

Data Path : Z:\HPCHEM1\BNA G\DATA\BG122117\
 Data File : BG031678.D
 Acq On : 21 Dec 2017 18:06
 Operator : SJ/JU
 Sample : I7001-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WP-1

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-BG122117.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	3.448	21	27	38	rBV	92060	190463	4.18%	0.838%
2	3.542	38	43	51	rVB2	30301	49852	1.09%	0.219%
3	6.245	496	503	515	rBV	330584	575267	12.63%	2.530%
4	7.920	781	788	804	rVB	212299	420369	9.23%	1.849%
5	8.343	851	860	871	rBV	642029	1231327	27.03%	5.416%
6	8.830	935	943	960	rVB	164393	332432	7.30%	1.462%
7	9.171	993	1001	1012	rVB	614330	1174440	25.79%	5.166%
8	9.618	1070	1077	1085	rBV2	23602	45735	1.00%	0.201%
9	10.029	1139	1147	1162	rBV	437367	831306	18.25%	3.656%
10	11.721	1426	1435	1442	rBV	252974	489738	10.75%	2.154%
11	12.826	1617	1623	1626	rBV	28771	46364	1.02%	0.204%
12	12.884	1626	1633	1637	rVV2	38707	106479	2.34%	0.468%
13	13.090	1657	1668	1673	rBV	72355	150558	3.31%	0.662%
14	13.143	1673	1677	1687	rVB	76797	129002	2.83%	0.567%
