

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012117\
 Data File : BG025569.D
 Acq On : 21 Jan 2017 12:03
 Operator : UM/SJ
 Sample : I1267-04
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-21

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-BG122116.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	5.234	402	408	417	rBV	226793	383096	4.32%	1.011%
2	5.716	484	490	505	rBV	816905	1501056	16.92%	3.962%
3	7.338	759	766	783	rBV	540534	1079104	12.16%	2.848%
4	7.708	822	829	841	rBV	1528588	2793284	31.48%	7.372%
5	8.178	902	909	922	rVB	289793	507385	5.72%	1.339%
6	8.501	957	964	975	rBV	1266705	2340423	26.38%	6.177%
7	9.365	1102	1111	1125	rBV	1135801	2247662	25.33%	5.932%
8	11.010	1383	1391	1409	rBV	332181	699757	7.89%	1.847%
9	13.430	1794	1803	1812	rBV	3051666	4971796	56.03%	13.121%
10	14.811	2031	2038	2050	rVB	614759	1037706	11.70%	2.739%
11	16.298	2284	2291	2302	rBV	3082729	4806051	54.16%	12.684%
12	17.555	2499	2505	2515	rBV2	820482	1337691	15.08%	3.530%
13	17.890	2557	2562	2571	rBV2	140628	404717	4.56%	1.068%
14	18.395	2644	2648	2653	rBV6	94255	133676	1.51%	0.353%
15	19.658	2859	2863	2869	rBV7	97549	149399	1.68%	0.394%
16	19.776	2879	2883	2892	rBV	275917	545555	6.15%	1.440%
17	20.134	2939	2944	2950	rBV	6285493	8873007	100.00%	23.417%
18	21.286	3136	3140	3150	rVB3	123858	246554	2.78%	0.651%
19	21.844	3228	3235	3244	rBV	1084403	1906548	21.49%	5.032%
20	25.223	3801	3810	3823	rVB2	626470	1926417	21.71%	5.084%

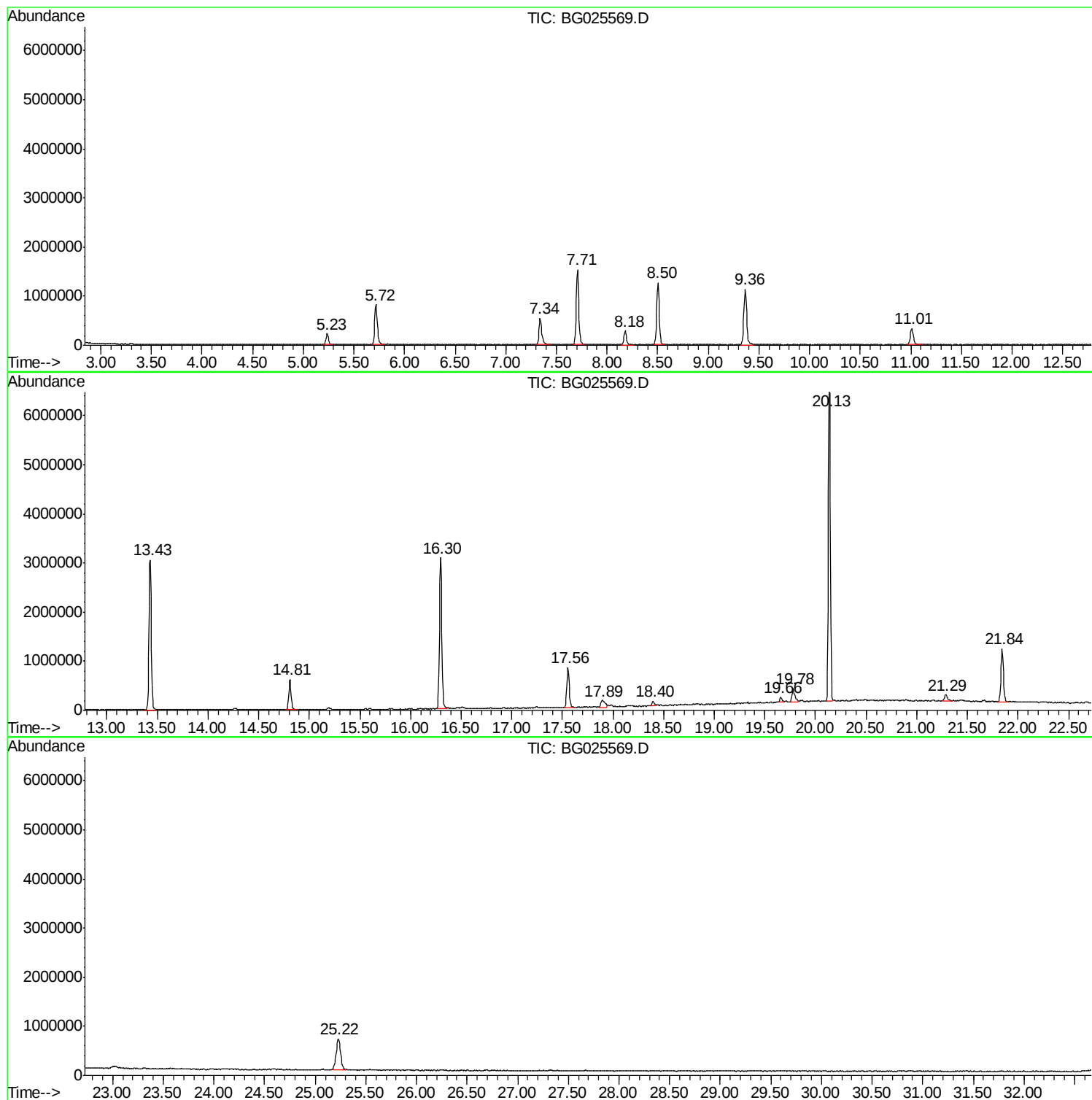
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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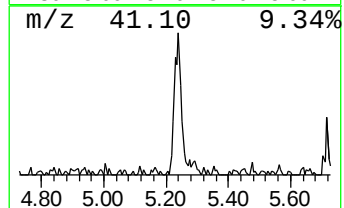
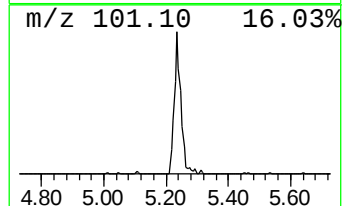
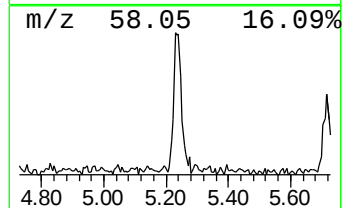
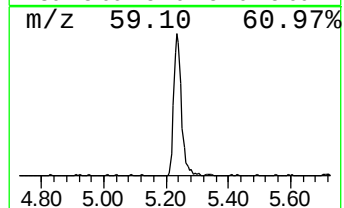
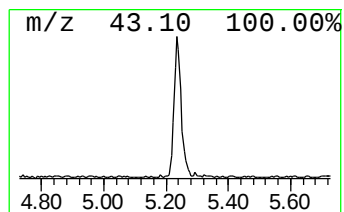
