

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101821\
 Data File : BG050624.D
 Acq On : 18 Oct 2021 19:34
 Operator : CG/JU
 Sample : M4251-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P287-DITCH

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-BG100621.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050624.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.791	384	392	405	rBV	346499	586005	17.68%	4.479%
2	7.389	657	664	674	rBV	220107	394622	11.90%	3.016%
3	8.253	804	811	822	rVB	150470	258821	7.81%	1.978%
4	9.422	1001	1010	1019	rBV	524475	945284	28.52%	7.225%
5	10.821	1241	1248	1255	rBV	64304	116350	3.51%	0.889%
6	11.079	1284	1292	1300	rBV	201793	375576	11.33%	2.871%
7	13.494	1695	1703	1715	rBV	1221834	1977449	59.65%	15.114%
8	14.869	1930	1937	1946	rVB	342777	550354	16.60%	4.207%
9	16.355	2183	2190	2203	rBV	960130	1544671	46.60%	11.806%
10	16.531	2213	2220	2230	rBV	86501	154631	4.66%	1.182%
11	17.613	2398	2404	2413	rBV	467187	730700	22.04%	5.585%
12	18.470	2545	2550	2560	rBV	119447	185176	5.59%	1.415%
13	19.734	2760	2765	2771	rBV2	52475	78596	2.37%	0.601%
14	20.204	2839	2845	2853	rBV	2538140	3314947	100.00%	25.337%
15	20.979	2973	2977	2982	rBV	108284	143021	4.31%	1.093%
16	21.514	3063	3068	3079	rVB3	60337	117640	3.55%	0.899%
17	21.913	3129	3136	3143	rBV	434702	762234	22.99%	5.826%
18	23.658	3428	3433	3440	rVB2	20771	41083	1.24%	0.314%
19	25.327	3706	3717	3728	rVB3	252781	770172	23.23%	5.887%
20	26.532	3917	3922	3930	rVB10	13272	36060	1.09%	0.276%

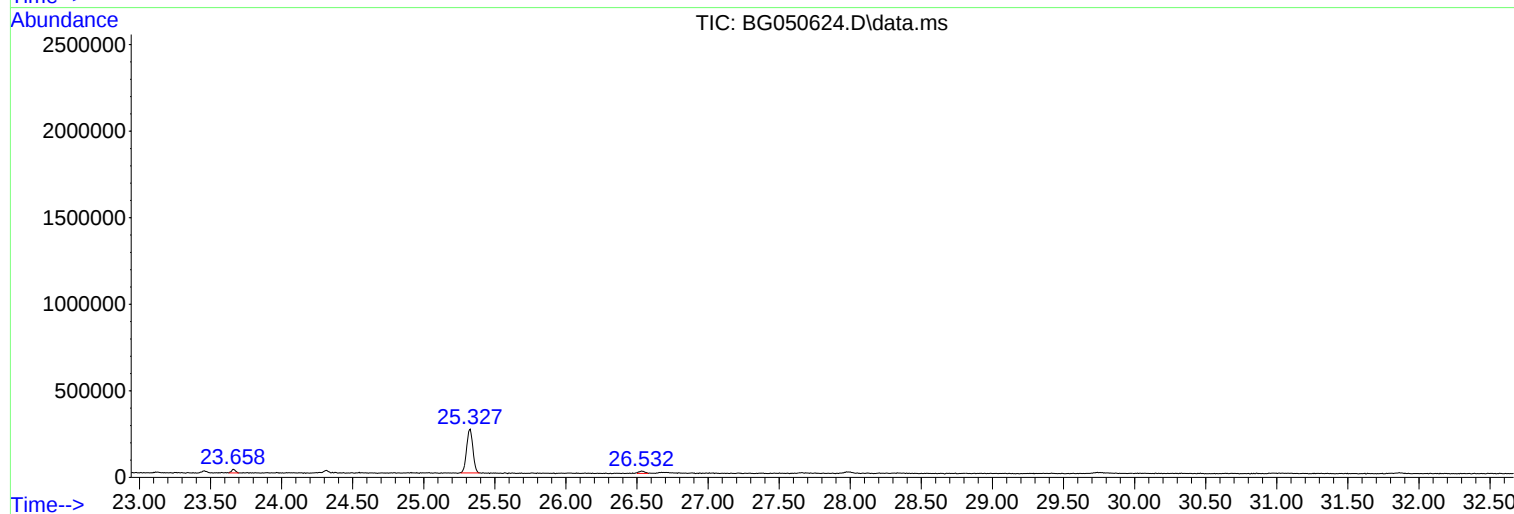
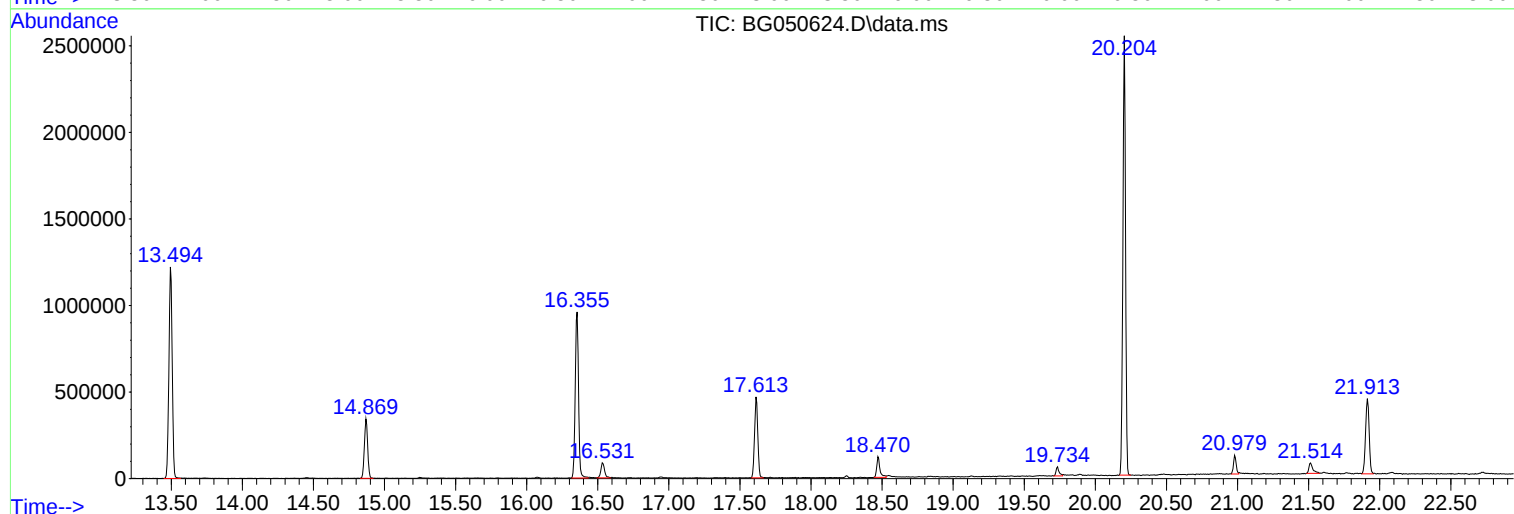
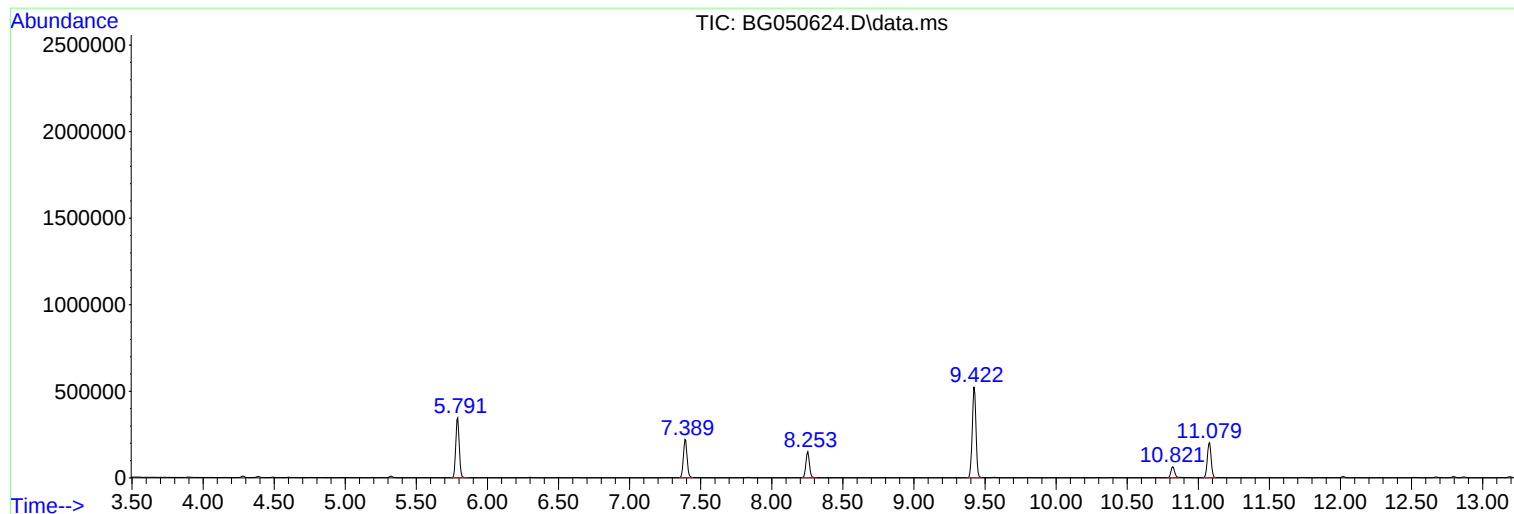
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Data File : BG050624.D
