

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
 Data File : BG043830.D
 Acq On : 17 Dec 2019 21:56
 Operator : JU
 Sample : K6317-08
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 178K-WC2

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-BG120919.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	3.195	14	18	28	rVB	198660	289895	4.44%	0.782%
2	5.111	338	344	353	rBV	335519	511406	7.83%	1.379%
3	5.581	416	424	442	rBV	1457610	2337919	35.80%	6.305%
4	7.161	686	693	708	rBV	1627390	2853499	43.70%	7.696%
5	7.537	747	757	769	rBV	1509448	2653492	40.63%	7.156%
6	8.002	827	836	844	rBV	365362	620669	9.50%	1.674%
7	8.325	883	891	899	rBV	1096227	1882642	28.83%	5.077%
8	9.153	1024	1032	1040	rBV	937241	1645810	25.20%	4.439%
9	10.804	1304	1313	1320	rBV	544115	974859	14.93%	2.629%
10	13.254	1722	1730	1743	rBV	2617201	4092846	62.67%	11.038%
11	14.077	1864	1870	1883	rVB	255037	398580	6.10%	1.075%
12	14.629	1956	1964	1972	rBV	979360	1622323	24.84%	4.375%
13	16.110	2210	2216	2239	rBV	1244447	2194551	33.60%	5.919%
14	17.367	2424	2430	2440	rBV	1374874	2125377	32.55%	5.732%
15	19.982	2869	2875	2882	rBV	4811514	6530484	100.00%	17.612%
16	20.675	2988	2993	2999	rBV	191274	442091	6.77%	1.192%
17	21.292	3093	3098	3109	rBV	429742	776152	11.89%	2.093%
18	21.627	3148	3155	3165	rBV2	1324095	2209628	33.84%	5.959%
19	21.856	3189	3194	3200	rVB2	107471	158030	2.42%	0.426%
20	22.461	3292	3297	3307	rVB2	127093	234773	3.60%	0.633%
21	23.148	3409	3414	3420	rVB	119529	207846	3.18%	0.561%
22	23.948	3544	3550	3557	rBV3	101978	218011	3.34%	0.588%
23	24.782	3682	3692	3704	rBV2	681076	2097883	32.12%	5.658%

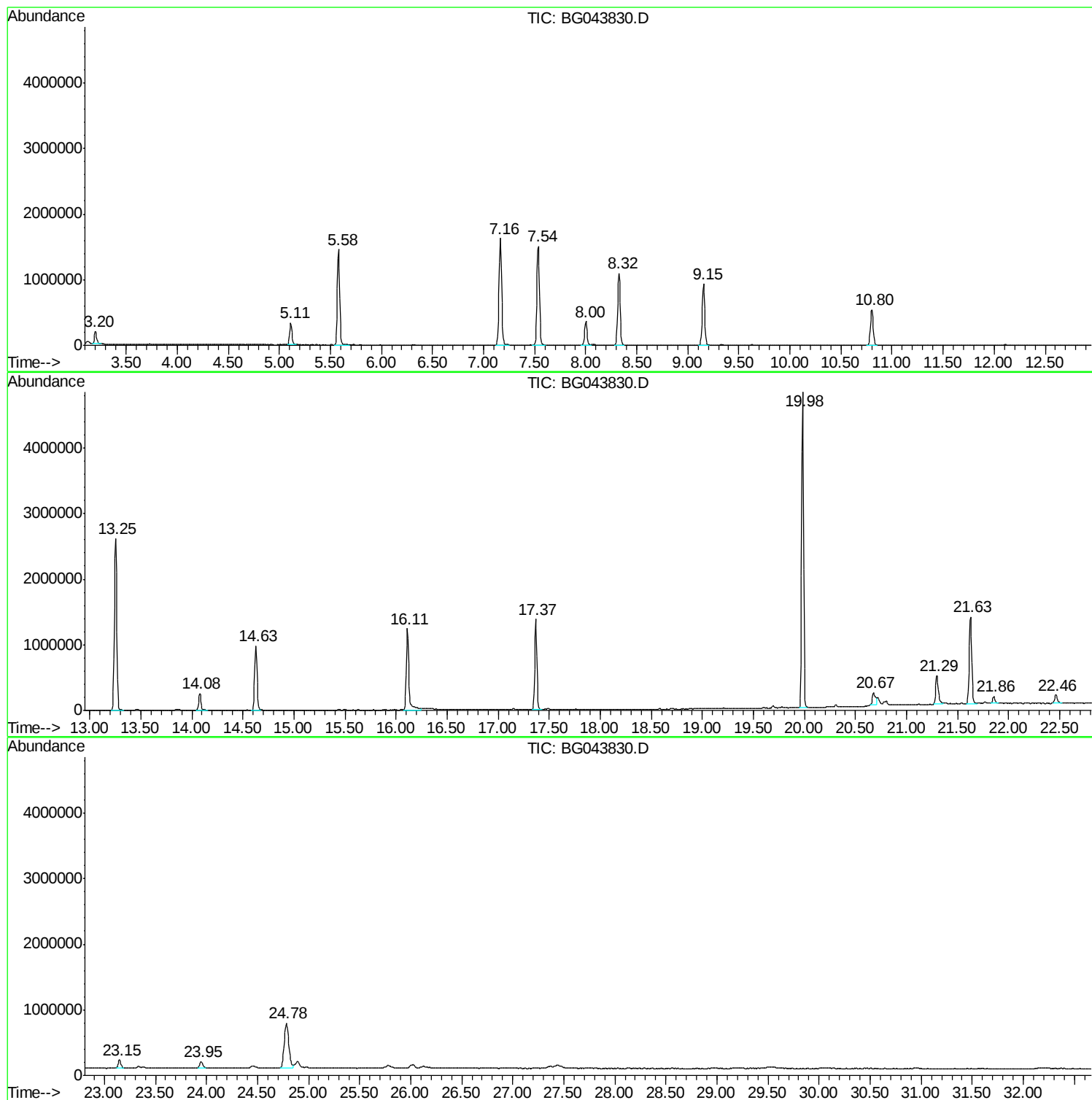
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG120919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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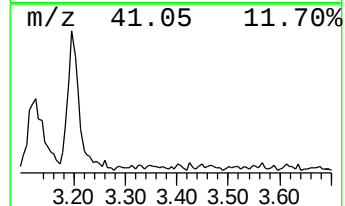