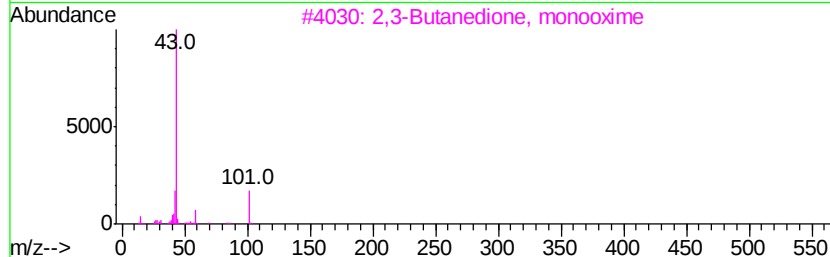
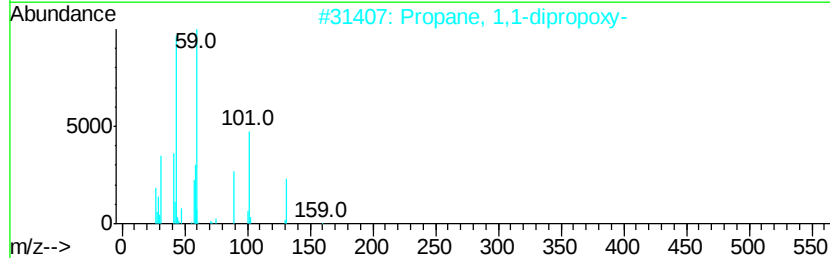
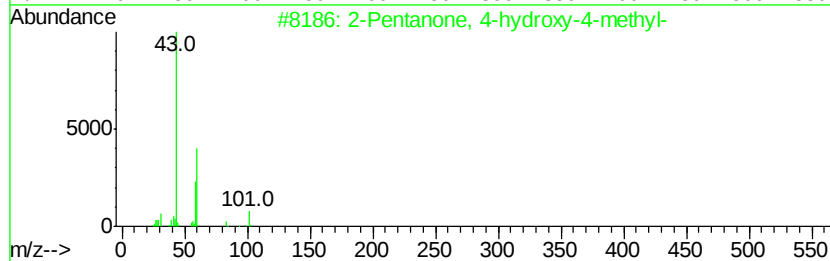
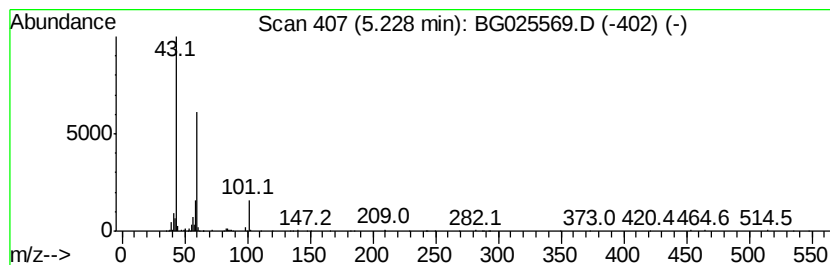
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	15.10 ng	383096	1,4-Dichlorobenzene-d4	8.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	47
2	Propane, 1,1-dipropoxy-	160	C9H20O2		004744-11-0	38
3	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	35
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2		000921-14-2	28
5	1,2-Butanediol	90	C4H10O2		000584-03-2	23



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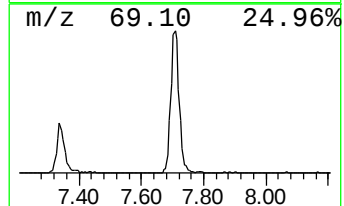
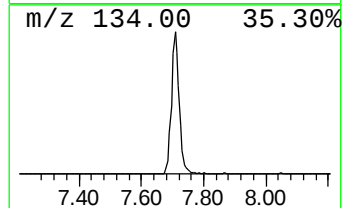
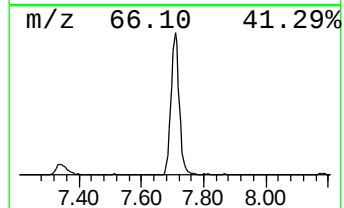
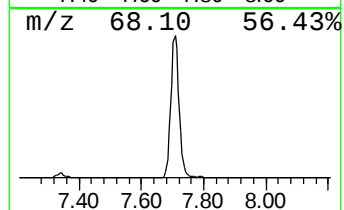
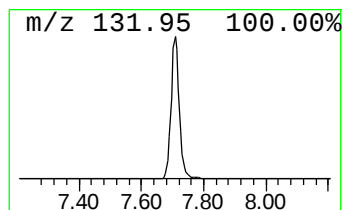
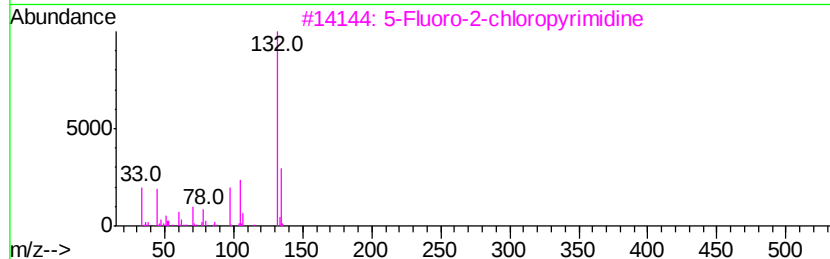
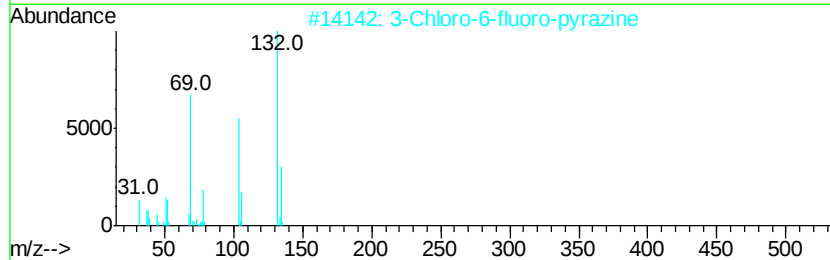
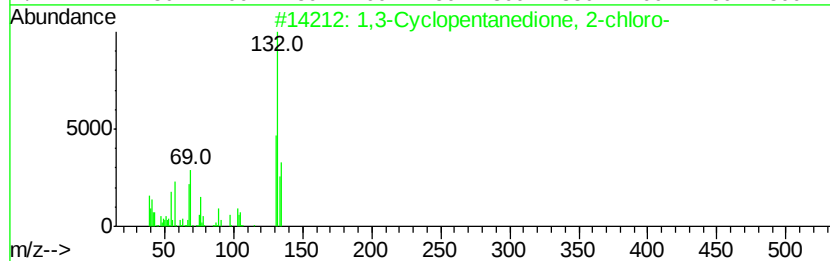
