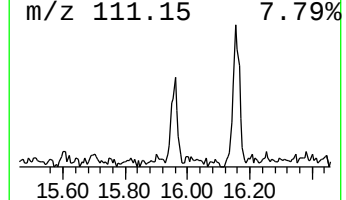
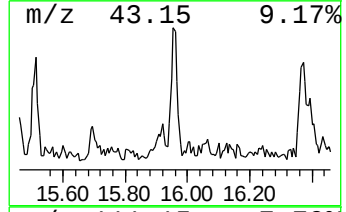
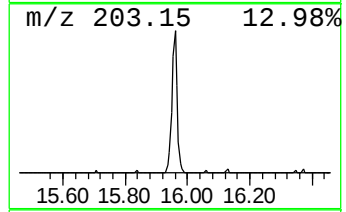
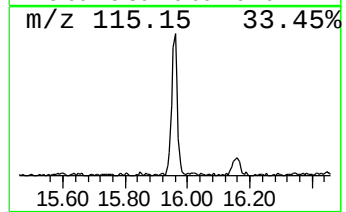
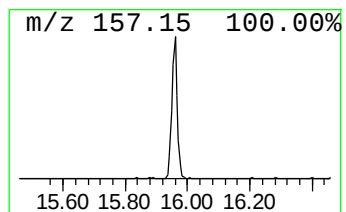
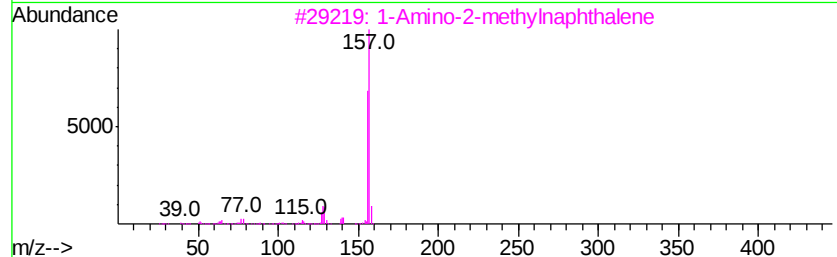
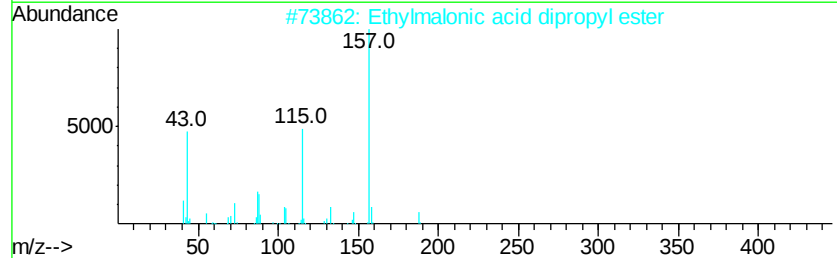
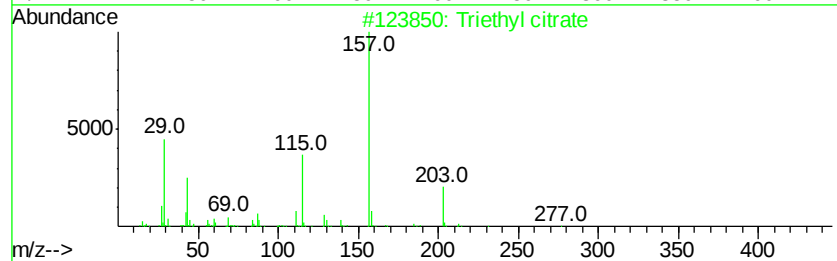
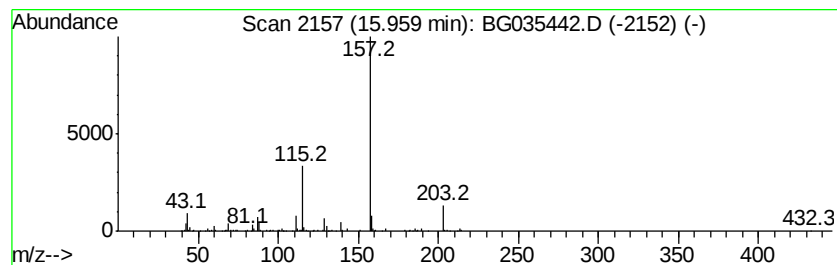
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 Triethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	5.74 ng	185544	Acenaphthene-d10	14.67

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	50
3		1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	40
4		Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	40
5		Adipic acid, ethyl pent-4-en-2-y...	242	C13H22O4	1000354-11-7	40