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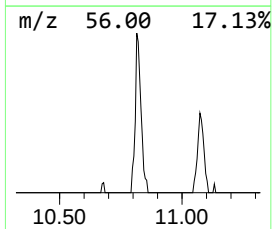
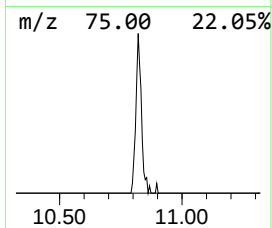
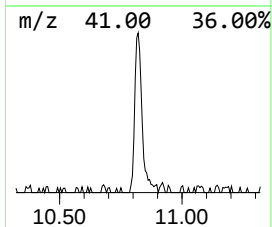
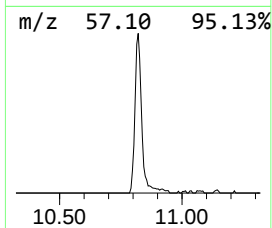
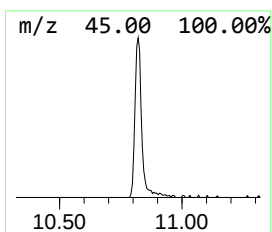
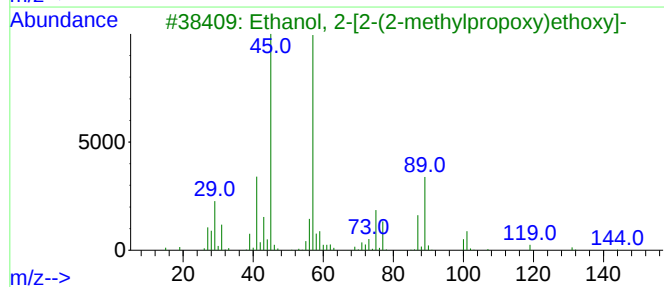
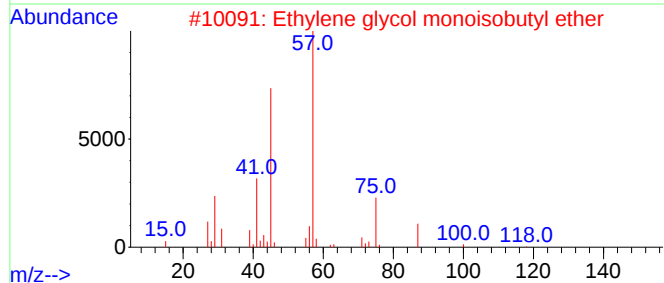
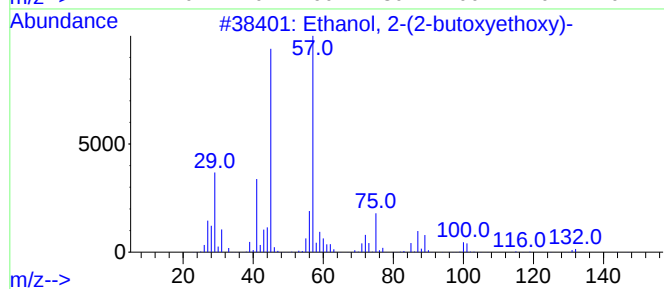
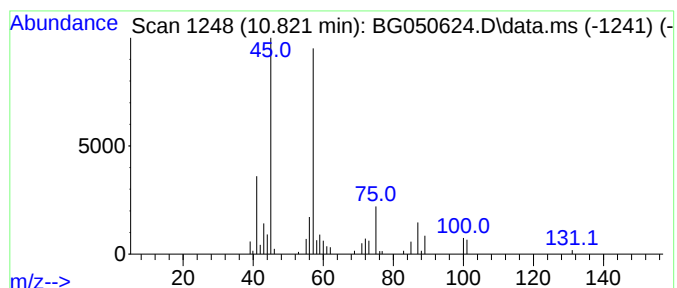
Instrument :
BNA_G
ClientSampleId :
P287-DITCH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.820	6.20 ng	116350	Naphthalene-d8	11.079	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	64
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45



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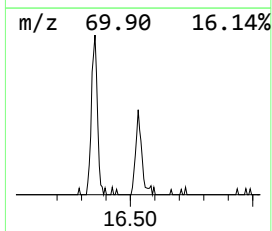
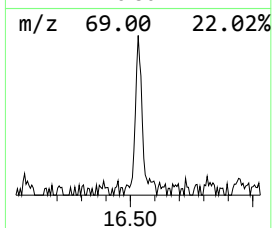