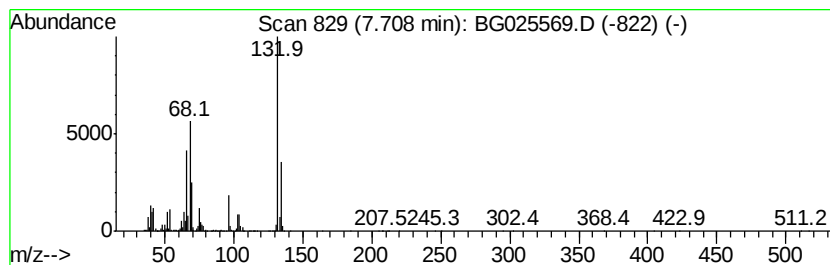
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Peak Number 2 unknown7.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.71	110.11 ng	2793280	1,4-Dichlorobenzene-d4	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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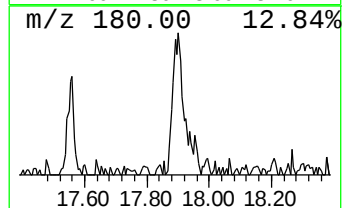
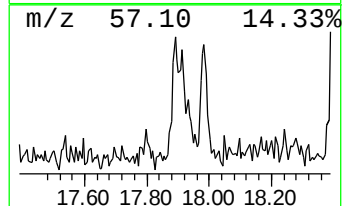
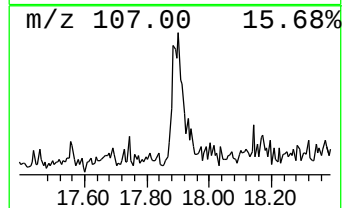
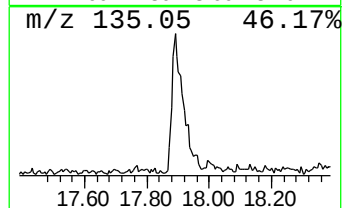
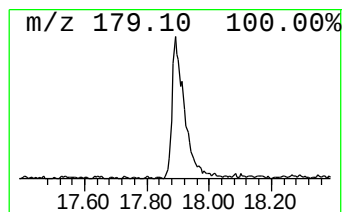
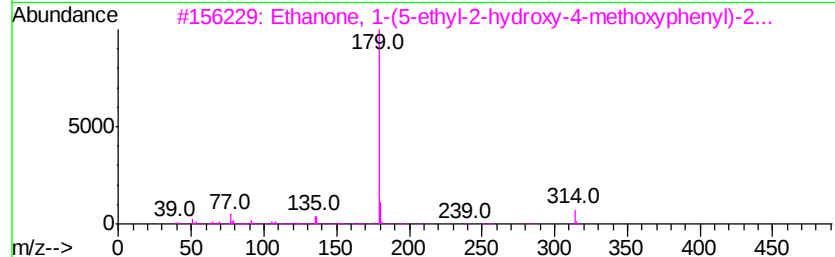
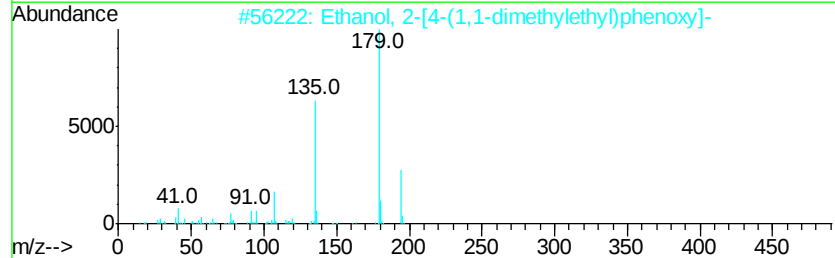
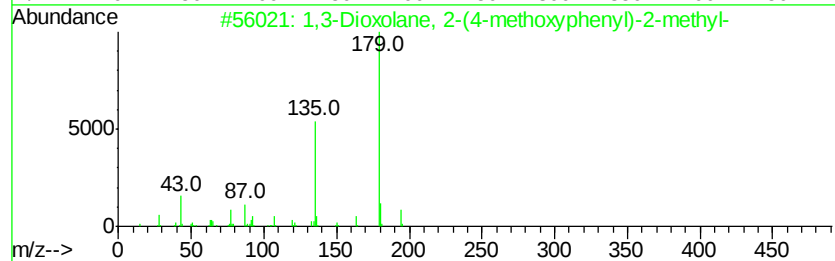
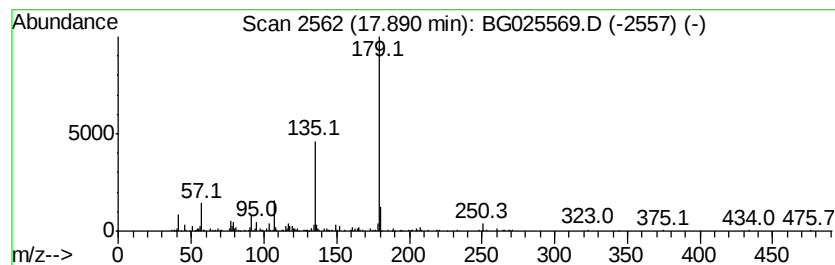
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Peak Number 4 1,3-Dioxolane, 2-(4-methoxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	6.05 ng	404717	Phenanthrene-d10	17.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-(4-methoxyphenyl)-2-methyl-	194	C11H14O3	036881-00-2	50
