

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042518\
 Data File : BG033993.D
 Acq On : 25 Apr 2018 19:08
 Operator : SJ/JU
 Sample : J2543-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TOTE

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-BG041918.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	5.439	359	366	378	rBV	583933	924444	13.21%	3.281%
2	6.402	524	530	541	rVB	88645	159154	2.27%	0.565%
3	6.996	624	631	644	rVB	400469	656537	9.38%	2.330%
4	7.360	686	693	711	rBV	1055085	1832817	26.19%	6.505%
5	7.830	764	773	779	rVB	219941	376947	5.39%	1.338%
6	8.147	819	827	839	rVB	1034412	1739862	24.86%	6.175%
7	8.976	955	968	976	rBV	866908	1535938	21.95%	5.451%
8	10.609	1239	1246	1254	rBV	340426	599472	8.57%	2.128%
9	13.083	1660	1667	1675	rBV	2697968	4088636	58.42%	14.511%
10	14.457	1893	1901	1910	rVB2	605912	945962	13.52%	3.357%
11	15.950	2148	2155	2165	rBV	2177215	3251576	46.46%	11.540%
12	16.144	2181	2188	2192	rBV	116953	176321	2.52%	0.626%
13	17.207	2363	2369	2376	rBV	825613	1276664	18.24%	4.531%
14	18.118	2520	2524	2535	rBV	151548	251285	3.59%	0.892%
15	19.405	2738	2743	2750	rBV2	108198	165066	2.36%	0.586%
16	19.845	2812	2818	2825	rBV	5079962	6998308	100.00%	24.837%
17	21.156	3036	3041	3047	rBV2	97415	158459	2.26%	0.562%
18	21.467	3087	3094	3101	rBV	994078	1549131	22.14%	5.498%
19	24.522	3603	3614	3624	rBV2	553732	1489944	21.29%	5.288%

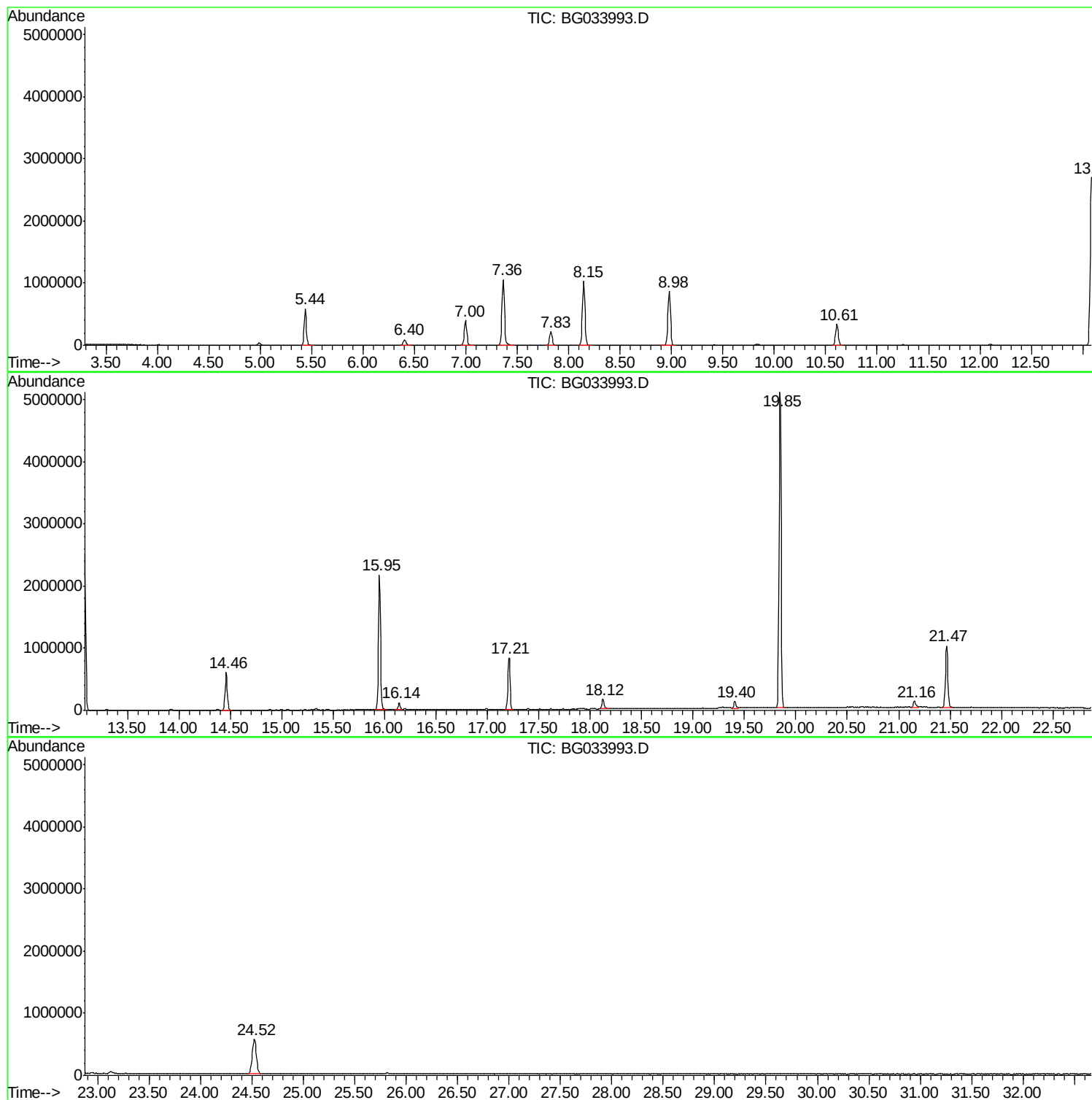
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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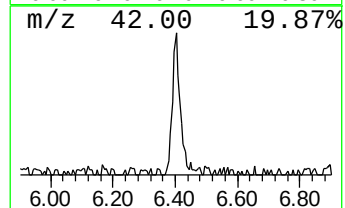
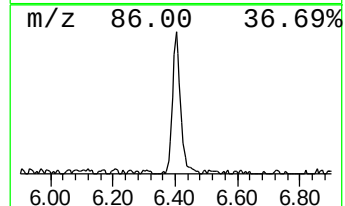
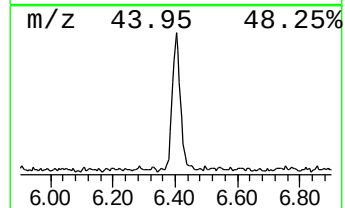