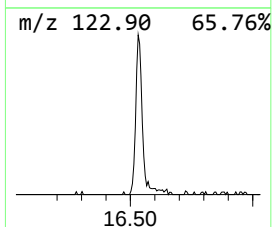
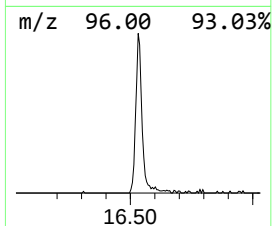
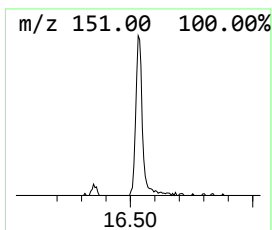
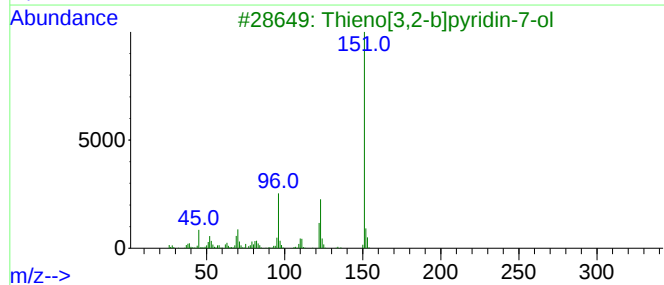
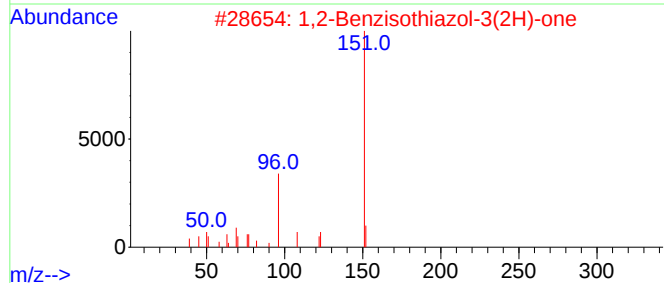
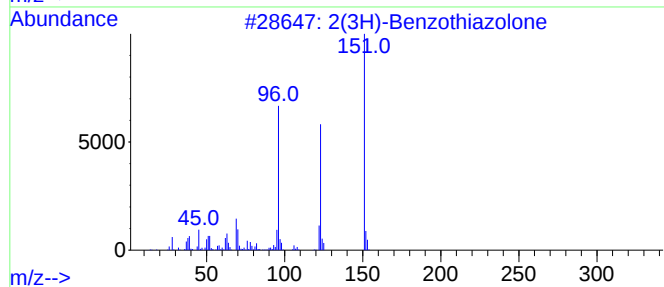
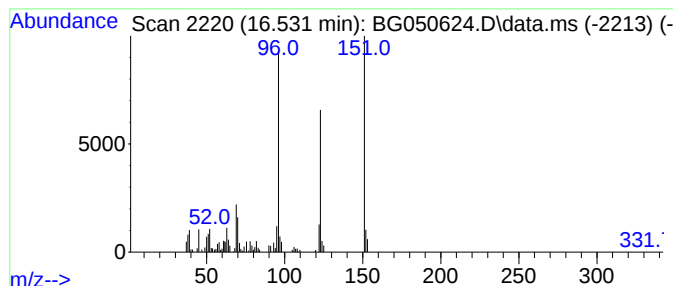
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 2(3H)-Benzothiazolone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.532	4.23 ng	154631	Phenanthrene-d10	17.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	93
2			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	59
3			Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	47
4			Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	38
5			2-Mercapto-1,3-benzoxazole	151	C7H5NOS	002382-96-9	35



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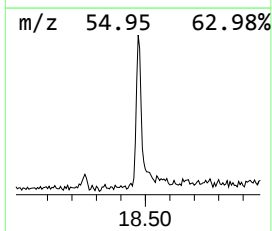