2		Ethanol, 2-[4-(1,1-dimethylethyl)phenoxy]-	194	C12H18O2	000713-46-2	38
3		Ethanone, 1-(5-ethyl-2-hydroxy-4-methoxyphenyl)-2-methyl-	314	C18H20O3	170241-39-1	37
4		Benzothiazole-6-carboxylic acid	179	C8H5NO2S	003622-35-3	33
5		Ethanol, 2-[4-(1,1-dimethylpropyl)phenoxy]-	208	C13H20O2	006382-07-6	28



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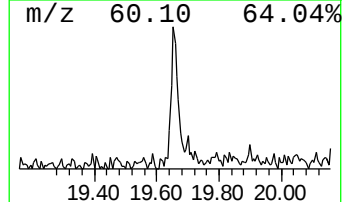
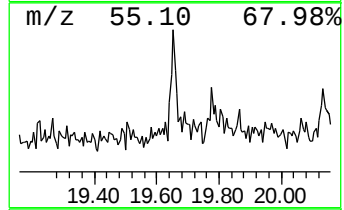
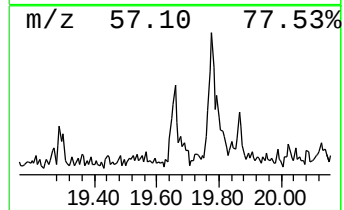
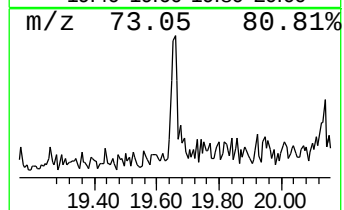
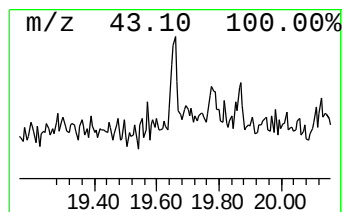
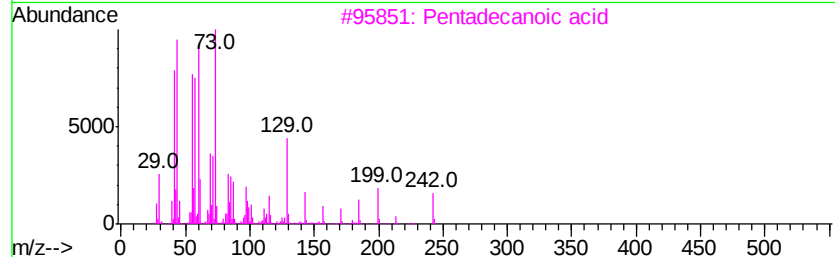
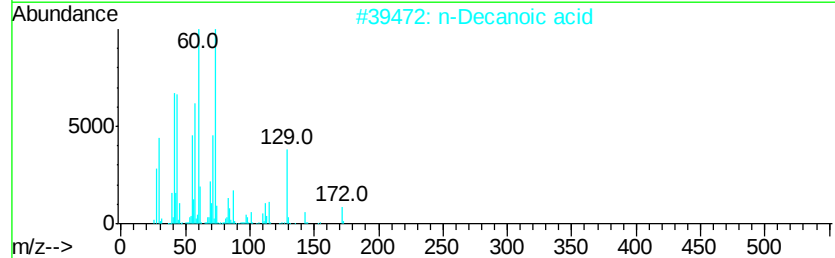
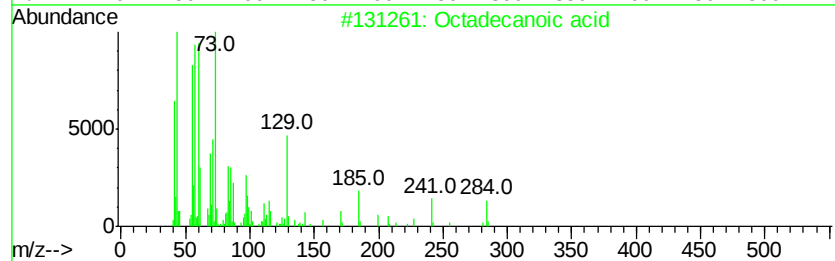
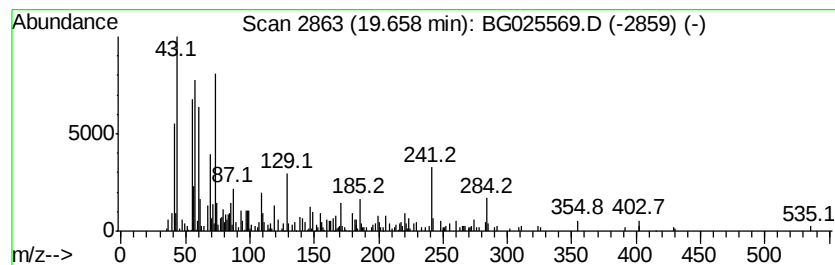
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Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.66	2.23 ng	149399	Phenanthrene-d10	17.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	64
