

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102521\
 Data File : BG050717.D
 Acq On : 25 Oct 2021 19:26
 Operator : CG/JU
 Sample : M4295-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RBR-251686

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: BG050717.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	385	392	400	rBV	647373	1088726	55.29%	7.384%
2	7.395	657	665	673	rBV	657625	1172597	59.55%	7.953%
3	8.247	801	810	823	rVB	149766	279178	14.18%	1.894%
4	8.359	823	829	837	rVB	16709	27707	1.41%	0.188%
5	9.422	1001	1010	1018	rBV	406293	754511	38.32%	5.118%
6	10.814	1239	1247	1262	rBV	101291	186053	9.45%	1.262%
7	11.073	1284	1291	1298	rBV	202324	379387	19.27%	2.573%
8	13.494	1694	1703	1713	rVB	963364	1531992	77.81%	10.391%
9	14.869	1930	1937	1944	rVB	307302	492550	25.02%	3.341%
10	16.349	2183	2189	2200	rBV	673799	1077142	54.70%	7.306%
11	16.543	2217	2222	2230	rBV3	52805	112565	5.72%	0.763%
12	17.260	2338	2344	2350	rBV3	58849	104782	5.32%	0.711%
13	17.330	2352	2356	2360	rVV	70903	86608	4.40%	0.587%
14	17.383	2361	2365	2369	rVB2	29402	41303	2.10%	0.280%
15	17.612	2398	2404	2408	rBV	361514	561030	28.49%	3.805%
16	17.654	2408	2411	2417	rVB	131120	192884	9.80%	1.308%
17	18.071	2479	2482	2487	rVB2	27413	39370	2.00%	0.267%
18	18.241	2508	2511	2516	rVB	57590	72303	3.67%	0.490%
19	18.470	2545	2550	2556	rBV2	135324	215658	10.95%	1.463%
20	18.758	2596	2599	2604	rBV	29458	37436	1.90%	0.254%
21	19.023	2640	2644	2651	rVB3	41495	67310	3.42%	0.457%
22	19.404	2705	2709	2713	rVB	356119	398072	20.22%	2.700%