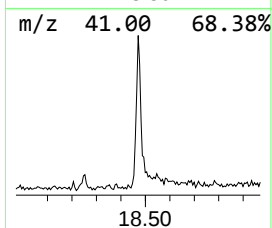
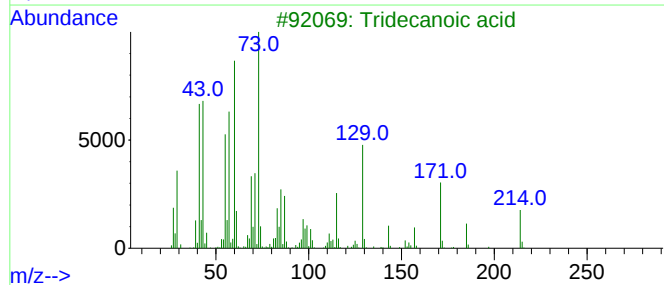
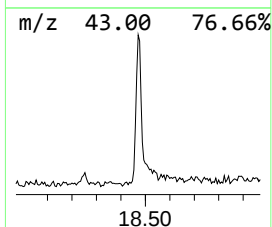
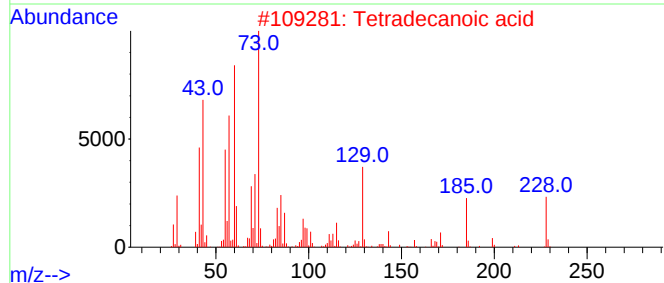
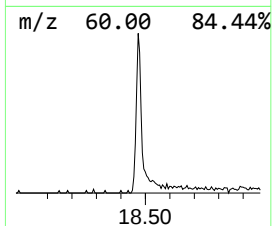
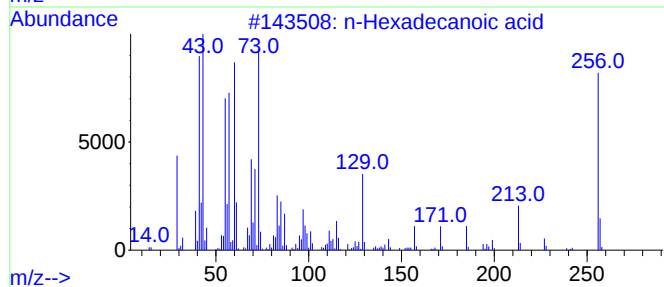
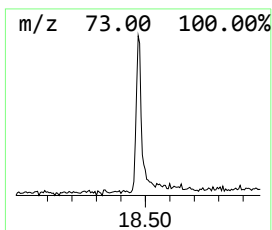
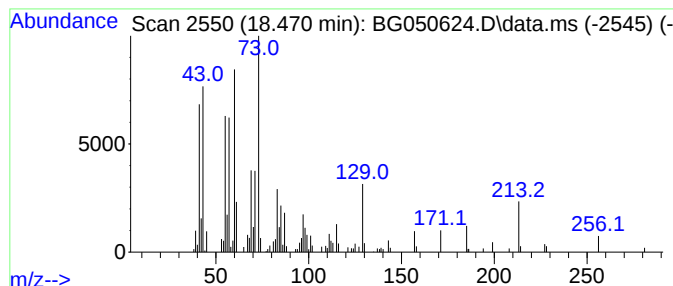
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.470	5.07 ng	185176	Phenanthrene-d10	17.613

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	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			Nonanoic acid	158	C9H18O2	000112-05-0	53



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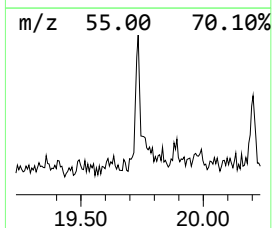
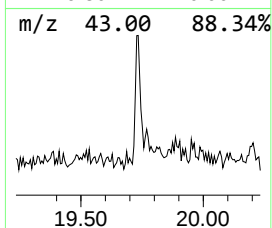
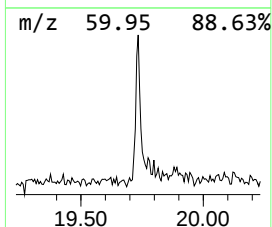
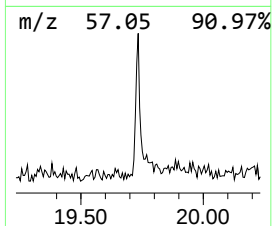
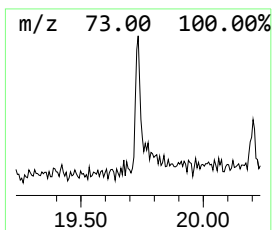