2		n-Decanoic acid	172	C10H20O2	000334-48-5	47
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	43
4		Undecanoic acid	186	C11H22O2	000112-37-8	38
5		Dodecanoic acid	200	C12H24O2	000143-07-7	38



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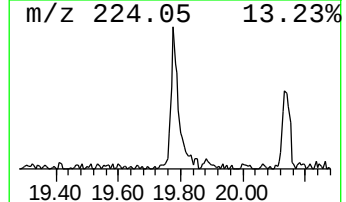
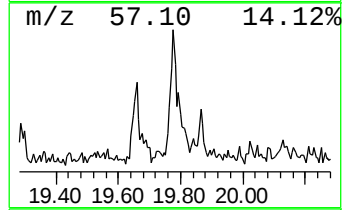
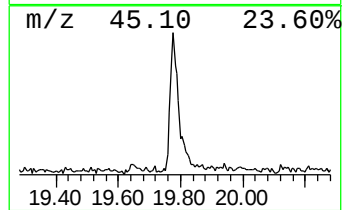
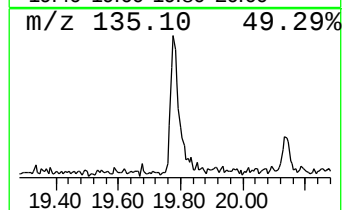
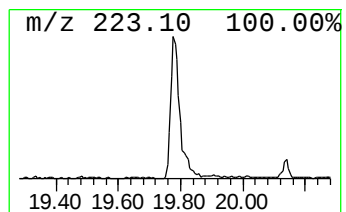
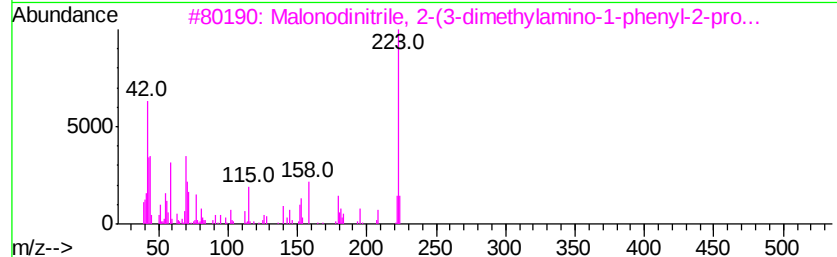
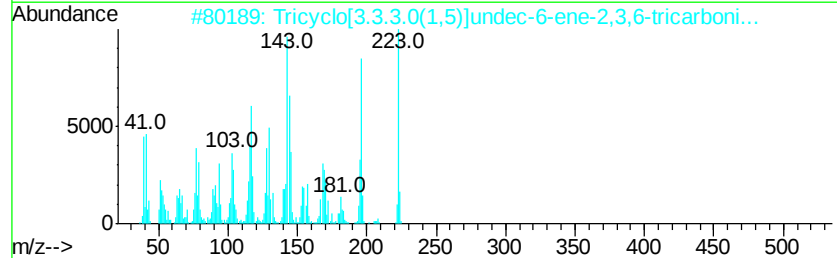
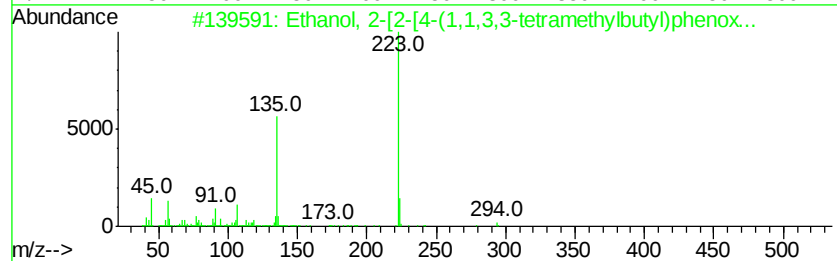
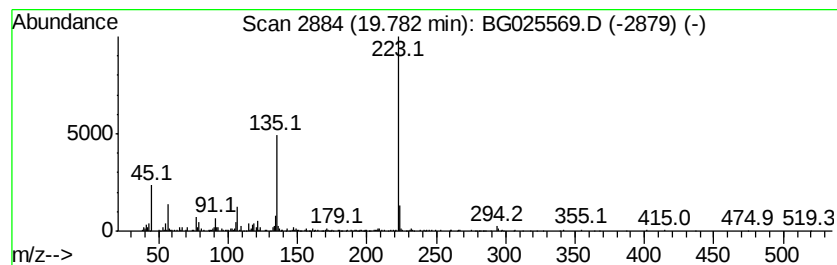
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.78	5.72 ng	545555	Chrysene-d12	21.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	72
2		Tricyclo[3.3.3.0(1,5)]undec-6-en...	223	C14H13N3	118894-71-6	50