23	19.534	2728	2731	2736	rVB2	77853	92269	4.69%	0.626%
24	19.651	2747	2751	2758	rVB	335910	503769	25.58%	3.417%
25	20.015	2809	2813	2820	rVB	288355	439899	22.34%	2.984%
26	20.198	2839	2844	2850	rVB	1405809	1969012	100.00%	13.355%
27	21.508	3064	3067	3076	rVB3	90887	150575	7.65%	1.021%
28	21.760	3106	3110	3118	rVB	581259	852599	43.30%	5.783%
29	21.913	3128	3136	3141	rBV2	337200	794639	40.36%	5.390%
30	21.960	3141	3144	3149	rVB	140663	216902	11.02%	1.471%
31	24.234	3525	3531	3538	rBV2	99168	286125	14.53%	1.941%
32	25.327	3709	3717	3726	rVB2	177621	518637	26.34%	3.518%

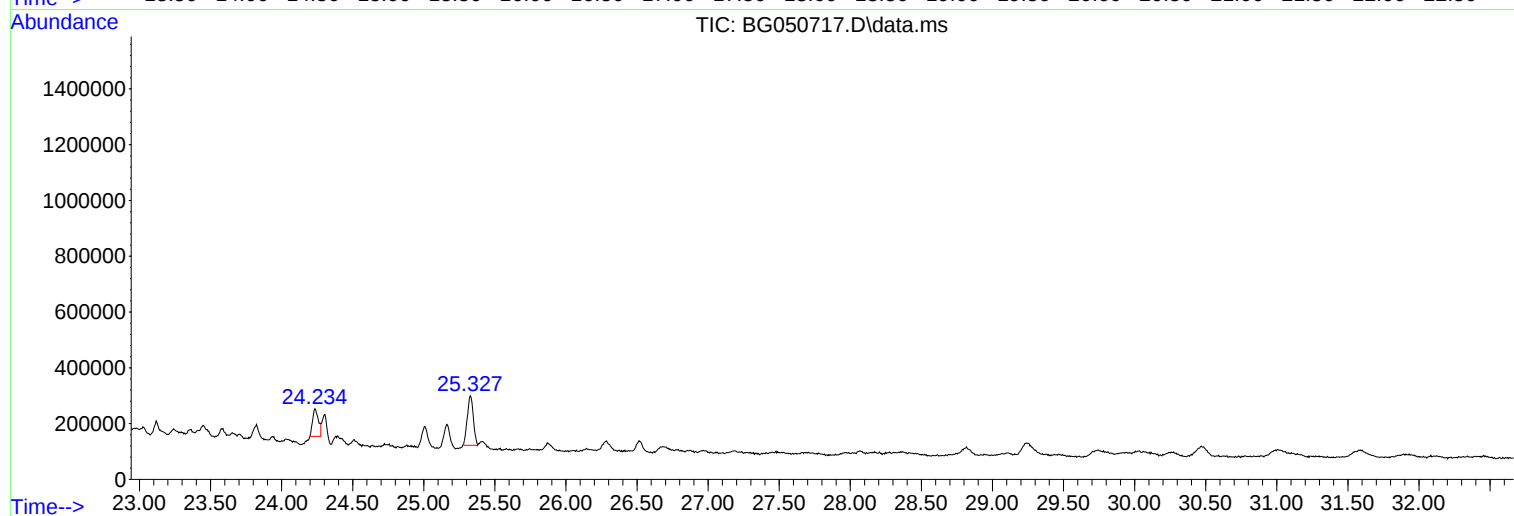
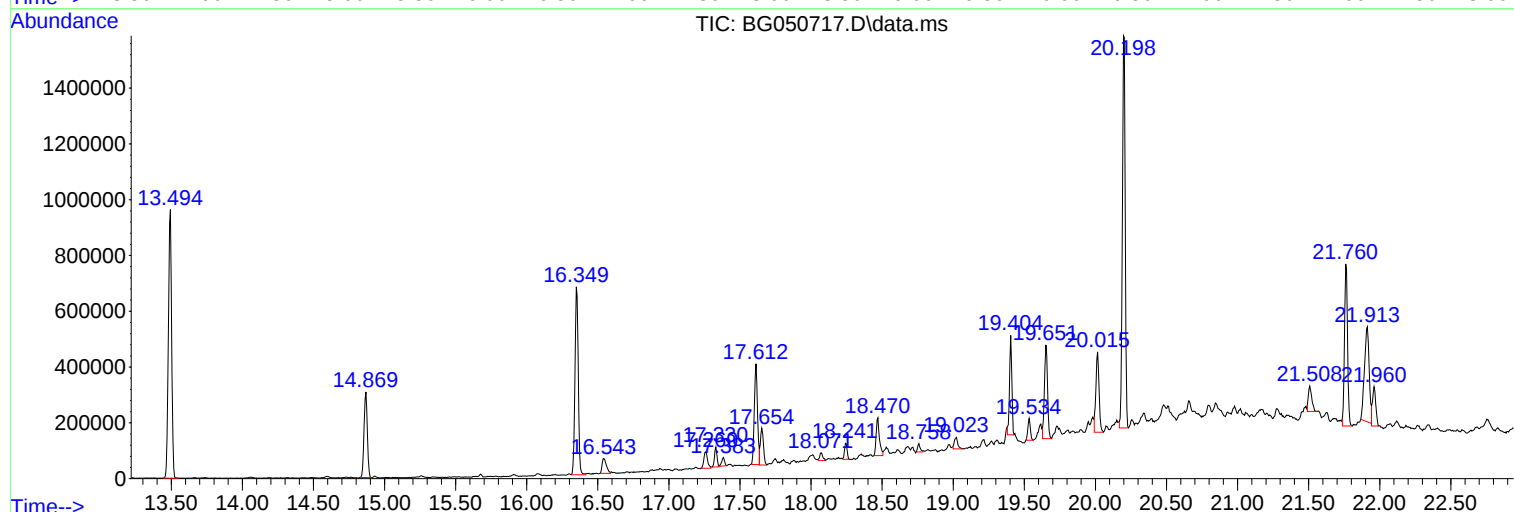
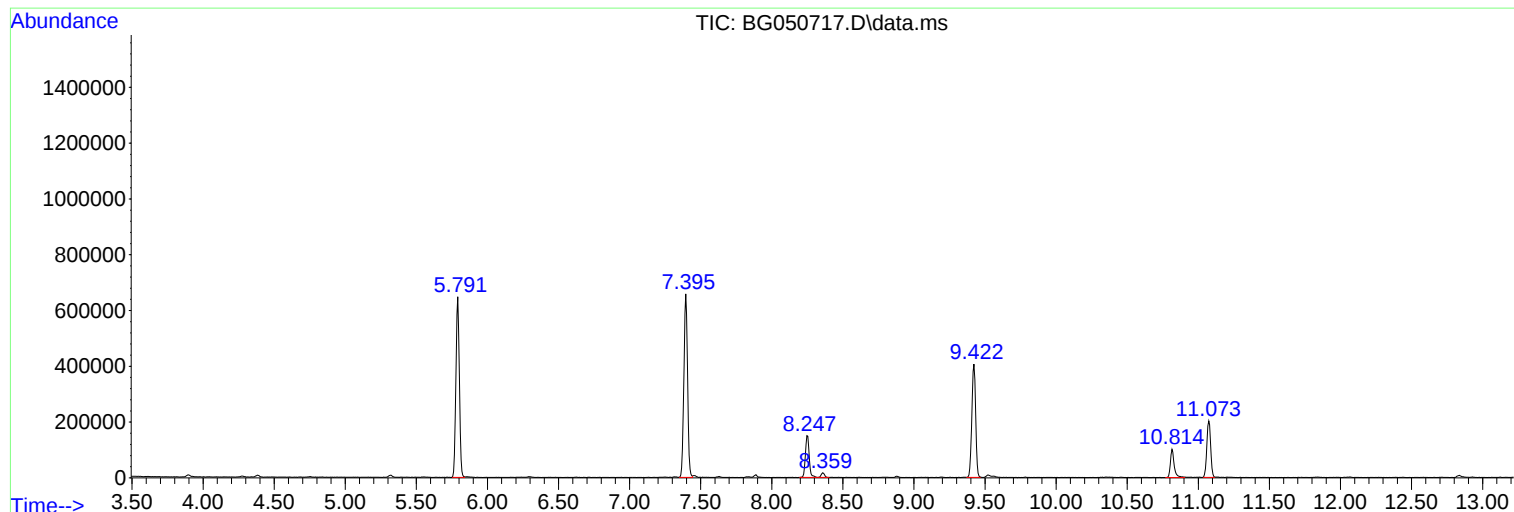
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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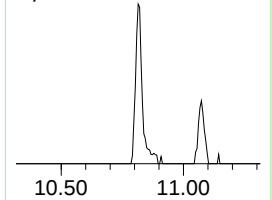