15	13.830	1785	1794	1800	rBV2	33424	66516	1.46%	0.293%
16	14.095	1827	1839	1853	rVB	1757649	2924250	64.20%	12.862%
17	15.375	2052	2057	2060	rBV	129493	208825	4.58%	0.918%
18	15.417	2060	2064	2067	rVV	95736	208180	4.57%	0.916%
19	15.464	2067	2072	2080	rVB2	455217	807049	17.72%	3.550%
20	16.163	2187	2191	2197	rVB2	47715	71135	1.56%	0.313%
21	16.768	2287	2294	2297	rBV	47270	75560	1.66%	0.332%
22	16.938	2315	2323	2332	rBV	1474868	2340550	51.39%	10.294%
23	17.062	2340	2344	2349	rVB5	41666	67693	1.49%	0.298%
24	17.115	2349	2353	2360	rBV7	25202	56691	1.24%	0.249%
25	17.291	2378	2383	2391	rBV4	32344	46955	1.03%	0.207%
26	18.202	2528	2538	2551	rBV2	612844	1042652	22.89%	4.586%
27	18.484	2578	2586	2592	rBV2	89805	207589	4.56%	0.913%
28	18.707	2618	2624	2629	rBV	72421	111706	2.45%	0.491%
29	19.024	2674	2678	2684	rBV3	76811	114167	2.51%	0.502%
30	19.306	2721	2726	2732	rBV	79593	123887	2.72%	0.545%
31	20.264	2885	2889	2896	rBV2	84671	128746	2.83%	0.566%
32	20.628	2947	2951	2955	rBV	31751	47127	1.03%	0.207%
33	20.734	2963	2969	2976	rVB	3340282	4554606	100.00%	20.032%