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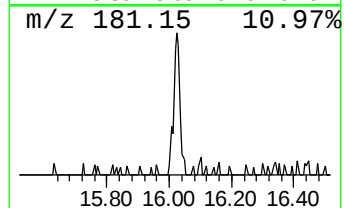
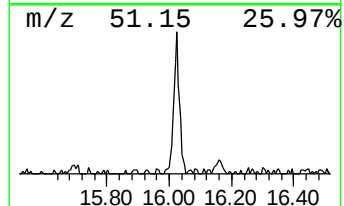
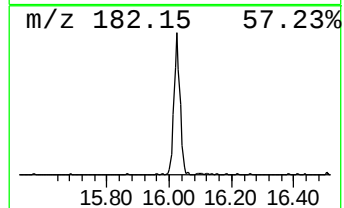
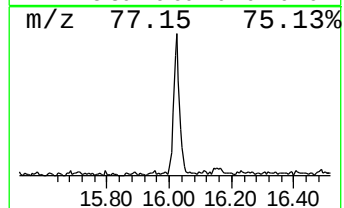
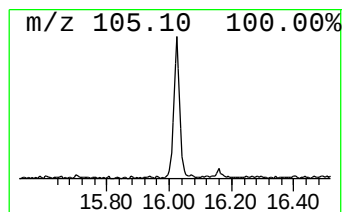
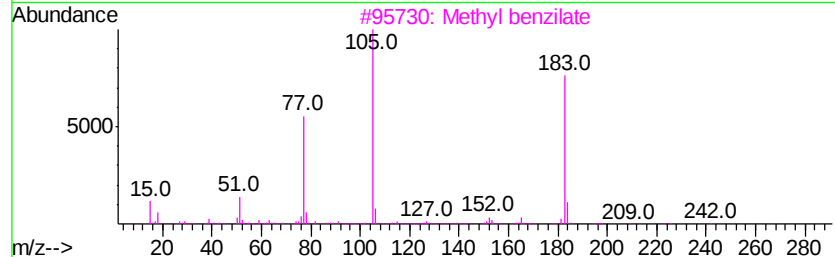
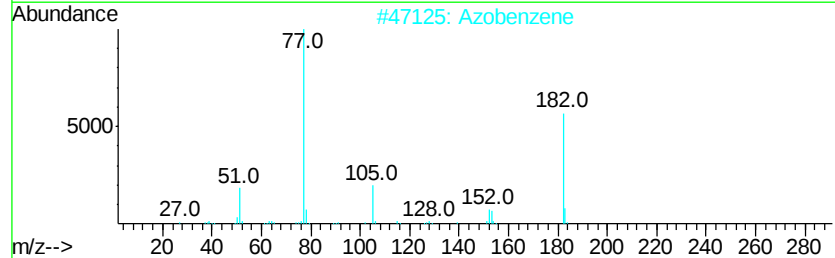
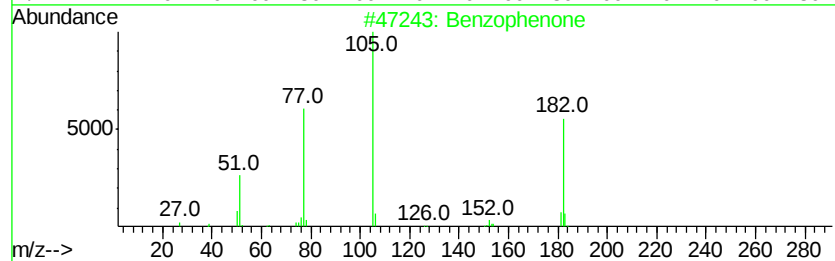
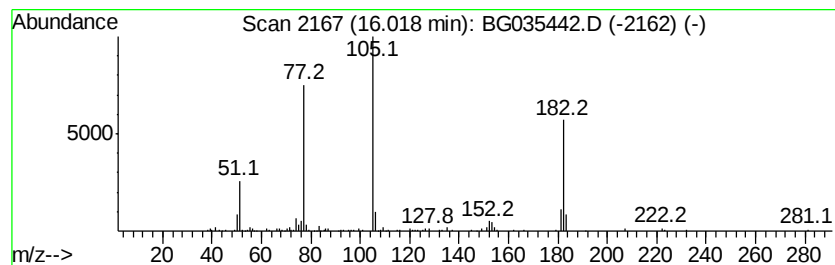
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	4.15 ng	133892	Acenaphthene-d10	14.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	97
2		Azobenzene	182	C12H10N2	000103-33-3	58
3		Methyl benzilate	242	C15H14O3	000076-89-1	47
4		Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	38
5		Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	38