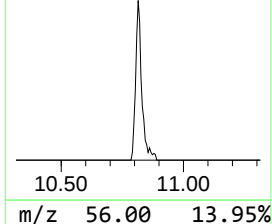
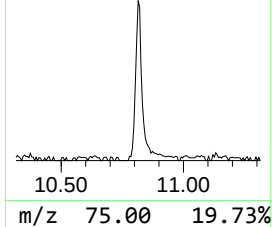
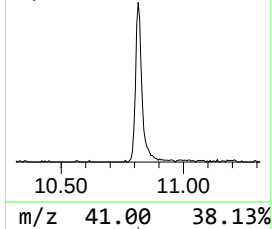
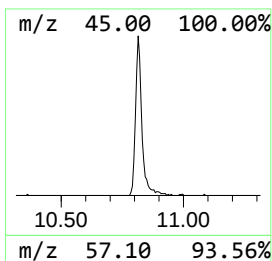
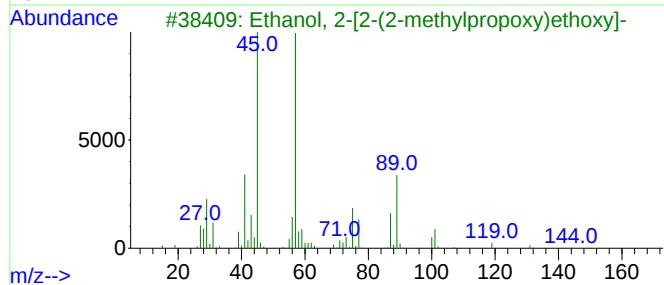
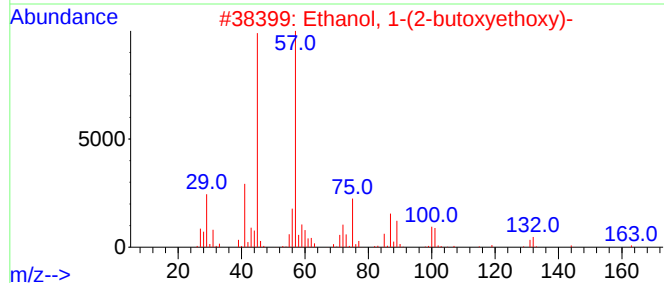
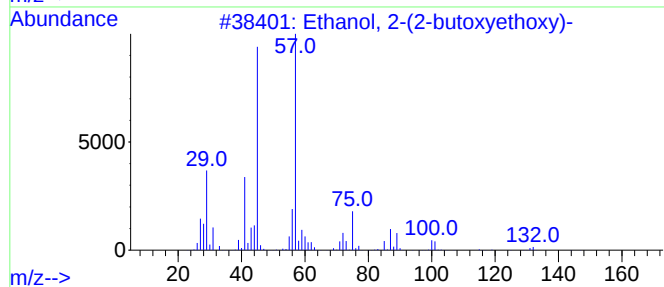
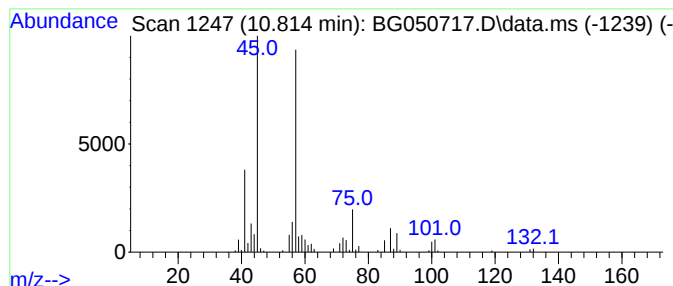
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.815	9.81 ng	186053	Naphthalene-d8	11.073	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	47
5	(+)-5-Methyl-2-hexanol	116	C7H16O	111768-09-3	43



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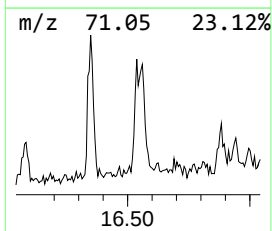
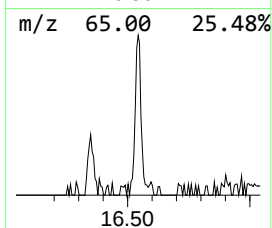
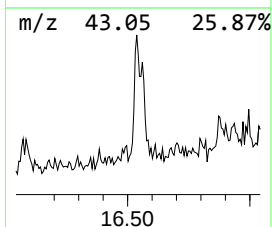