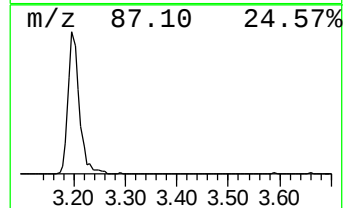
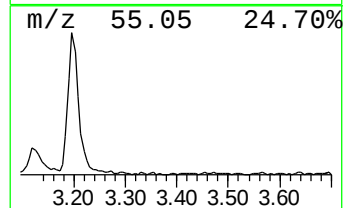
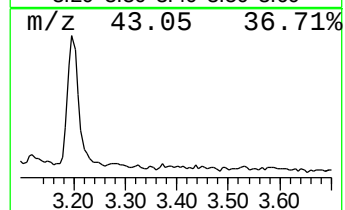
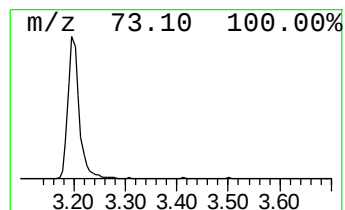
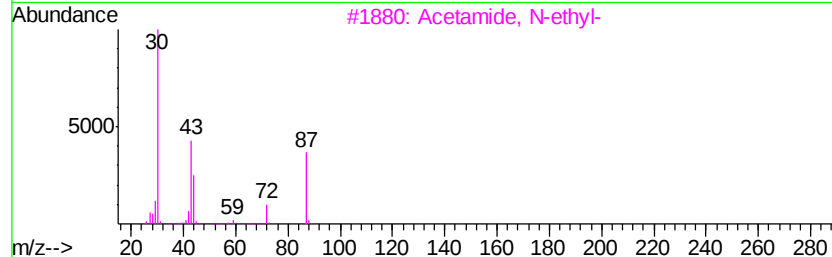
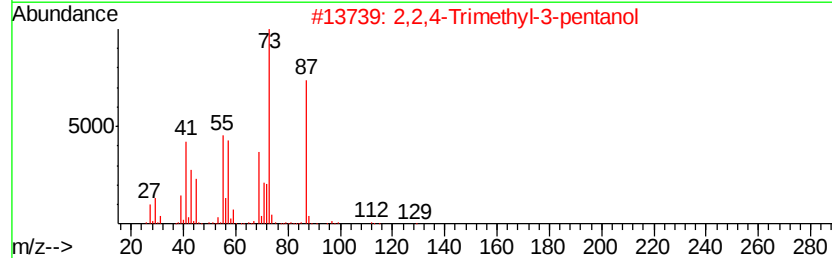
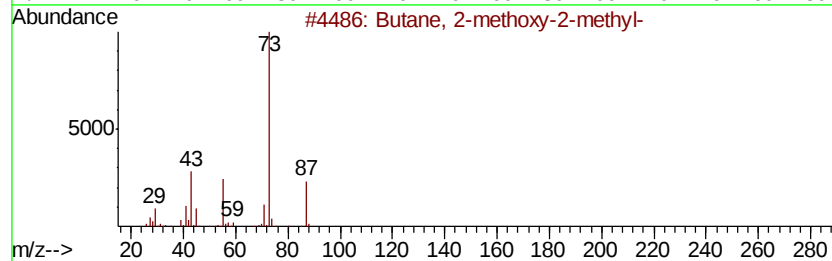
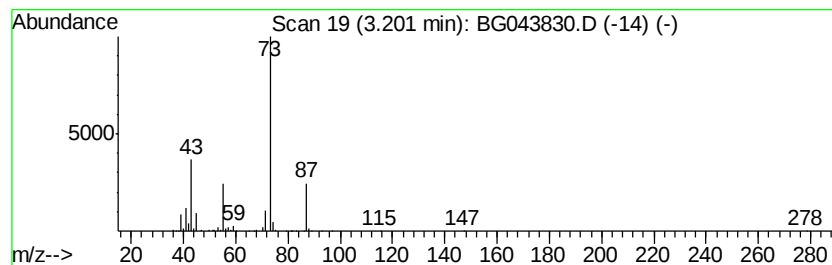
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	9.34 ng	289895	1,4-Dichlorobenzene-d4	8.00

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	40
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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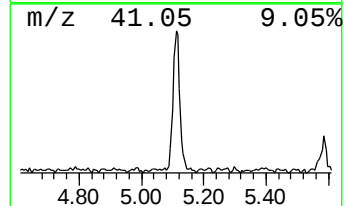
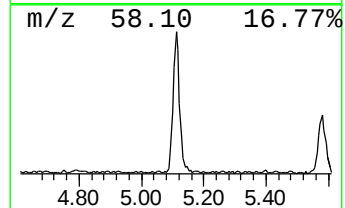
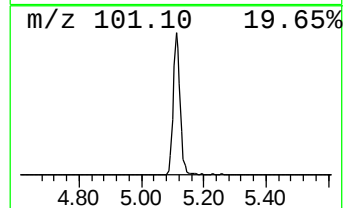
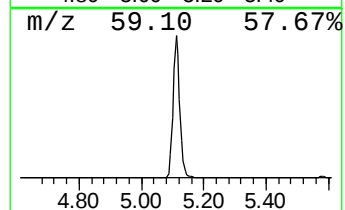
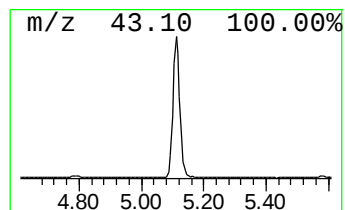
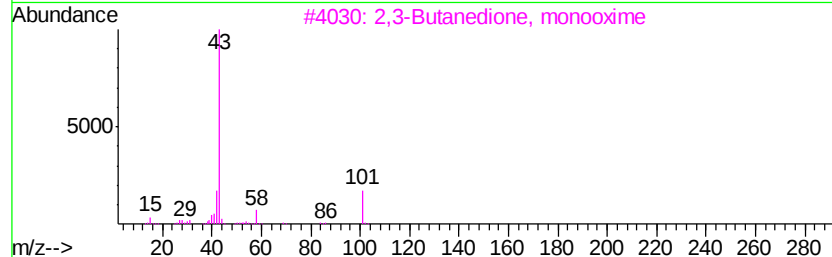