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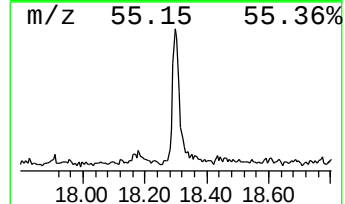
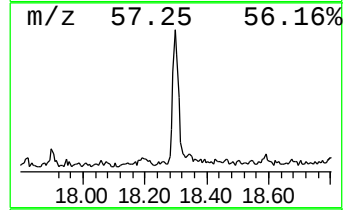
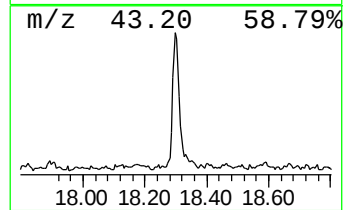
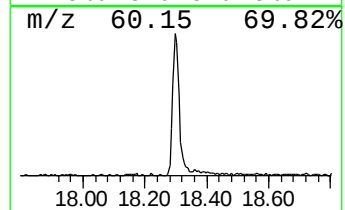
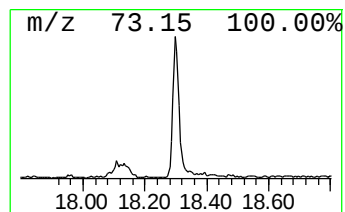
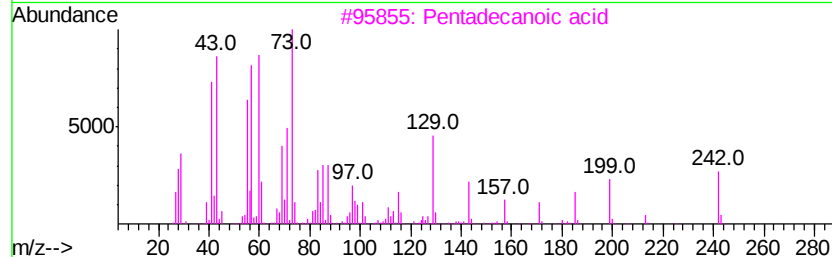
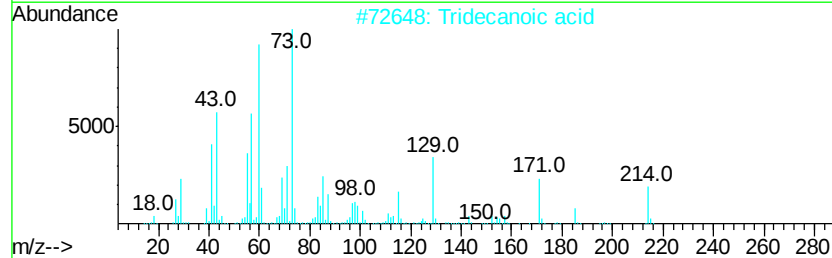
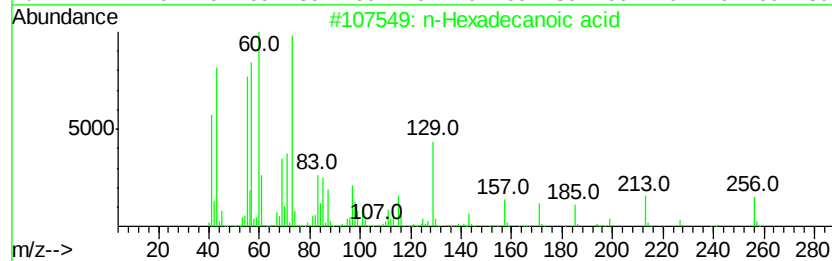
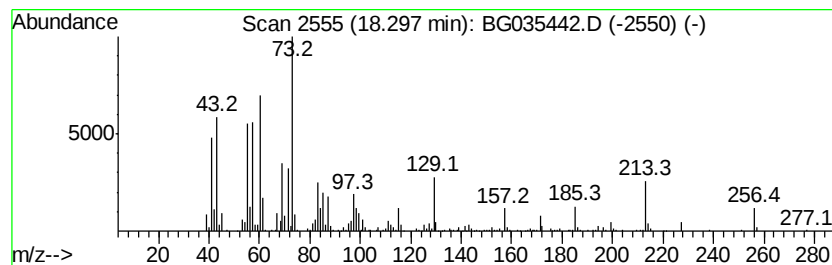
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	11.84 ng	525263	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Silane, decyldiethylmethyl-	242	C15H34Si	1000152-02-0	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062618\
Data File : BG035442.D
Acq On : 27 Jun 2018 12:23
Operator : JU/SJ
Sample : J3570-12
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20180375-COMPOSITE-CS-1A-ELU