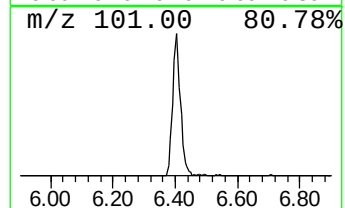
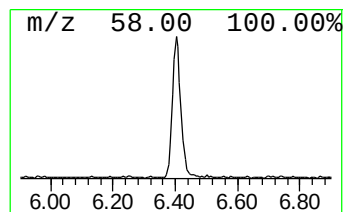
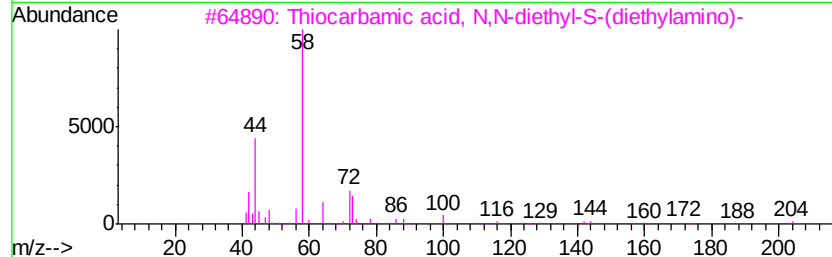
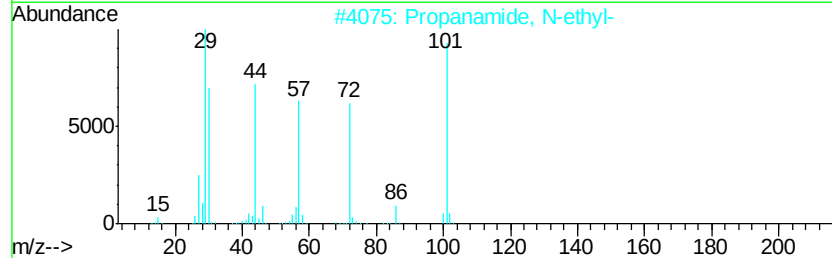
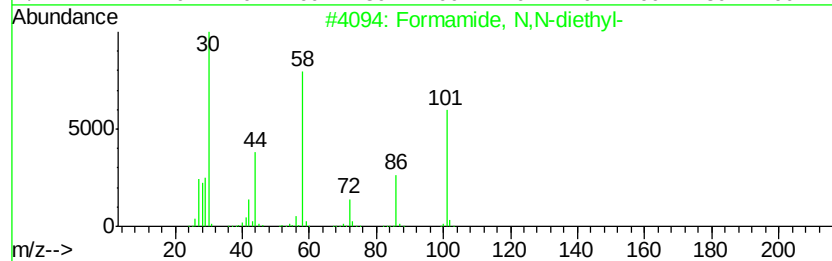
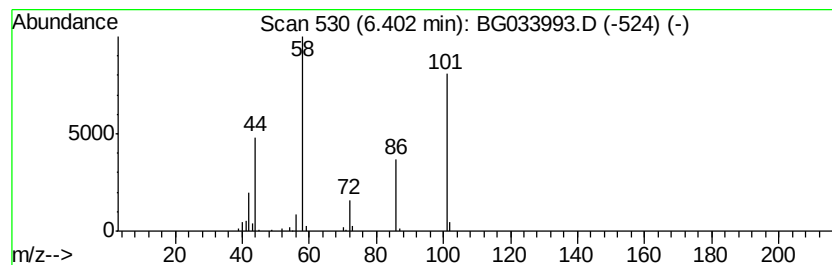
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Peak Number 1 Formamide, N,N-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	8.44 ng	159154	1,4-Dichlorobenzene-d4	7.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	91
2			Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	32
3			Thiocarbamic acid, N,N-diethyl-S...	204	C9H20N2OS	070151-21-2	25
4			N,N,N'-Trimethyl-1,3-propanediamine	116	C6H16N2	004543-96-8	25
5			1,2-Ethanediamine, N,N,N'-trimet...	102	C5H14N2	000142-25-6	16



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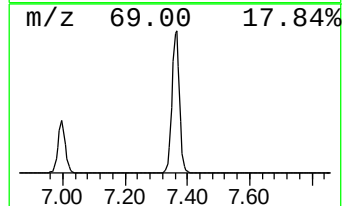