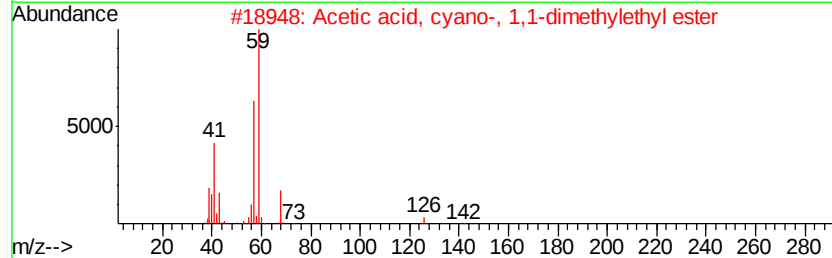
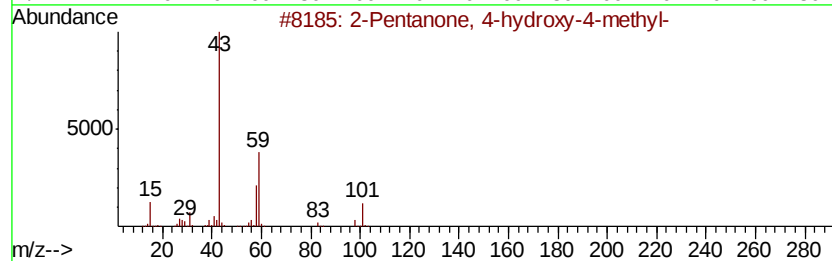
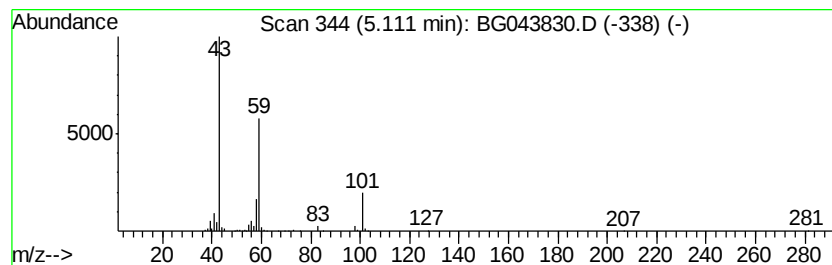
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	16.48 ng	511406	1,4-Dichlorobenzene-d4	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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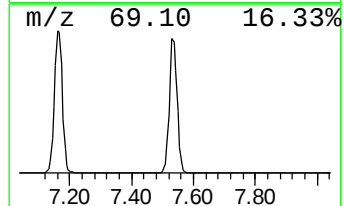
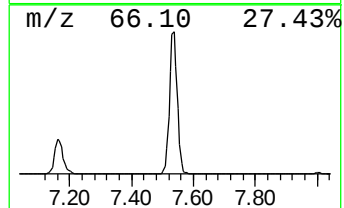
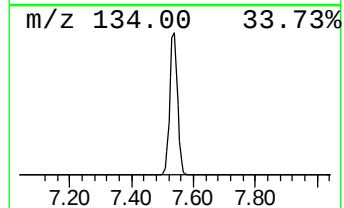
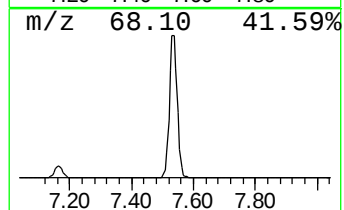
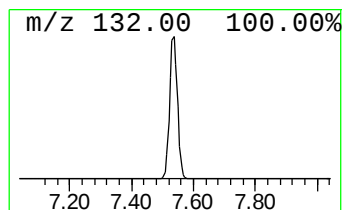
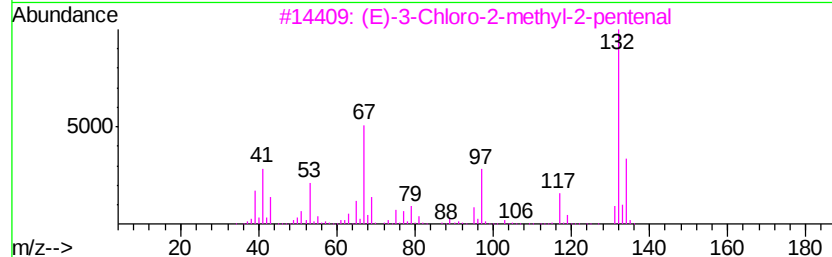
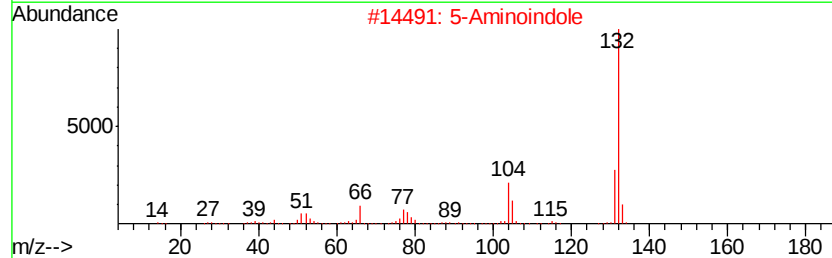
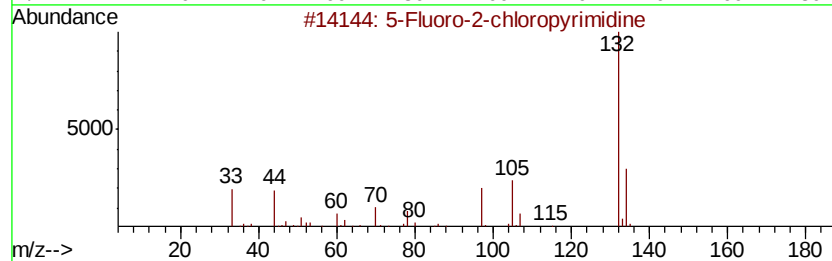
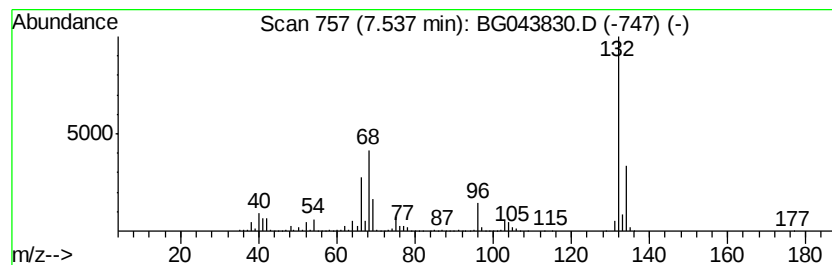
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Peak Number 3 unknown7.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	85.50 ng	2653490	1,4-Dichlorobenzene-d4	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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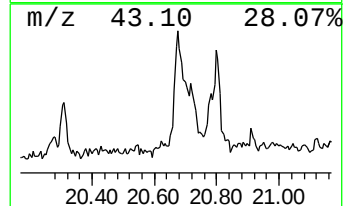