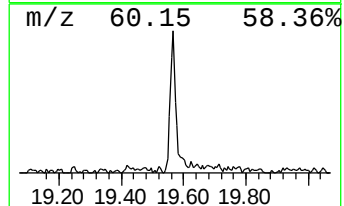
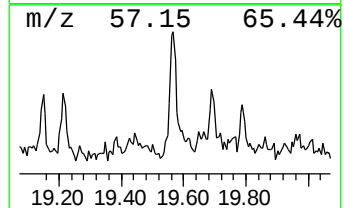
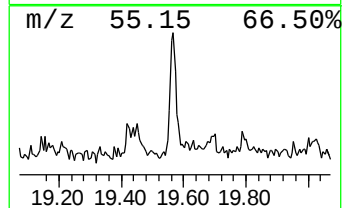
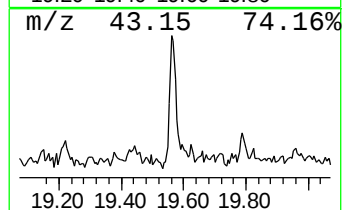
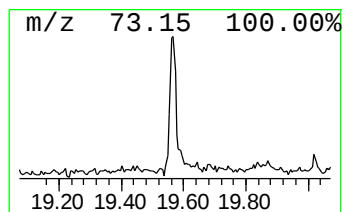
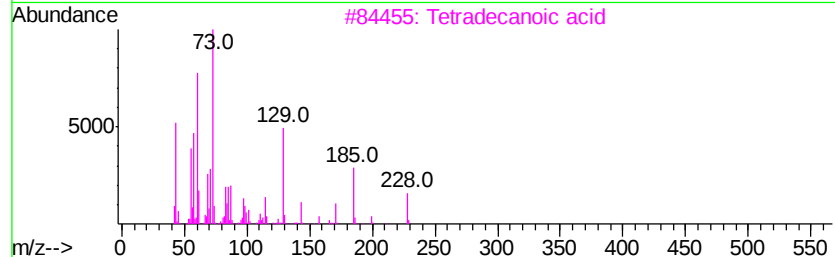
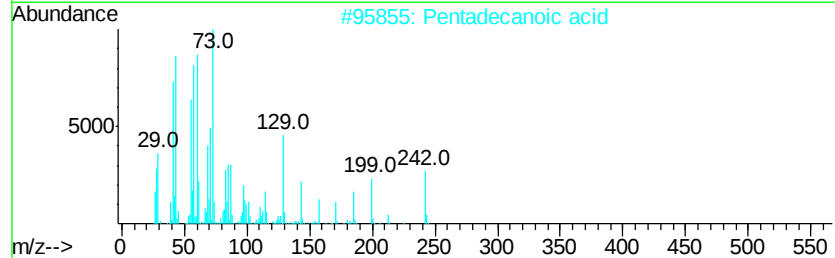
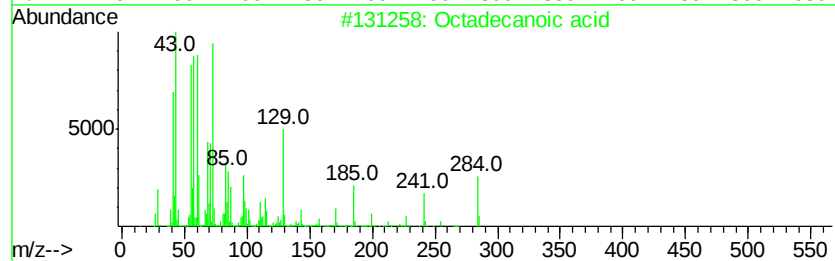
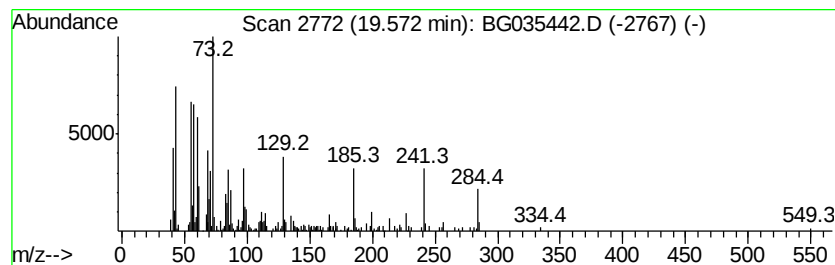
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.57	4.26 ng	207276	Chrysene-d12	21.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Tridecanoic acid	214	C13H26O2	000638-53-9	59
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062618\
Data File : BG035442.D
Acq On : 27 Jun 2018 12:23
Operator : JU/SJ
Sample : J3570-12
Misc :
ALS Vial : 33 Sample Multiplier: 1