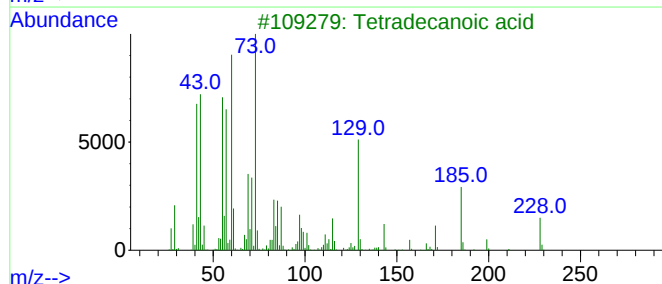
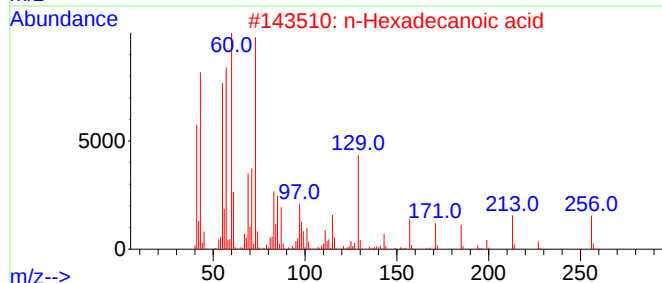
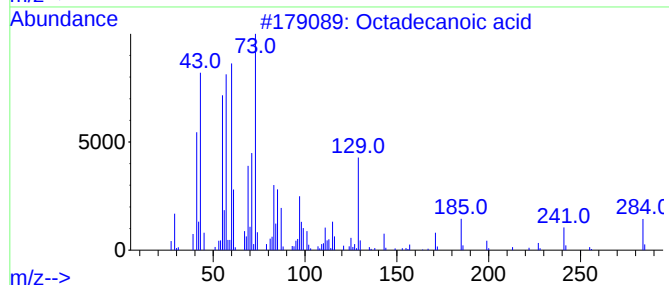
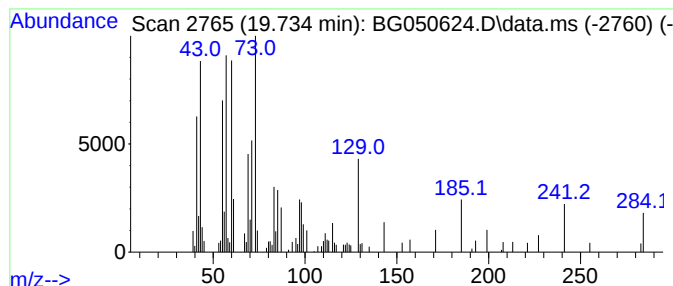
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.734	2.15 ng	78596	Phenanthrene-d10	17.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			Tridecanoic acid	214	C13H26O2	000638-53-9	59



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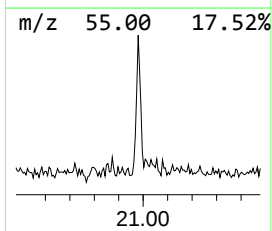
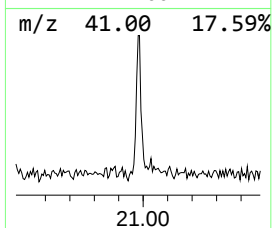
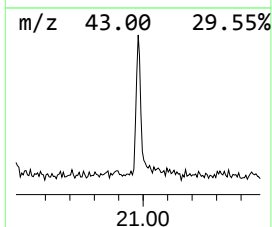
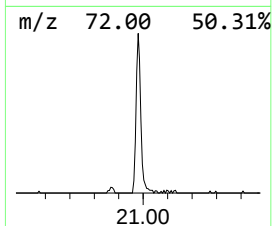
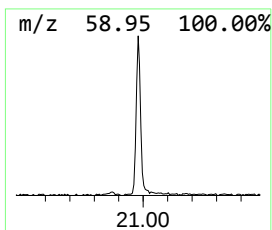
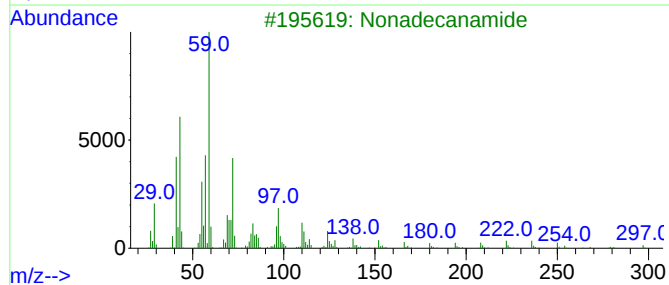
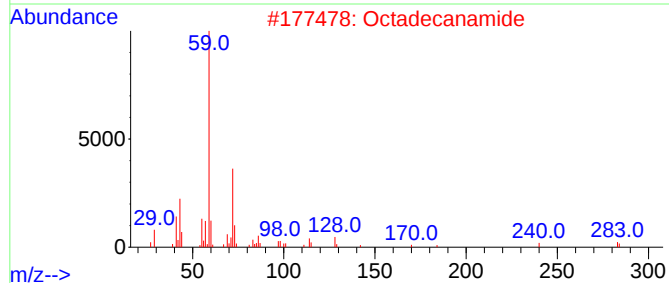
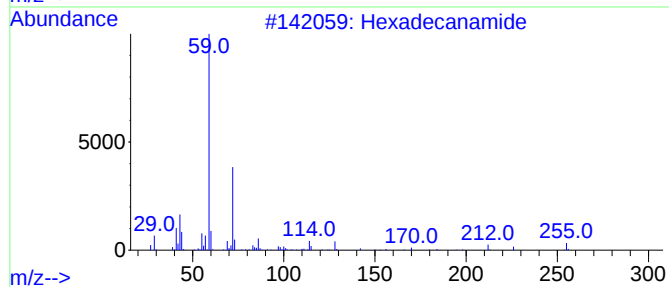
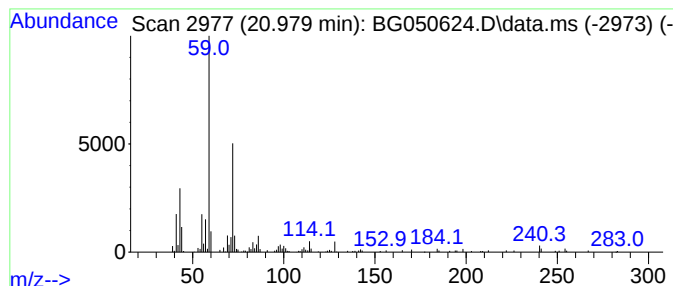