34	20.887	2990	2995	3002	rBV	112031	153587	3.37%	0.676%

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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 >
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35	21.527	3099	3104	3113	rBV	497111	639323	14.04%	2.812%
36	22.408	3250	3254	3257	rBV	40806	67061	1.47%	0.295%
37	22.444	3257	3260	3267	rVB4	53100	80943	1.78%	0.356%
38	22.561	3272	3280	3290	rBV2	651006	1229855	27.00%	5.409%
39	24.559	3611	3620	3631	rVB2	129824	325813	7.15%	1.433%
40	26.351	3912	3925	3938	rVB2	375493	1262410	27.72%	5.552%

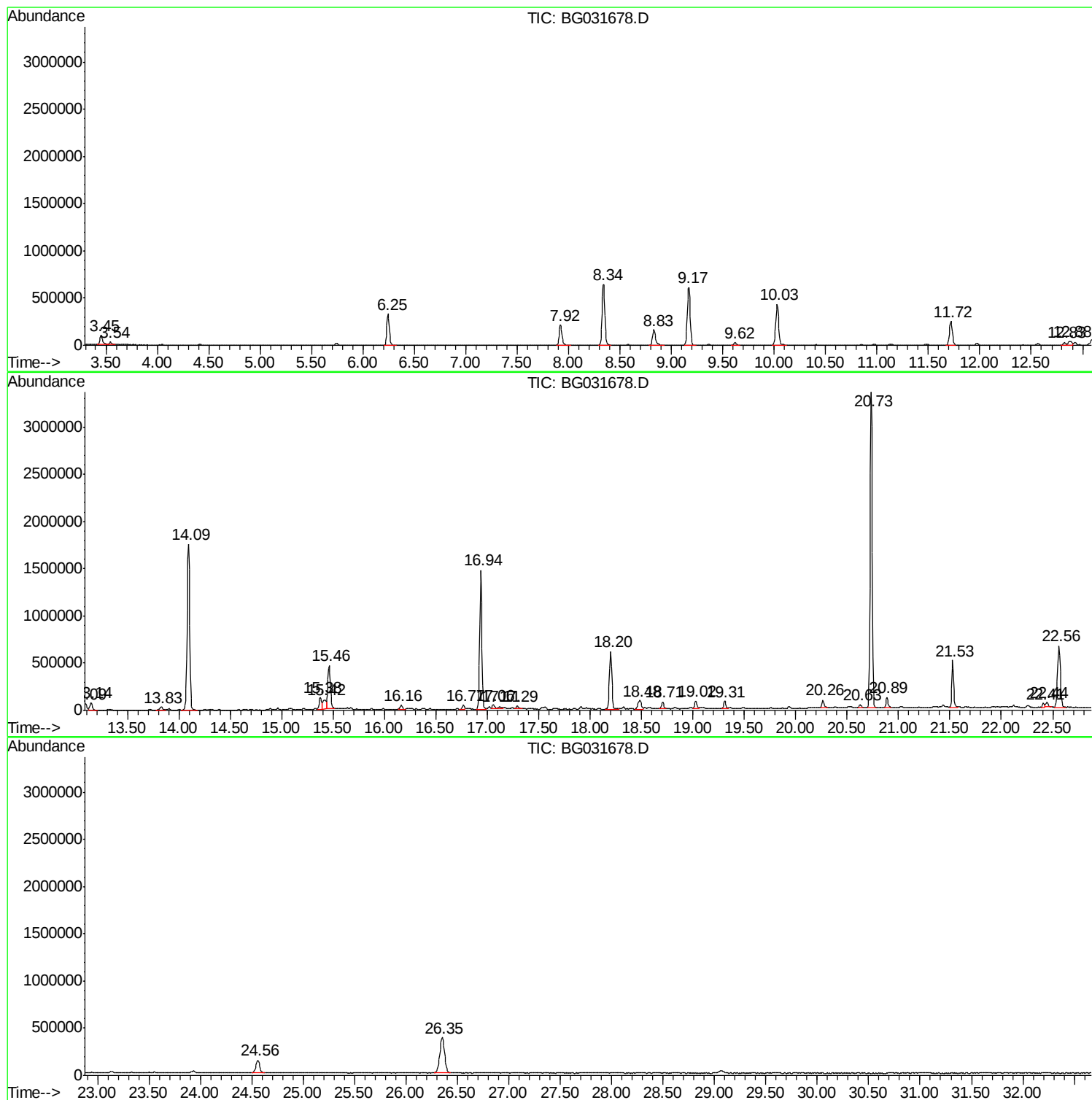
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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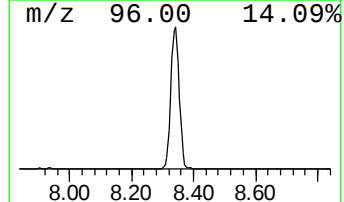
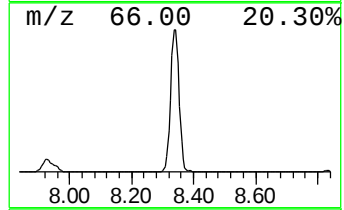
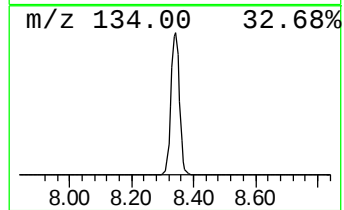
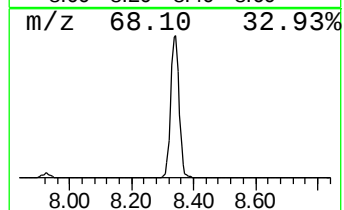
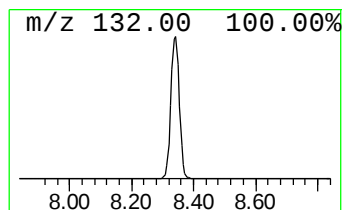
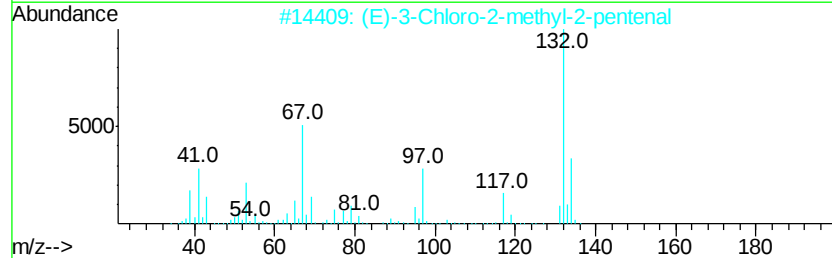
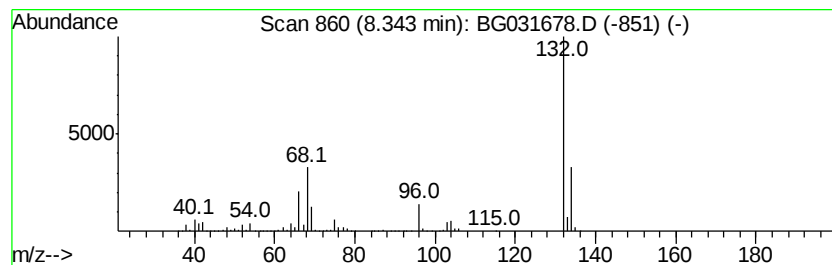