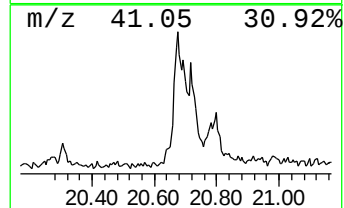
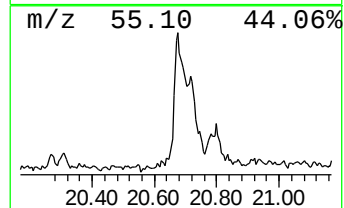
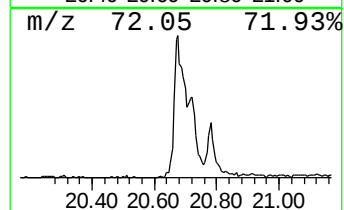
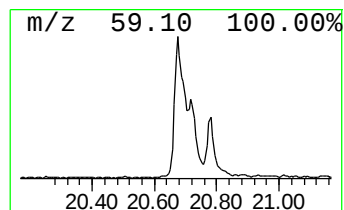
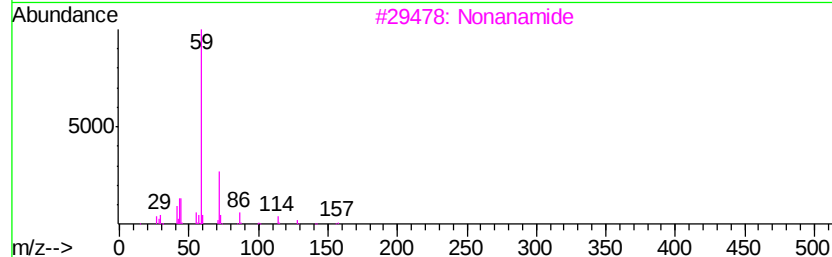
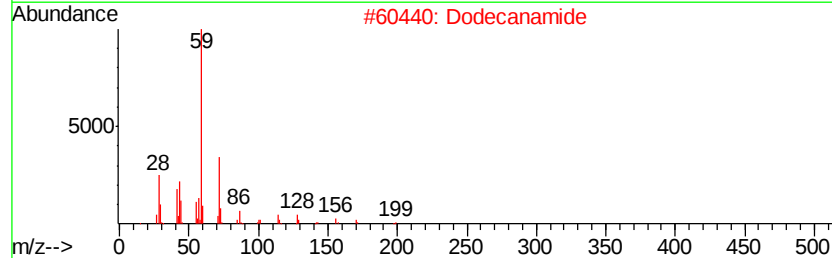
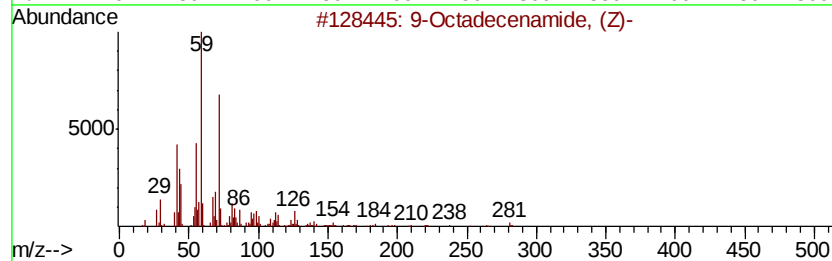
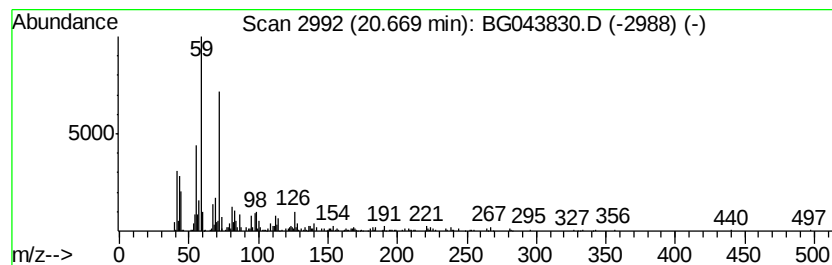
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.67	4.00 ng	442091	Chrysene-d12	21.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		Dodecanamide	199	C12H25NO	001120-16-7	68
3		Nonanamide	157	C9H19NO	001120-07-6	64
4		Hexadecanamide	255	C16H33NO	000629-54-9	59
5		Octanamide	143	C8H17NO	000629-01-6	53



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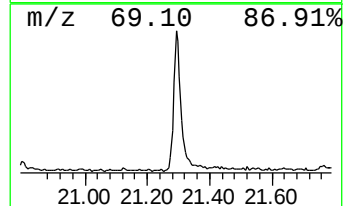
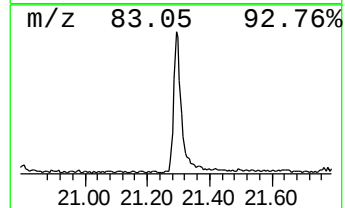