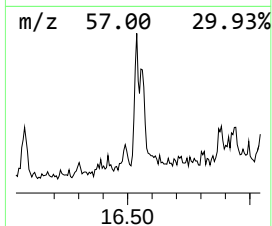
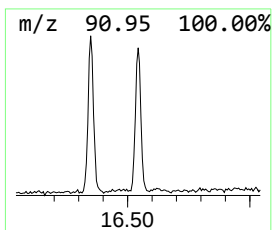
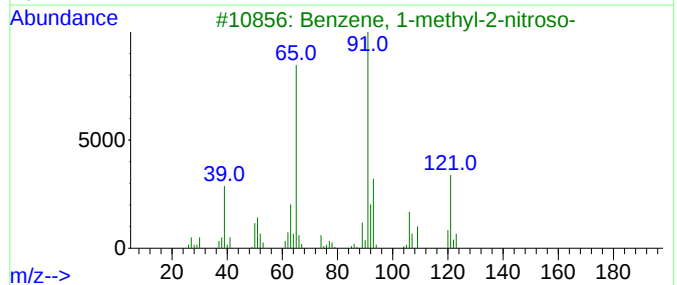
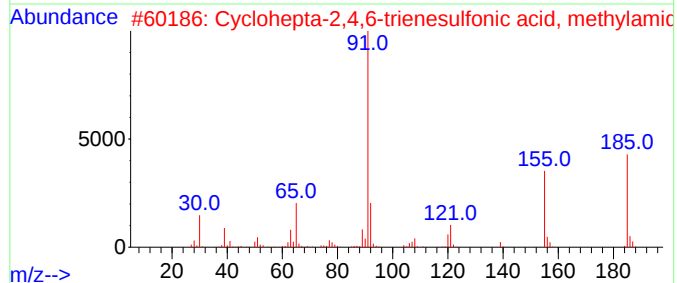
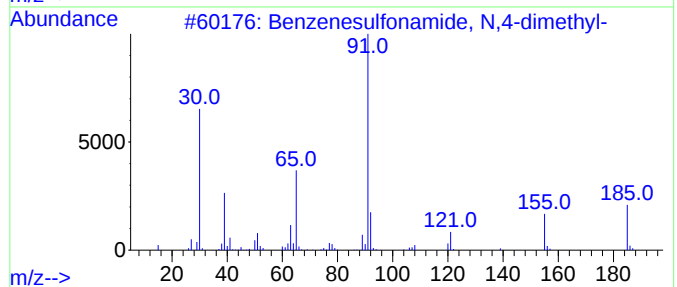
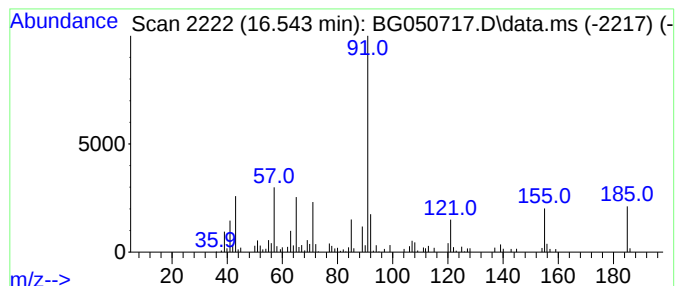
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.543	4.01 ng	112565	Phenanthrene-d10	17.612	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	81
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	50
3	Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	46
4	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	43
5	Benzeneethanamine	121	C8H11N	000064-04-0	30



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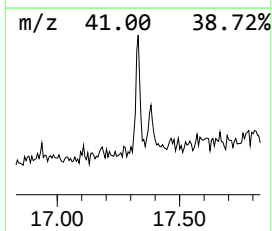
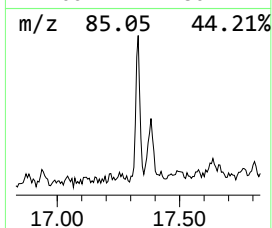
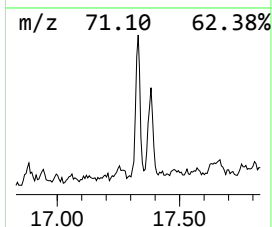