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Peak Number 2 unknown8.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	74.08 ng	1231330	1,4-Dichlorobenzene-d4	8.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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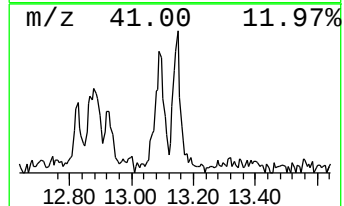
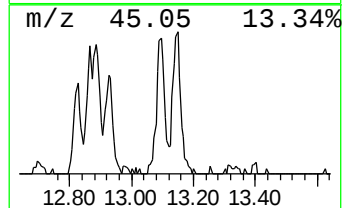
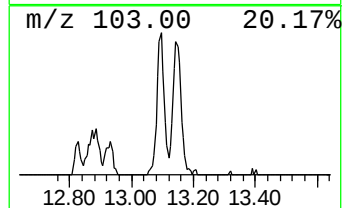
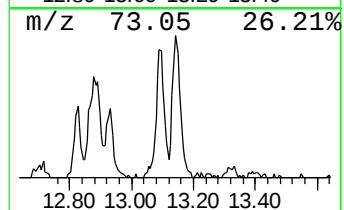
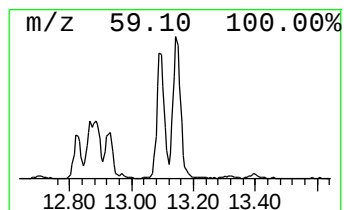
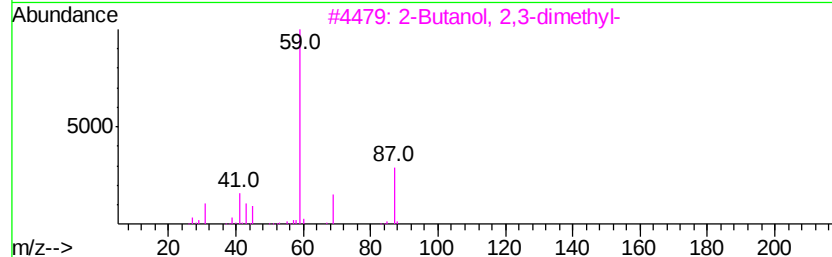
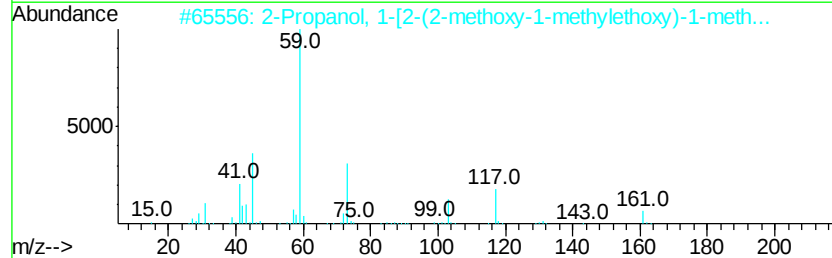
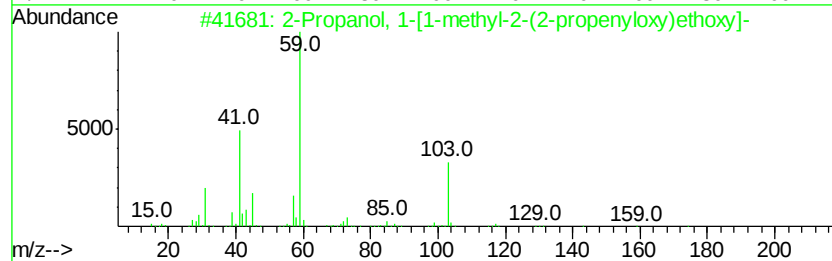
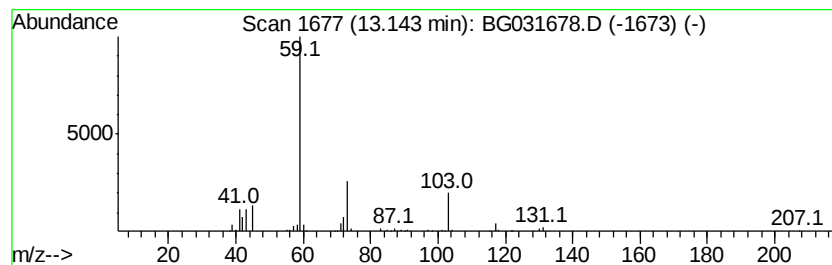
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Peak Number 6 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	5.27 ng	129002	Naphthalene-d8	11.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
2		2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	50
3		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	47
4		Pentane, 2-methoxy-	102	C6H14O	006795-88-6	47
5		Methane, diethoxy-	104	C5H12O2	000462-95-3	45