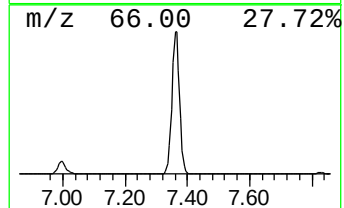
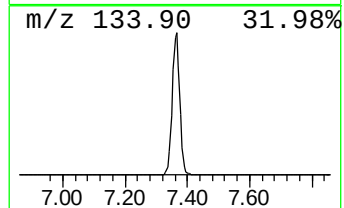
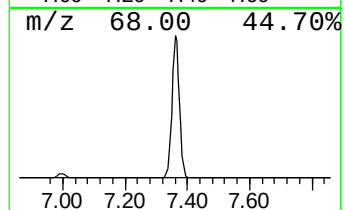
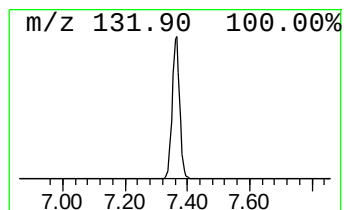
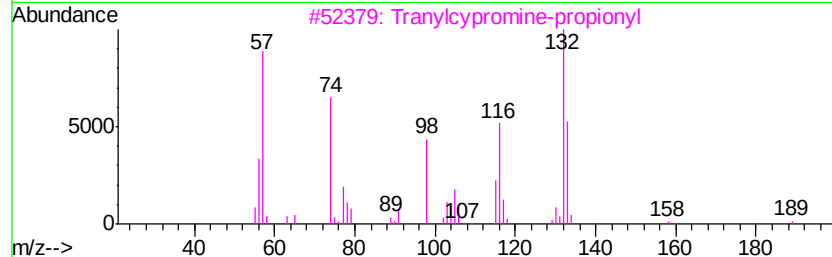
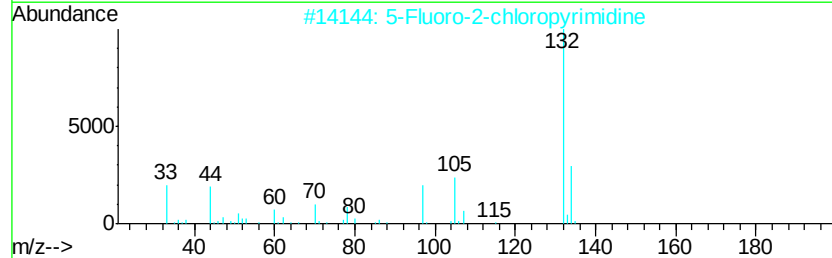
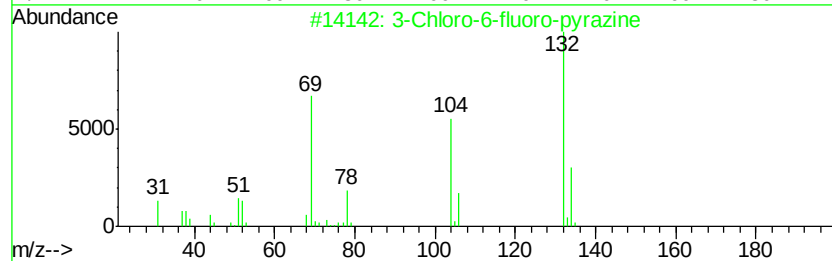
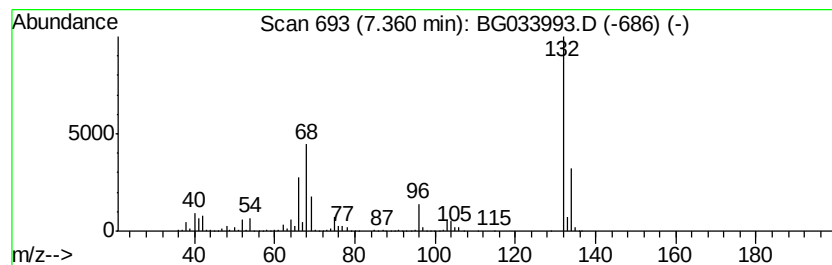
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Peak Number 2 unknown7.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	97.25 ng	1832820	1,4-Dichlorobenzene-d4	7.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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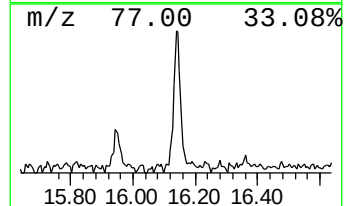
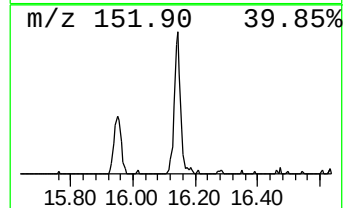
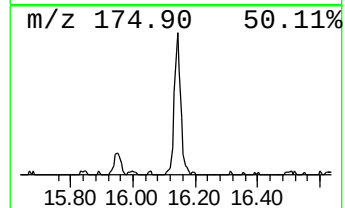
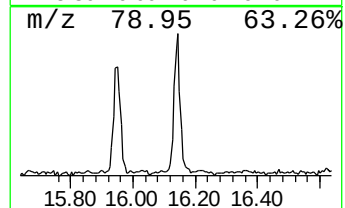
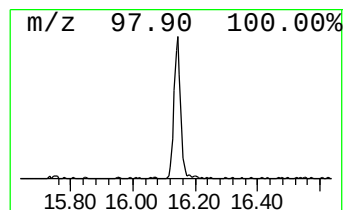
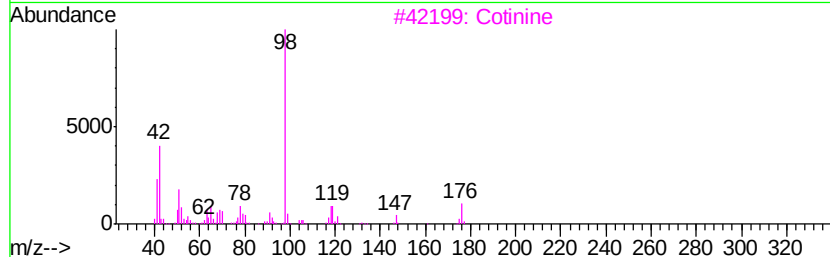