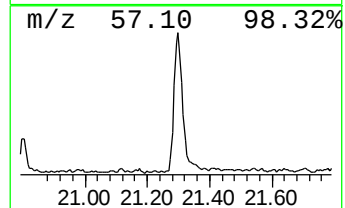
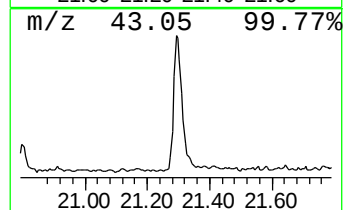
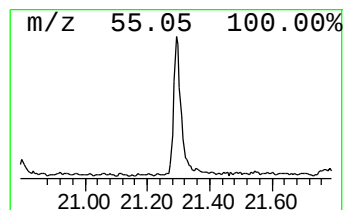
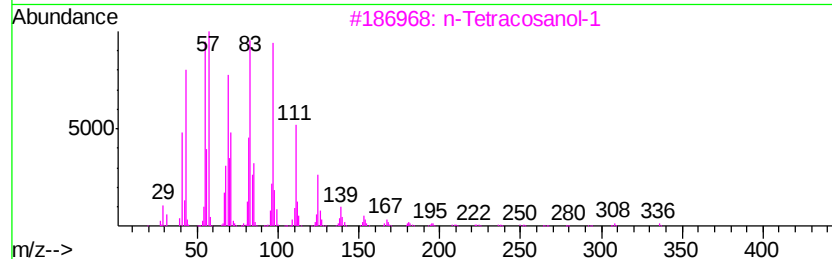
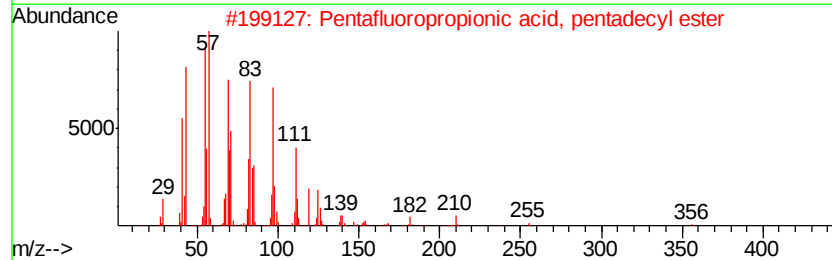
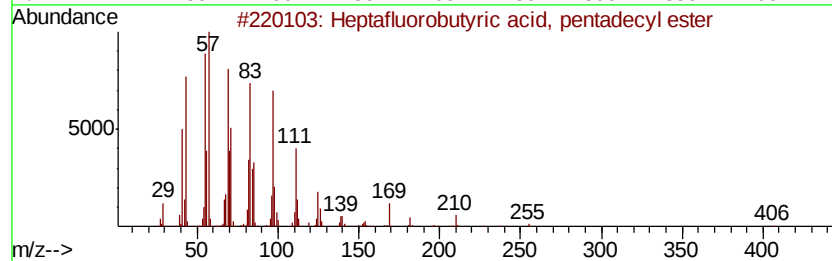
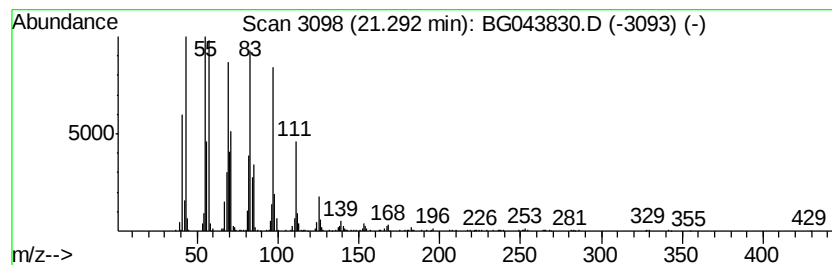
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	7.03 ng	776152	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91



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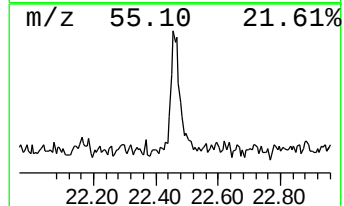
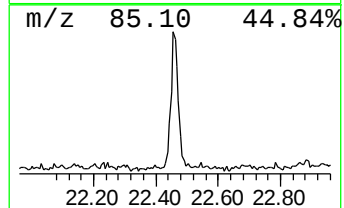
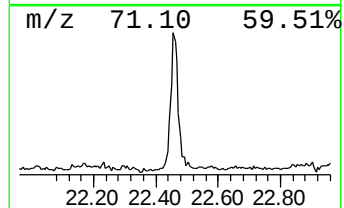
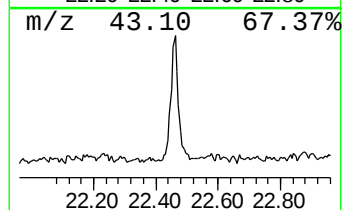
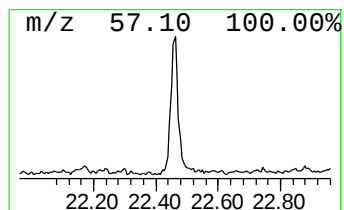
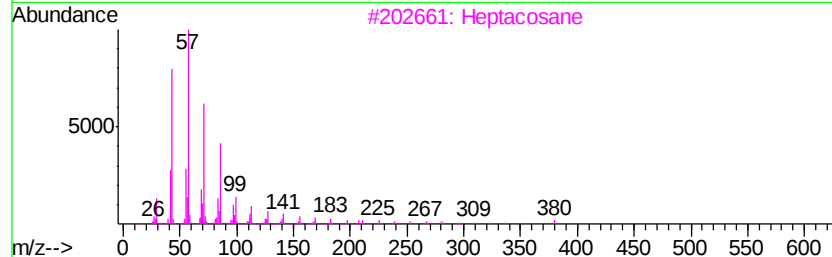
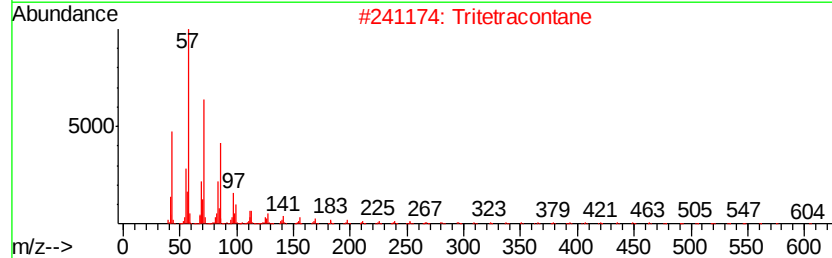
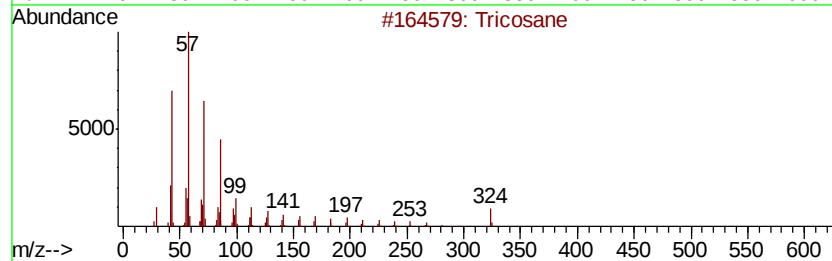
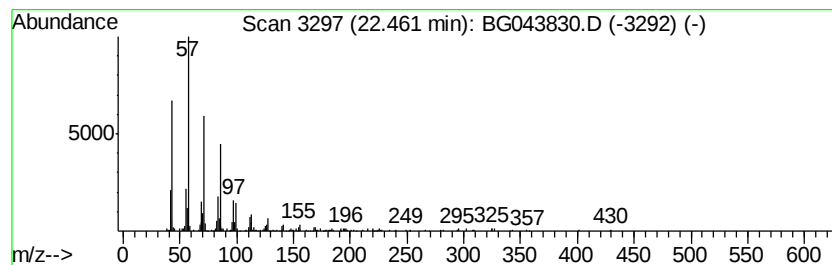