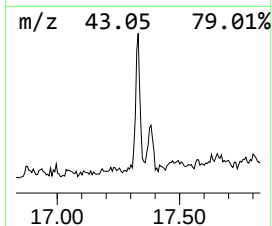
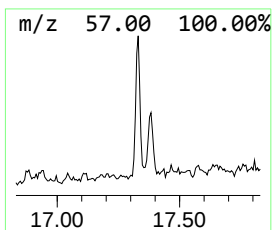
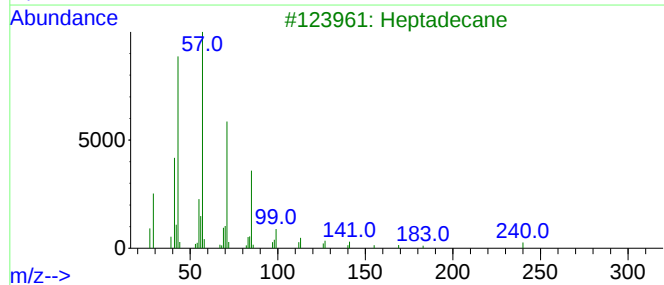
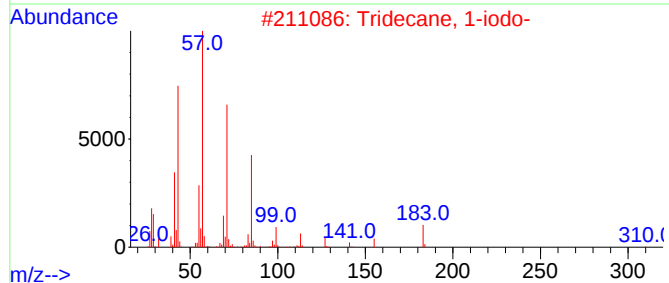
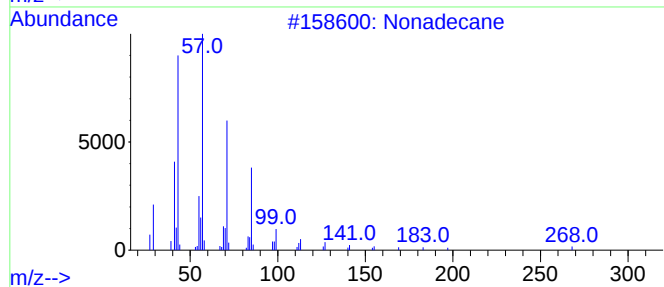
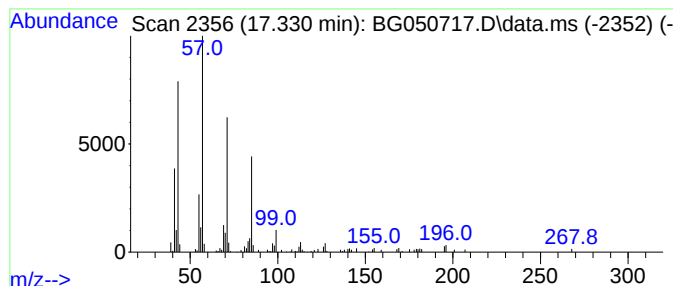
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.330	3.09 ng	86608	Phenanthrene-d10	17.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	97
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3			Heptadecane	240	C17H36	000629-78-7	86
4			Pentadecane	212	C15H32	000629-62-9	86
5			Tetradecane	198	C14H30	000629-59-4	86



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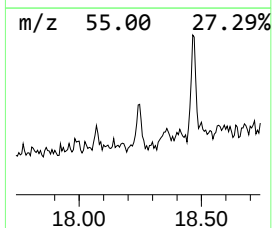
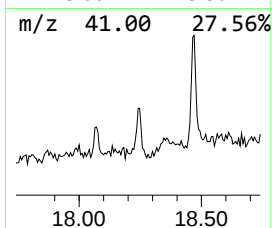
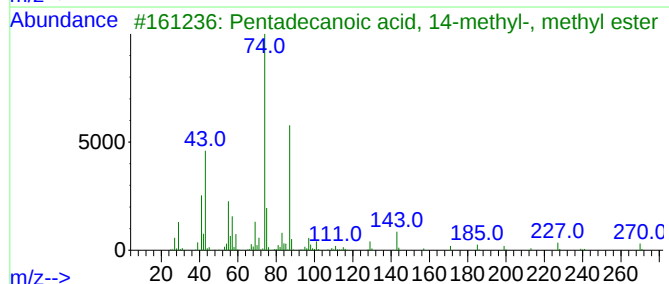