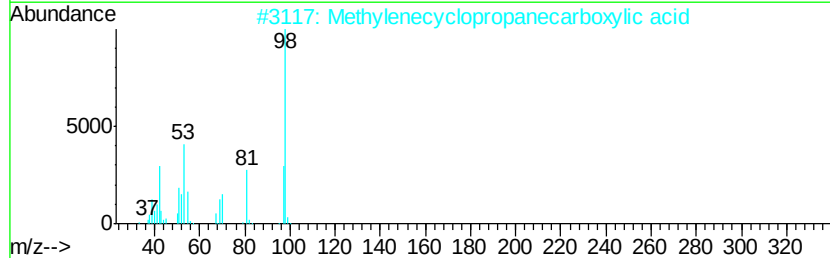
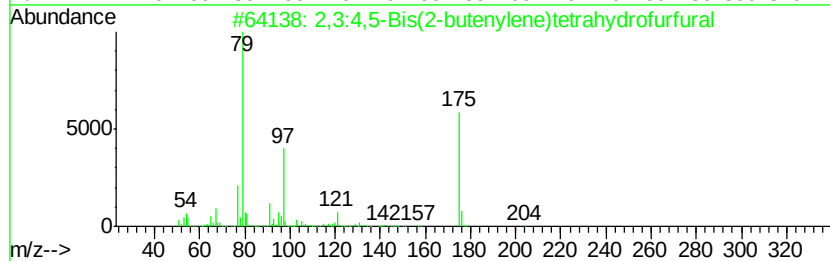
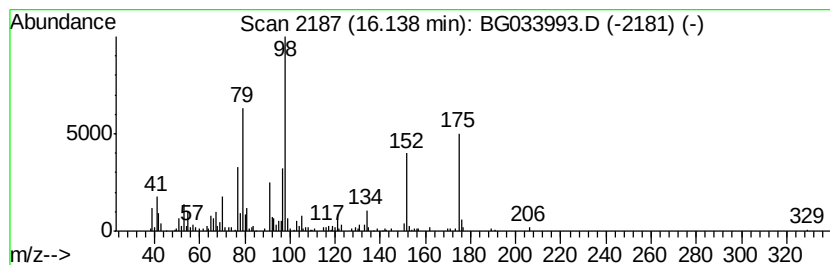
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Peak Number 4 unknown-16.14 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	2.76 ng	176321	Phenanthrene-d10	17.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3:4,5-Bis(2-butenylene)tetrahy...	204	C13H16O2	000126-15-8	38		
2	Methylenecyclopropanecarboxylic ...	98	C5H6O2	062266-36-8	27		
3	Cotinine	176	C10H12N2O	000486-56-6	22		
4	3-Furanmethanol	98	C5H6O2	004412-91-3	16		
5	3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	14		



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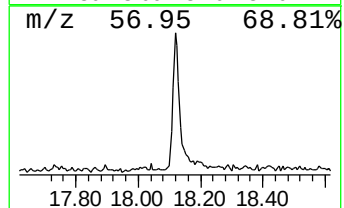
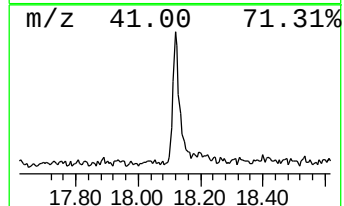
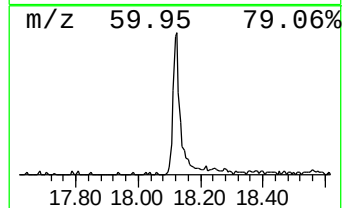