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tricosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.46	2.13 ng	234773	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosane	324	C23H48	000638-67-5	91
2		Tritetracontane	605	C43H88	007098-21-7	90
3		Heptacosane	380	C27H56	000593-49-7	90
4		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043830.D
Acq On : 17 Dec 2019 21:56
Operator : JU
Sample : K6317-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
178K-WC2

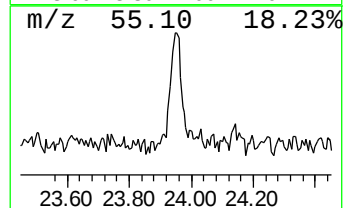
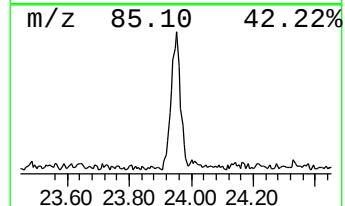
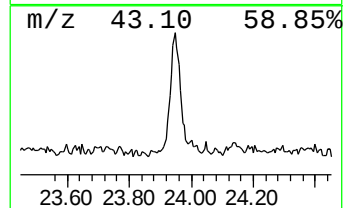
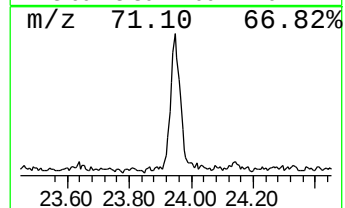
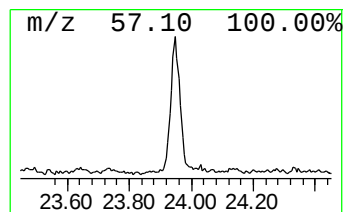
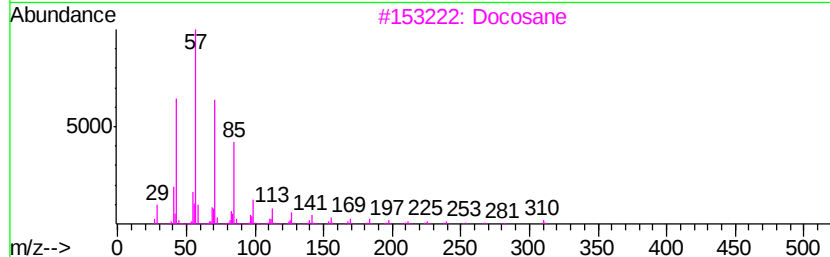
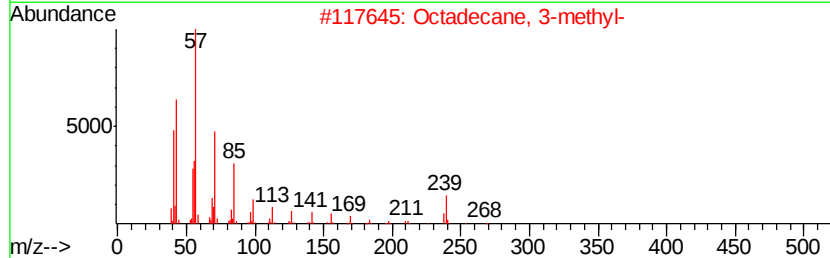
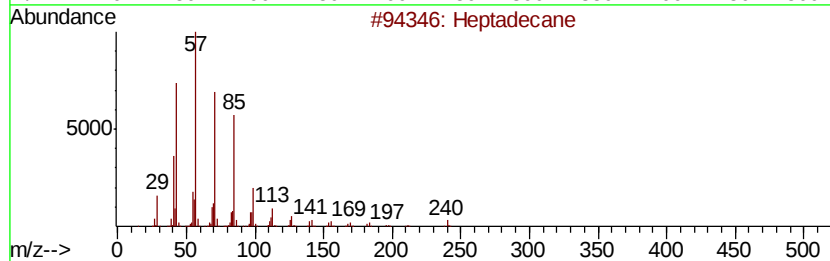
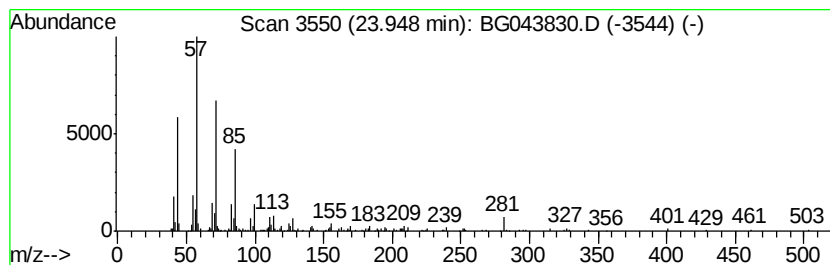
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.95	2.08 ng	218011	Perylene-d12	24.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	83
2		Octadecane, 3-methyl-	268	C19H40	006561-44-0	83
3		Docosane	310	C22H46	000629-97-0	83
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
5		2-Bromo dodecane	248	C12H25Br	013187-99-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121719\
Data File : BG043830.D
Acq On : 17 Dec 2019 21:56
Operator : JU
Sample : K6317-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
178K-WC2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.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...	3.20	9.3	ng	289895	1	8.00	620669	20.0
2-Pentanone, 4-hy...	5.11	16.5	ng	511406	1	8.00	620669	20.0
unknown7.54	7.54	85.5	ng	2653490	1	8.00	620669	20.0
9-Octadecenamide, ...	20.67	4.0	ng	442091	5	21.63	2209630	20.0
Heptafluorobutyri...	21.29	7.0	ng	776152	5	21.63	2209630	20.0
Tricosane	22.46	2.1	ng	234773	5	21.63	2209630	20.0
Heptadecane	23.95	2.1	ng	218011	6	24.78	2097880	20.0