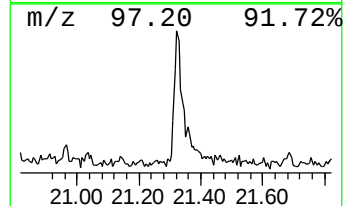
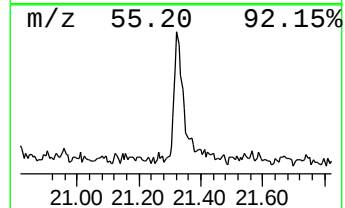
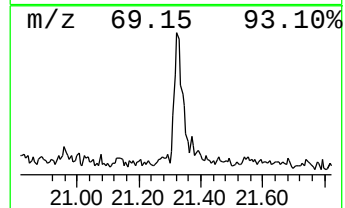
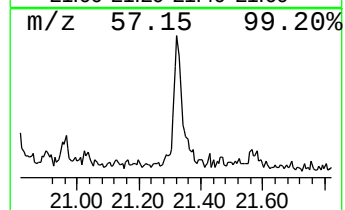
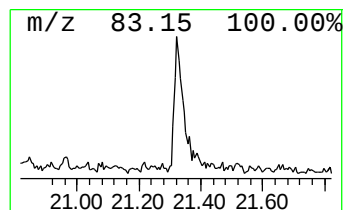
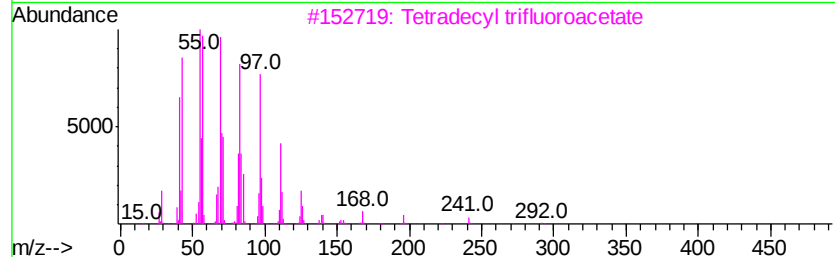
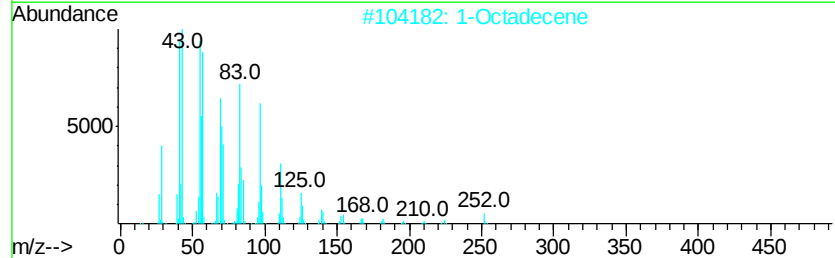
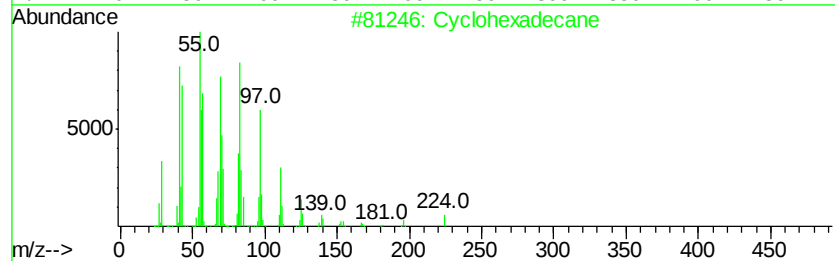
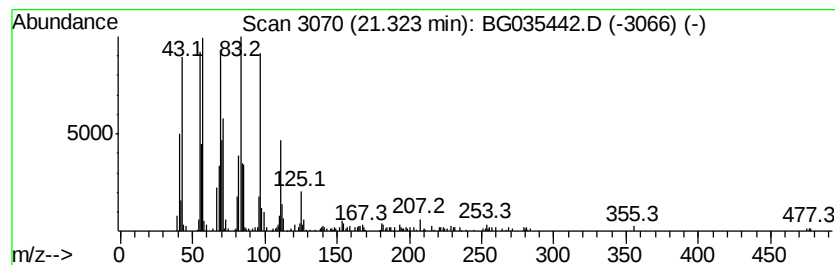
Instrument :
BNA_G
ClientSampleId :
20180375-COMPOSITE-CS-1A-ELU

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	6.02 ng	293011	Chrysene-d12	21.68
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 94
2		1-Octadecene	252 C18H36	000112-88-9 93
3		Tetradecyl trifluoroacetate	310 C16H29F3O2	006222-02-2 91
4		Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2 91
5		Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062618\