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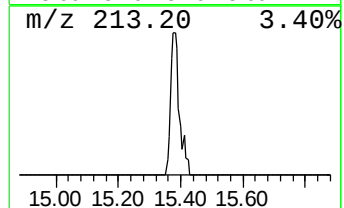
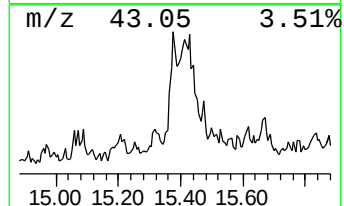
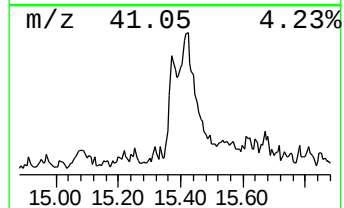
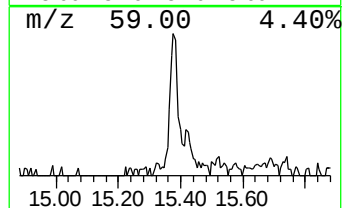
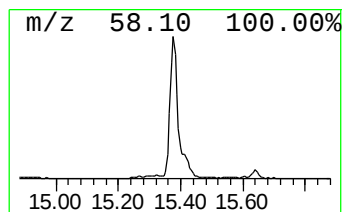
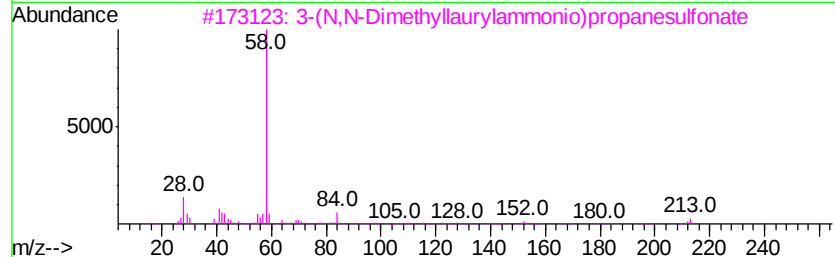
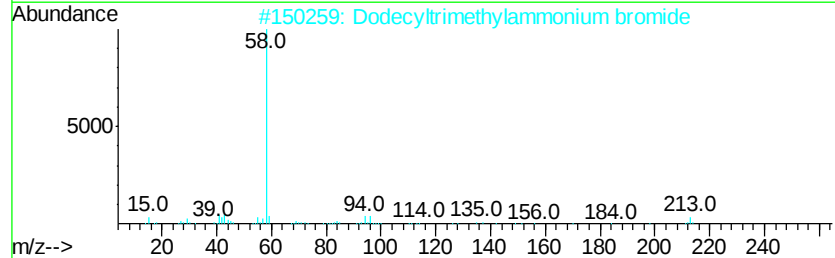
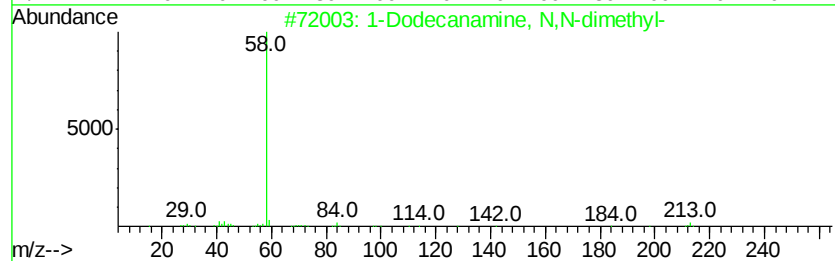
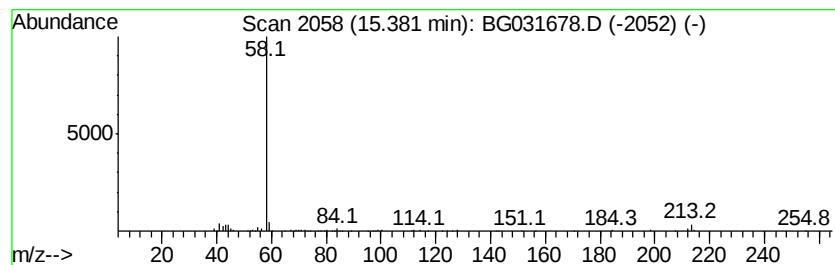
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 1-Dodecanamine, N,N-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.38	5.18 ng	208825	Acenaphthene-d10	15.46
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Dodecanamine, N,N-dimethyl-	213 C14H31N	000112-18-5 87
2		Dodecyltrimethylammonium bromide	307 C15H34BrN	001119-94-4 86
3		3-(N,N-Dimethylaurylammonio)pro...	335 C17H37N03S	014933-08-5 74
4		1-Heptanamine, N,N-dimethyl-	143 C9H21N	005277-11-2 72
5		Dimantine	297 C20H43N	000124-28-7 72



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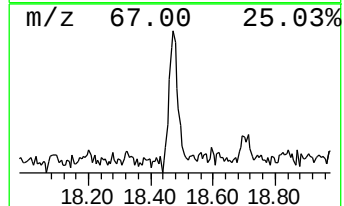
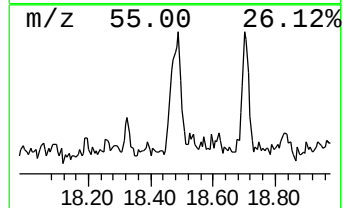