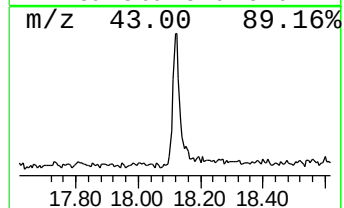
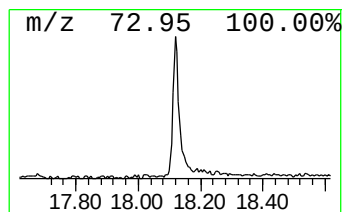
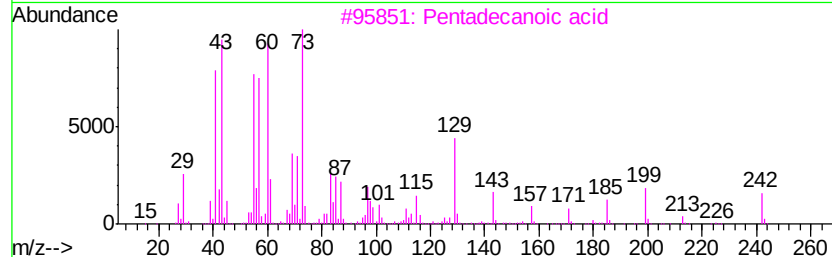
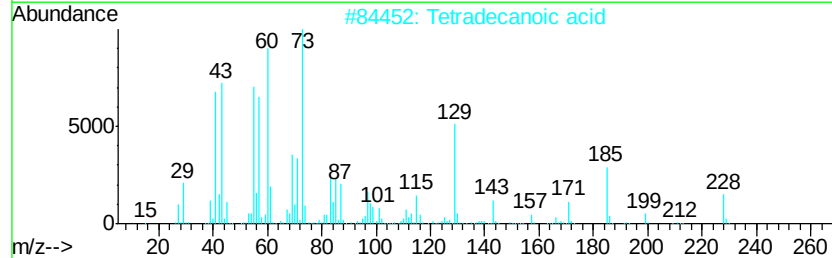
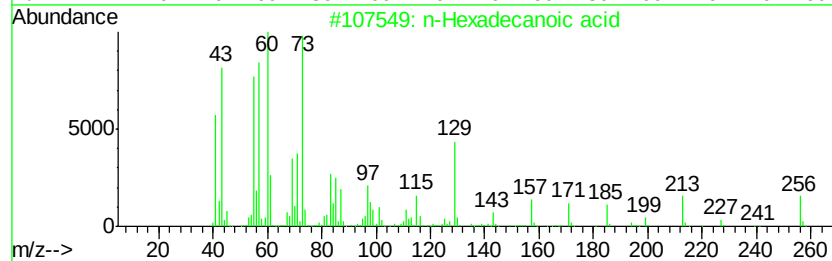
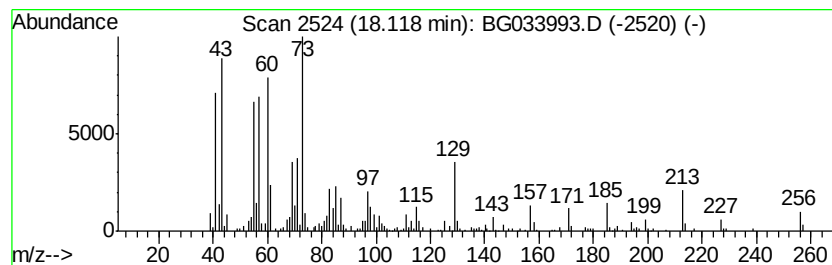
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.12	3.94 ng	251285	Phenanthrene-d10	17.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tridecanoic acid	214	C13H26O2	000638-53-9	76
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



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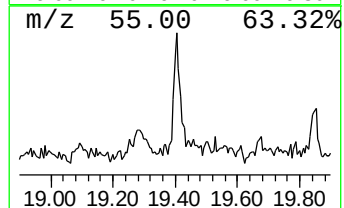
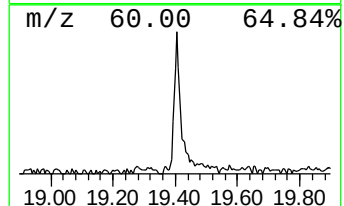
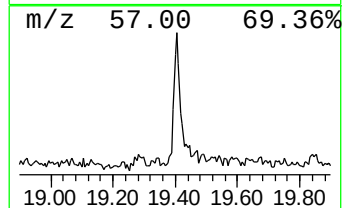
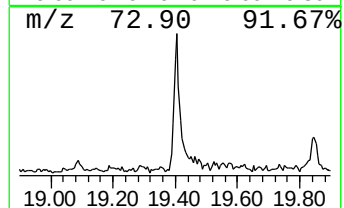
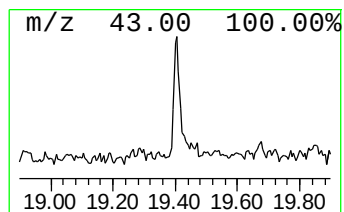
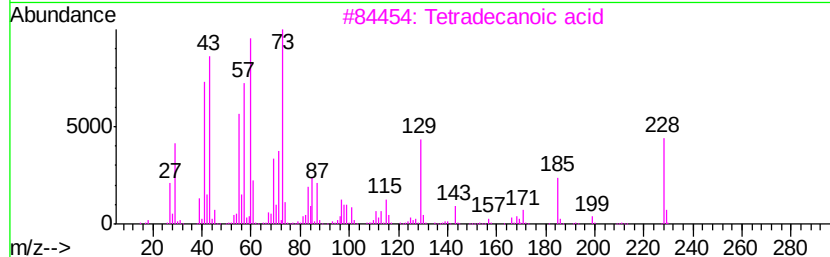
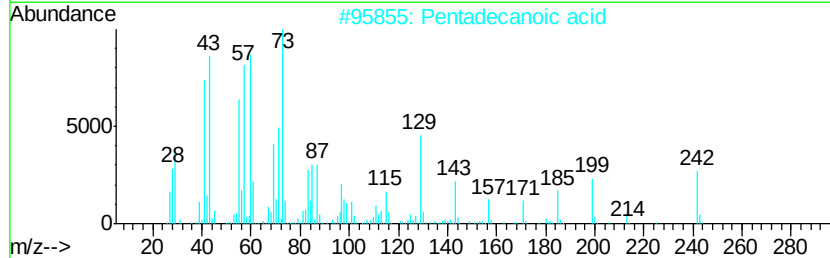