Data File : BG035442.D
Acq On : 27 Jun 2018 12:23
Operator : JU/SJ
Sample : J3570-12
Misc :
ALS Vial : 33 Sample Multiplier: 1

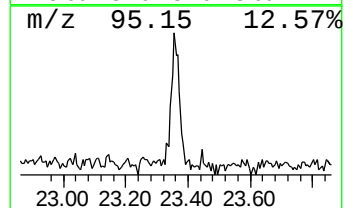
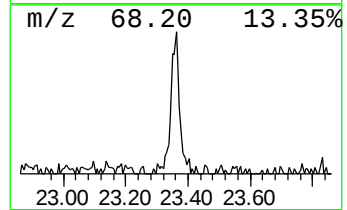
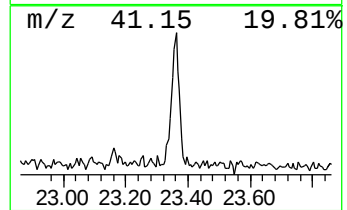
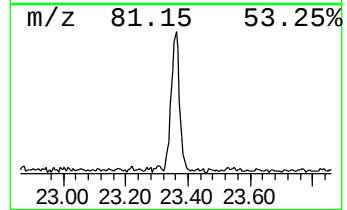
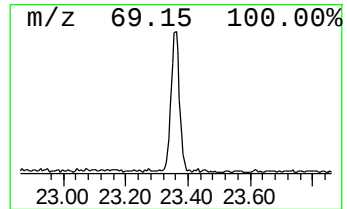
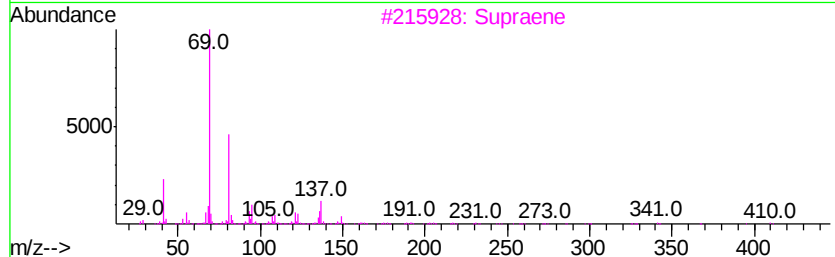
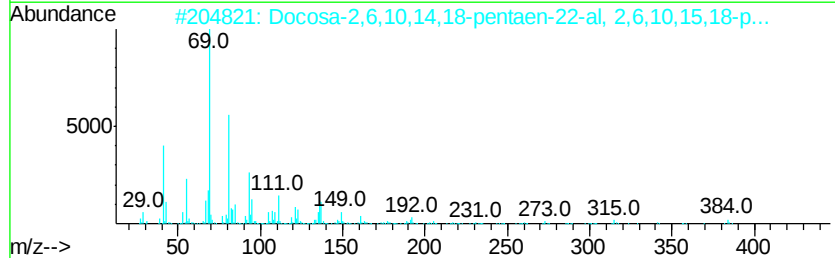
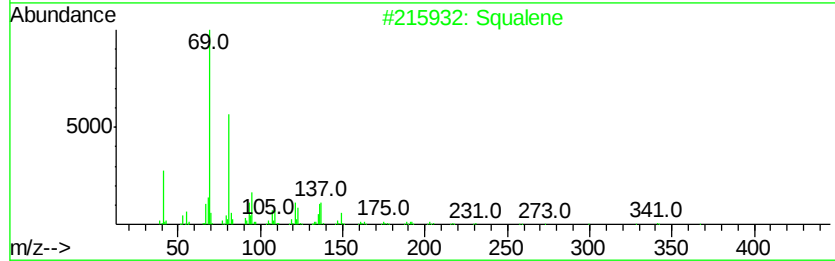
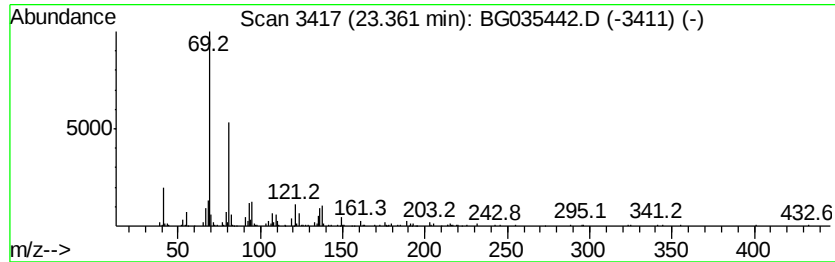
Instrument :
BNA_G
ClientSampleId :
20180375-COMPOSITE-CS-1A-ELU

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.36	5.31 ng	256529	Perylene-d12	24.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3	Supraene	410	C30H50	007683-64-9	87
4	trans-Farnesol	222	C15H26O	000106-28-5	80
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG062618\
Data File : BG035442.D
Acq On : 27 Jun 2018 12:23
Operator : JU/SJ
Sample : J3570-12
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20180375-COMPOSITE-CS-1A-ELU

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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
2-Pentanone, 4-hy...	5.17	2.9	ng	43124	1	8.05	296336	20.0
unknown7.58	7.58	84.7	ng	1255270	1	8.05	296336	20.0
Triethyl citrate	15.96	5.7	ng	185544	3	14.67	645953	20.0
Benzophenone	16.02	4.2	ng	133892	3	14.67	645953	20.0
n-Hexadecanoic acid	18.30	11.8	ng	525263	4	17.41	887338	20.0
Octadecanoic acid	19.57	4.3	ng	207276	5	21.68	973833	20.0
Cyclohexadecane	21.32	6.0	ng	293011	5	21.68	973833	20.0
Squalene	23.36	5.3	ng	256529	6	24.89	966279	20.0