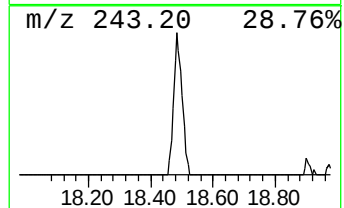
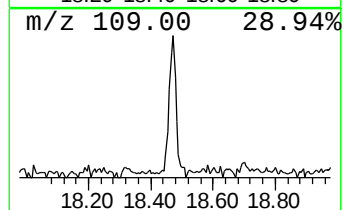
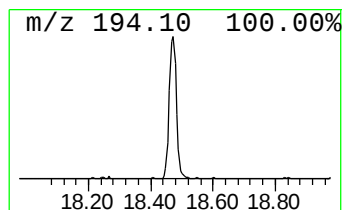
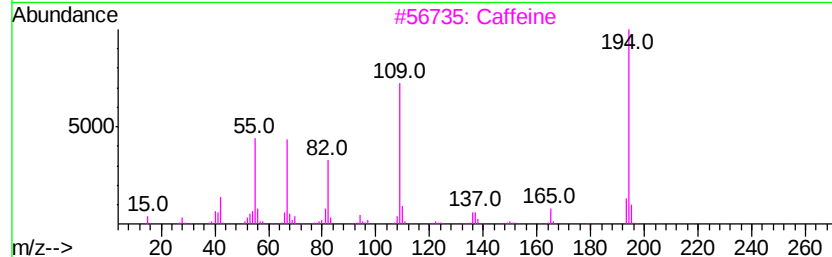
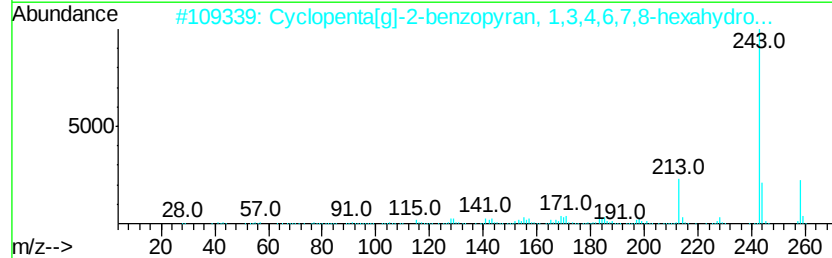
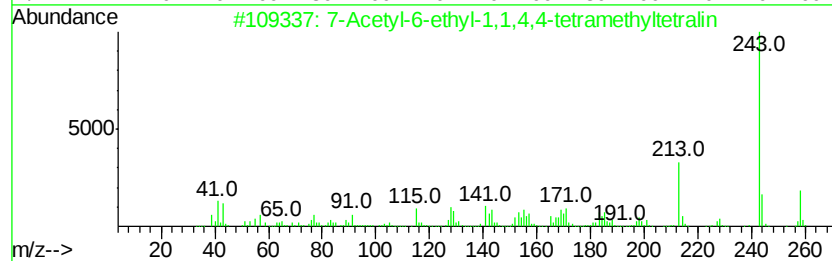
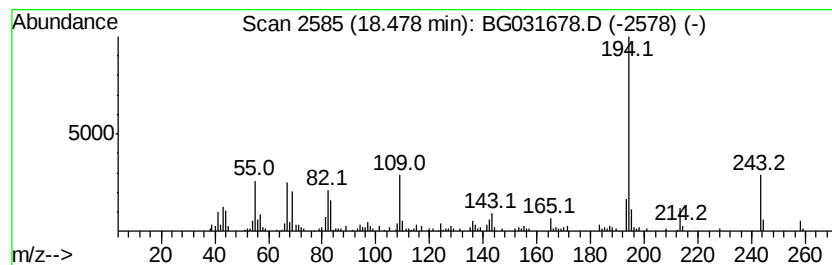
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TIC Library : C:\Database\NIST11.L
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 Peak Number 8 7-Acetyl-6-ethyl-1,1,4,4-te... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.48	3.98 ng	207589	Phenanthrene-d10	18.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Acetyl-6-ethyl-1,1,4,4-tetrame...	258	C18H26O	000088-29-9	91
2		Cyclopenta[<i>q</i>]-2-benzopyran, 1,3,...	258	C18H26O	001222-05-5	59
3		Caffeine	194	C8H10N4O2	000058-08-2	30
4		5-Methyl-1,10-phenanthroline	194	C13H10N2	003002-78-6	25
5		Phenazine, 1-methyl-	194	C13H10N2	001016-59-7	22



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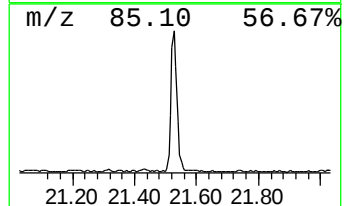
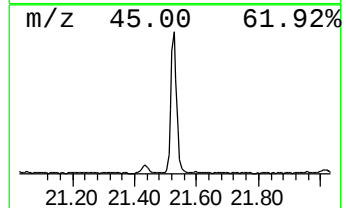