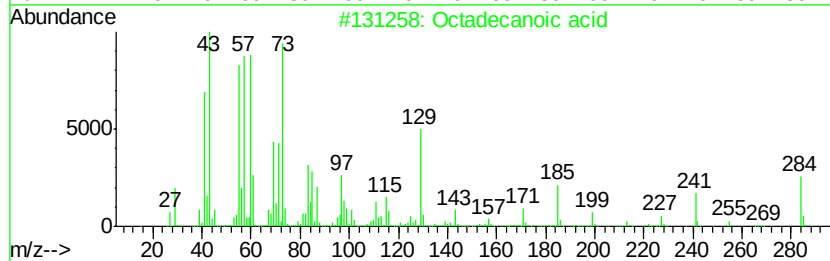
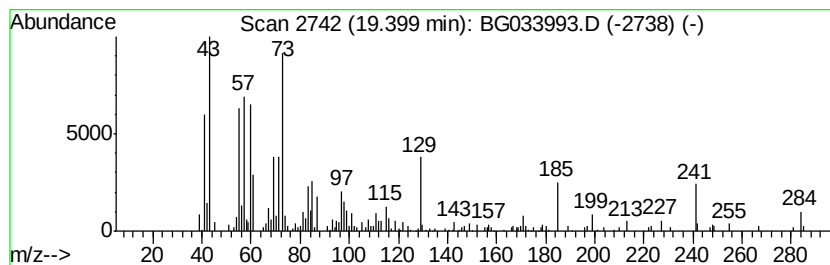
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Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.40	2.13 ng	165066	Chrysene-d12	21.47	
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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76



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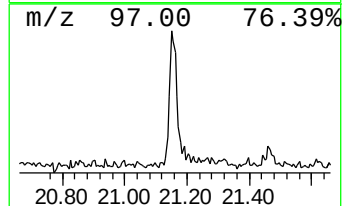
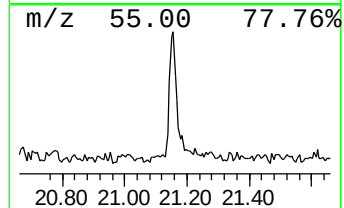
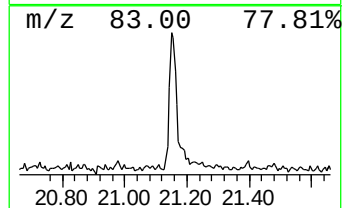
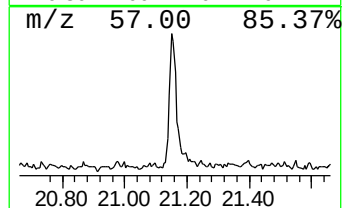
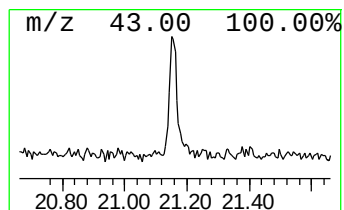
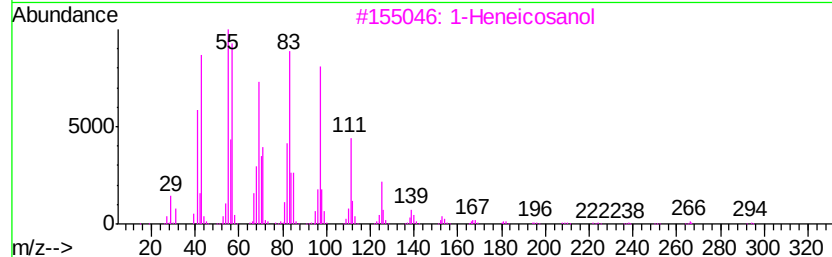
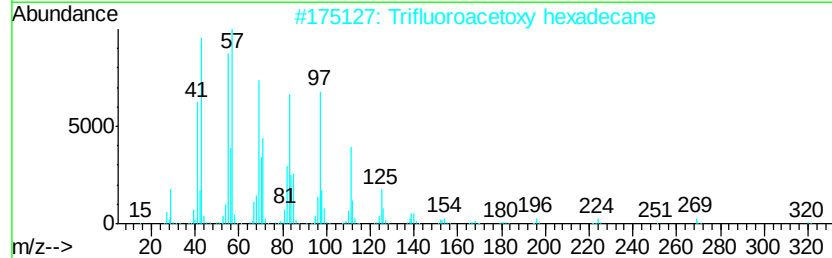
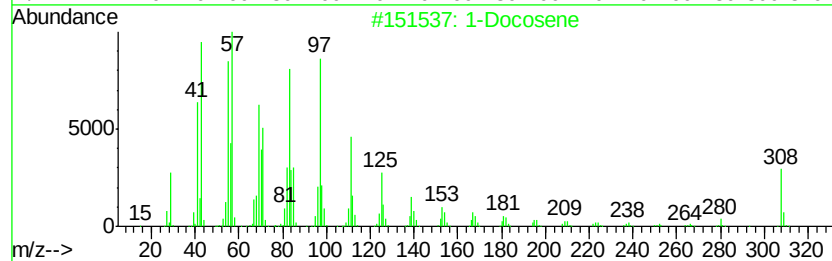
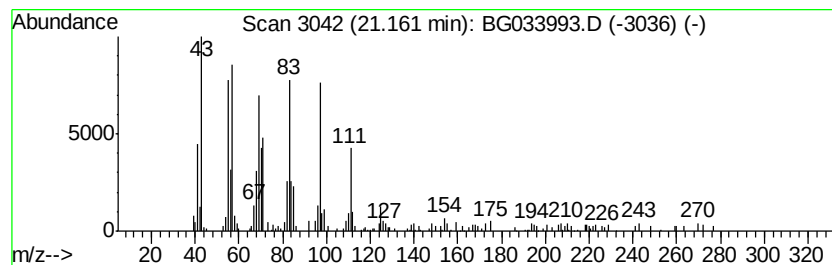
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Peak Number 7 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.16	2.05 ng	158459	Chrysene-d12	21.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	99
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
5	Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG042518\
Data File : BG033993.D
Acq On : 25 Apr 2018 19:08
Operator : SJ/JU
Sample : J2543-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TOTE

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.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
Formamide, N,N-di...	6.40	8.4	ng	159154	1	7.82	376947	20.0
unknown7.36	7.36	97.3	ng	1832820	1	7.82	376947	20.0
unknown-16.14	16.14	2.8	ng	176321	4	17.21	1276660	20.0
n-Hexadecanoic acid	18.12	3.9	ng	251285	4	17.21	1276660	20.0
Octadecanoic acid	19.40	2.1	ng	165066	5	21.47	1549130	20.0
1-Docosene	21.16	2.0	ng	158459	5	21.47	1549130	20.0