3		Malonodinitrile, 2-(3-dimethylam...	223	C14H13N3	065996-13-6	43
4		Benzenamine, 3-(5-methyl-1H-1,3-...	223	C14H13N3	1000319-43-9	38
5		9-[4-[1,3-Diphenyl-2-imidazolidi...	542	C28H30N8O4	1000214-46-0	32



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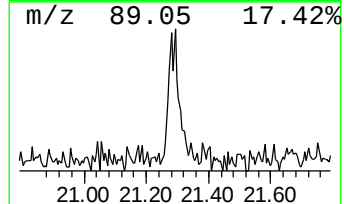
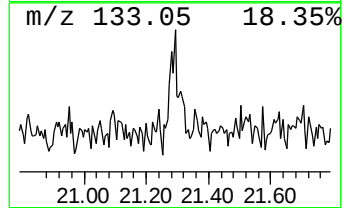
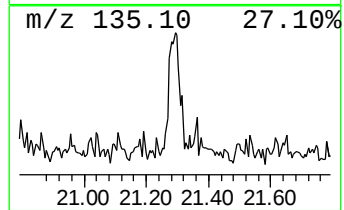
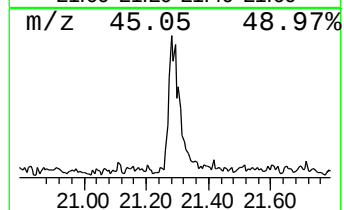
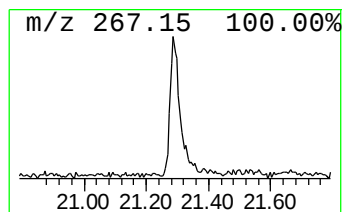
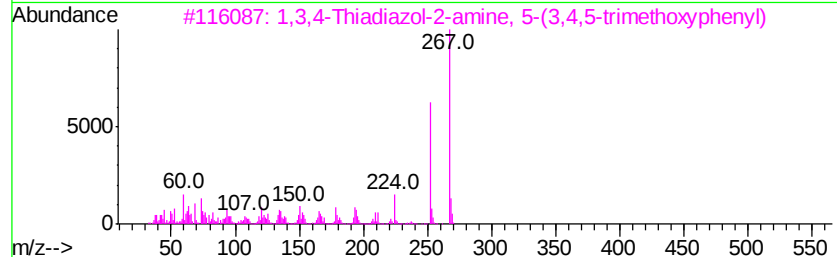
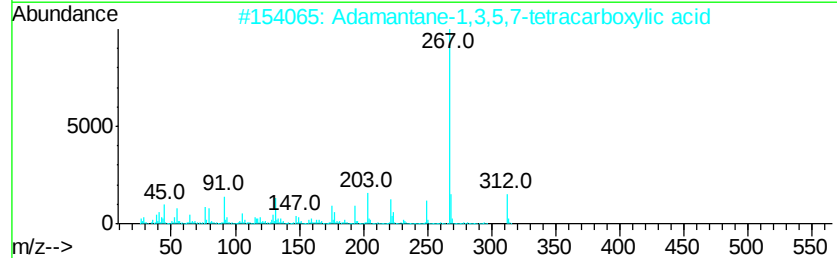
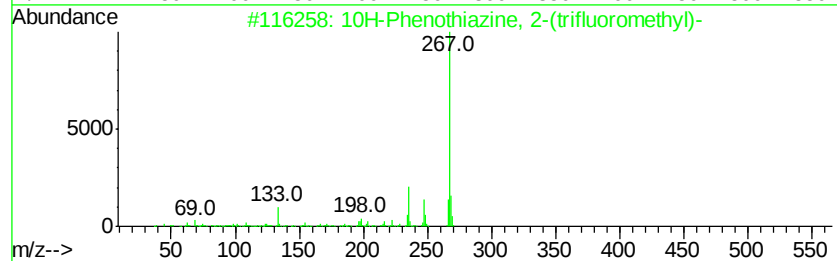
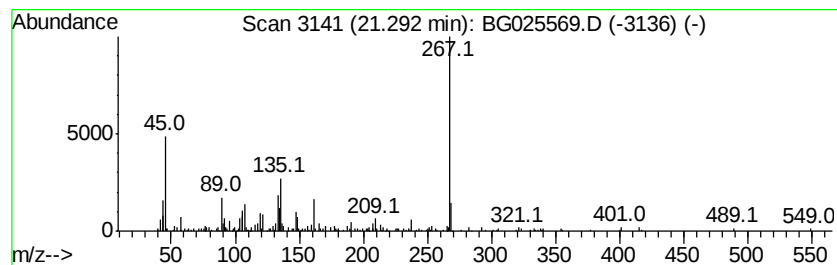
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown21.29 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	2.59 ng	246554	Chrysene-d12	21.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	10H-Phenothiazine, 2-(trifluorom...	267	C13H8F3NS	000092-30-8	46
2		Adamantane-1,3,5,7-tetracarboxyl...	312	C14H16O8	100884-80-8	43
3		1,3,4-Thiadiazol-2-amine, 5-(3,4...	267	C11H13N3O3S	028004-59-3	43
4		Benzimidazole-2-methanol, .alpha...	298	C17H18N2O3	309724-70-7	40
5		Ethanol, 2-[2-[2-[4-(1,1,3,3-tet...	338	C20H34O4	002315-62-0	39



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012117\
Data File : BG025569.D
Acq On : 21 Jan 2017 12:03
Operator : UM/SJ
Sample : I1267-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-21

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.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...	5.23	15.1	ng	383096	1	8.18	507385	20.0
unknown7.71	7.71	110.1	ng	2793280	1	8.18	507385	20.0
1,3-Dioxolane, 2-...	17.89	6.0	ng	404717	4	17.56	1337690	20.0
Octadecanoic acid	19.66	2.2	ng	149399	4	17.56	1337690	20.0
Ethanol, 2-[2-[4-...	19.78	5.7	ng	545555	5	21.84	1906550	20.0
unknown21.29	21.29	2.6	ng	246554	5	21.84	1906550	20.0