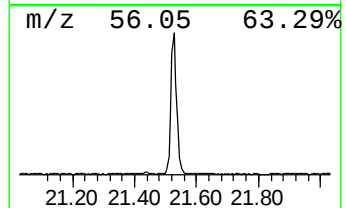
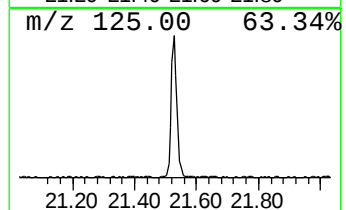
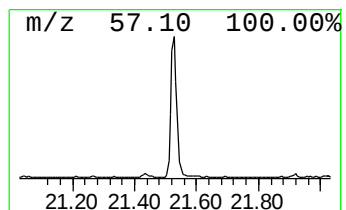
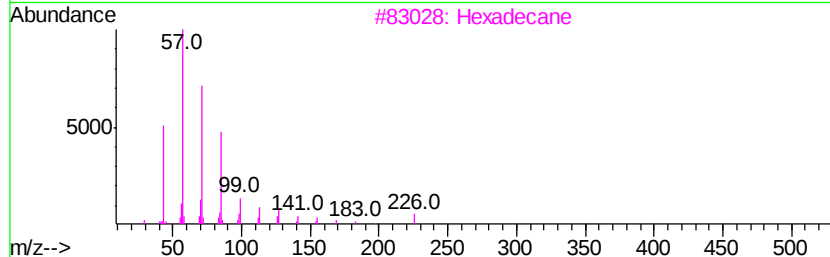
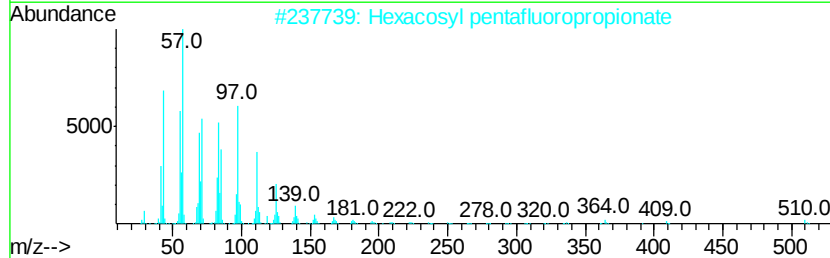
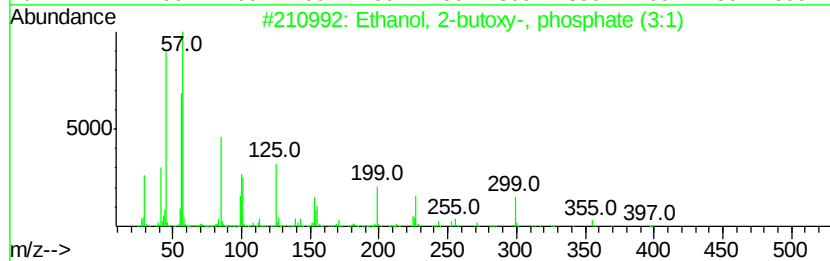
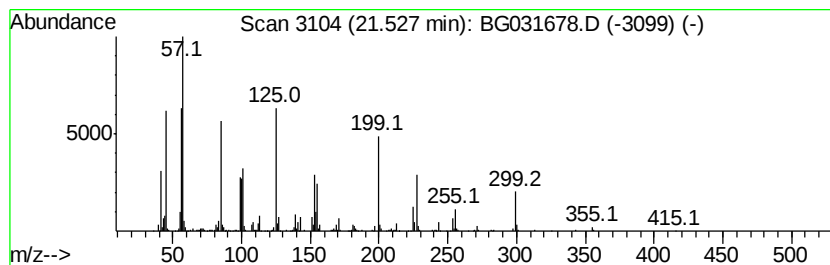
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Peak Number 9 Ethanol, 2-butoxy-, phospho... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.53	10.40 ng	639323	Chrysene-d12	22.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	86	
2	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	22	
3	Hexadecane	226	C16H34	000544-76-3	15	
4	Heptadecane	240	C17H36	000629-78-7	10	
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	10	



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WP-1

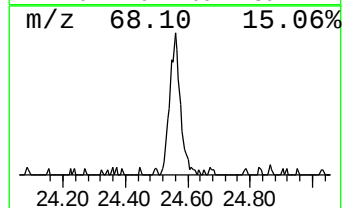
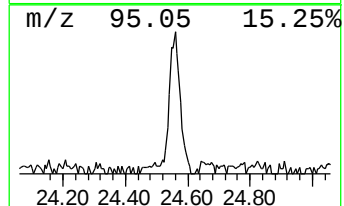
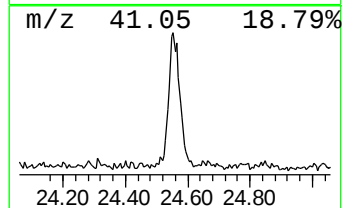
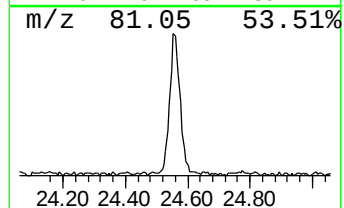
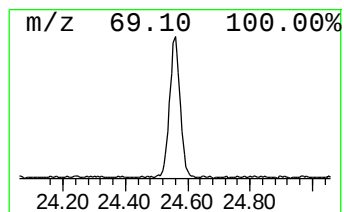
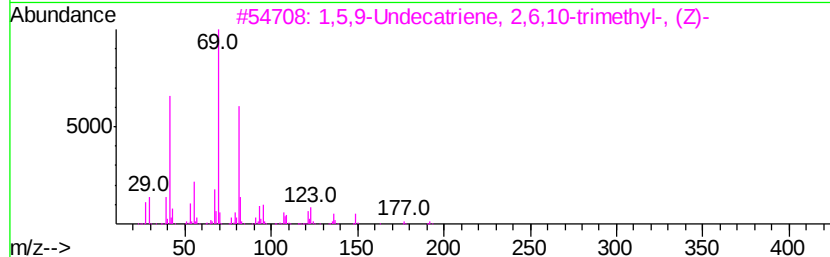
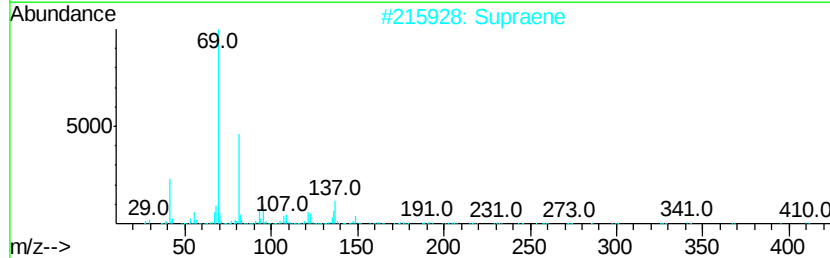