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Peak Number 5 Hexadecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.979	3.75 ng	143021	Chrysene-d12	21.913

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanamide	255	C16H33NO	000629-54-9	78
2			Octadecanamide	283	C18H37NO	000124-26-5	72
3			Nonadecanamide	297	C19H39NO	058185-32-3	64
4			Tetradecanamide	227	C14H29NO	000638-58-4	64
5			Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	59



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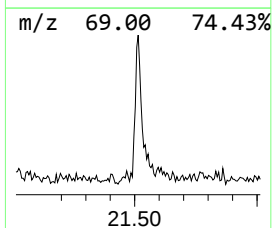
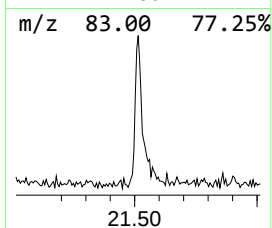
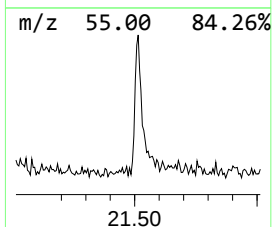
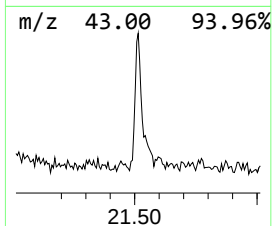
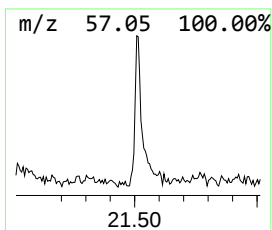
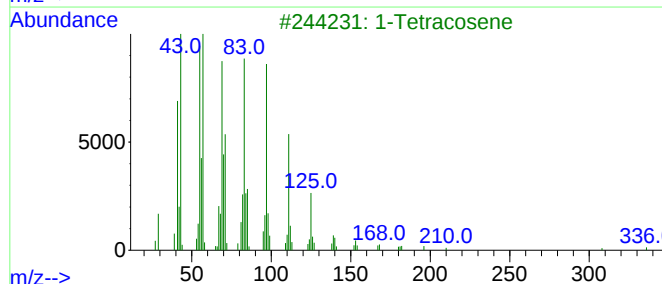
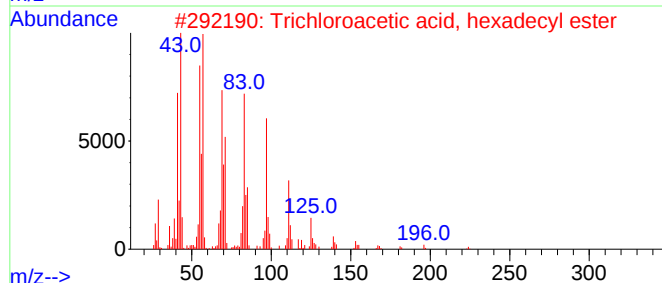
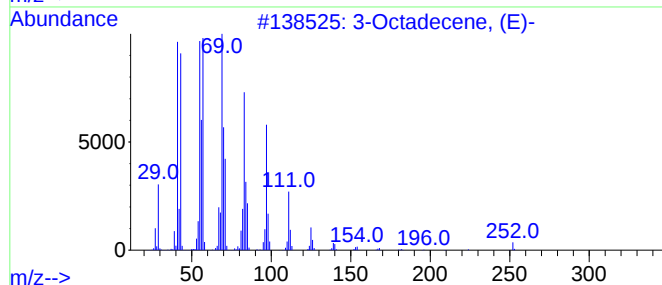
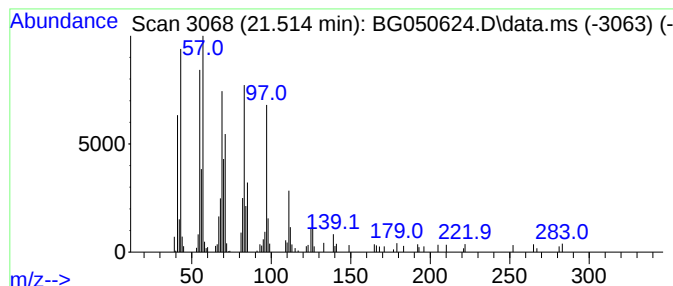
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.514	3.09 ng	117640	Chrysene-d12	21.913

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octadecene, (E)-	252	C18H36	007206-19-1	96
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			1-Tetracosene	336	C24H48	010192-32-2	91
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101821\
Data File : BG050624.D
Acq On : 18 Oct 2021 19:34
Operator : CG/JU
Sample : M4251-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P287-DITCH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.820	6.2	ng	116350	2	11.079	375576	20.0
2(3H)-Benzothia...	16.532	4.2	ng	154631	4	17.613	730700	20.0
n-Hexadecanoic ...	18.470	5.1	ng	185176	4	17.613	730700	20.0
Octadecanoic acid	19.734	2.1	ng	78596	4	17.613	730700	20.0
Hexadecanamide	20.979	3.8	ng	143021	5	21.913	762234	20.0
3-Octadecene, (E)-	21.514	3.1	ng	117640	5	21.913	762234	20.0