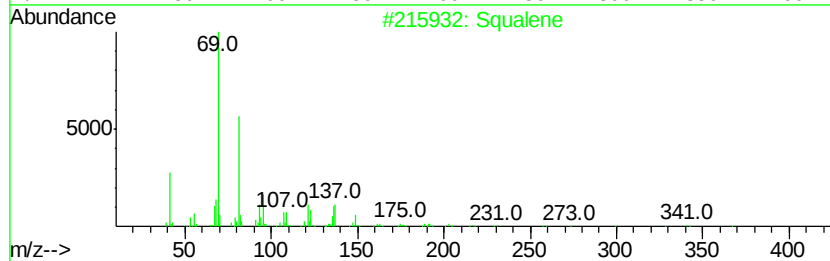
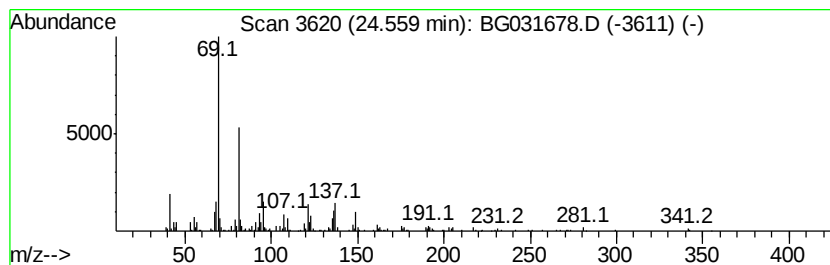
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.56	5.16 ng	325813	Perylene-d12	26.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	83
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
4		Farnesol isomer a	222	C15H26O	1000108-92-4	62
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122117\
Data File : BG031678.D
Acq On : 21 Dec 2017 18:06
Operator : SJ/JU
Sample : I7001-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WP-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.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
unknown8.34	8.34	74.1	ng	1231330	1	8.83	332432	20.0
2-Propanol, 1-[2-...	12.88	4.3	ng	106479	2	11.72	489738	20.0
2-Propanol, 1-[1-...	13.14	5.3	ng	129002	2	11.72	489738	20.0
1-Dodecanamine, N...	15.38	5.2	ng	208825	3	15.46	807049	20.0
7-Acetyl-6-ethyl-...	18.48	4.0	ng	207589	4	18.20	1042650	20.0
Ethanol, 2-butoxy...	21.53	10.4	ng	639323	5	22.56	1229860	20.0
Squalene	24.56	5.2	ng	325813	6	26.35	1262410	20.0