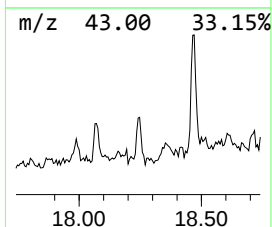
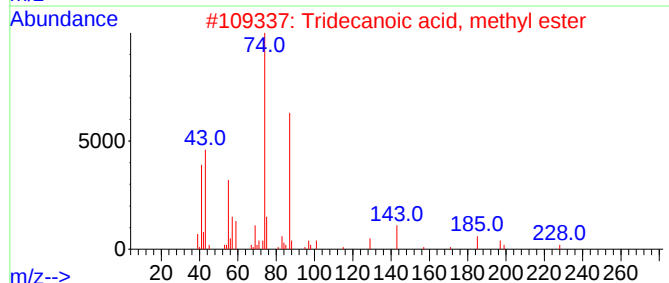
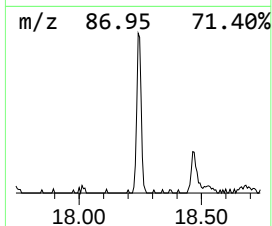
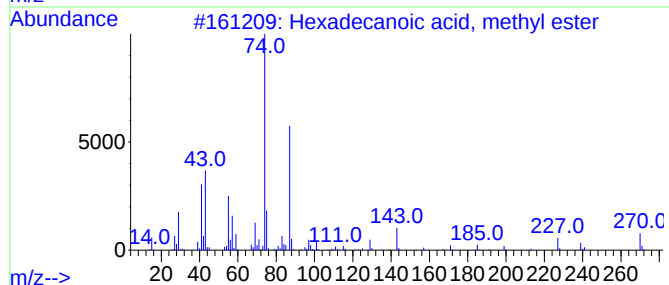
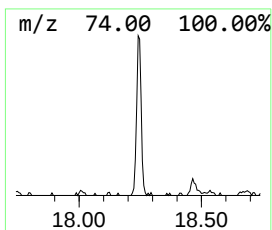
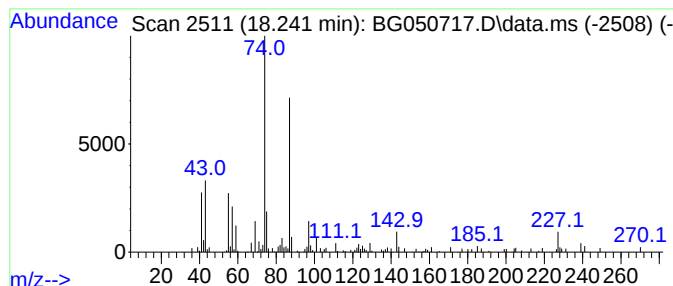
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.241	2.58 ng	72303	Phenanthrene-d10	17.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	81
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	74
4			Methyl 8-methyl-decanoate	200	C12H24O2	1010336-49-1	72
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	72



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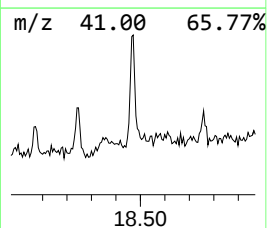
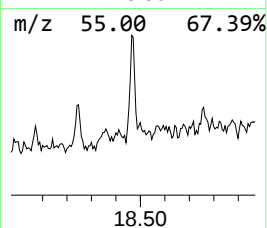
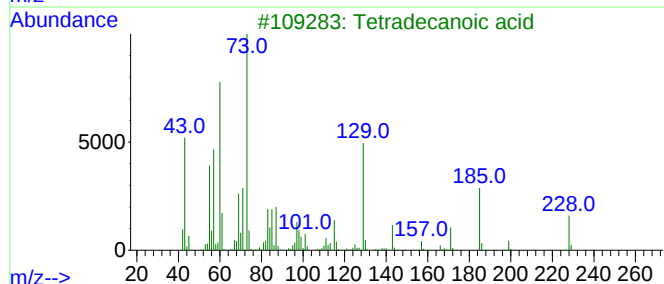
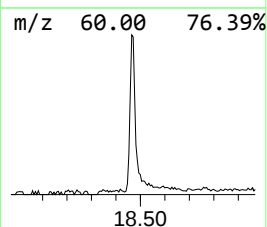
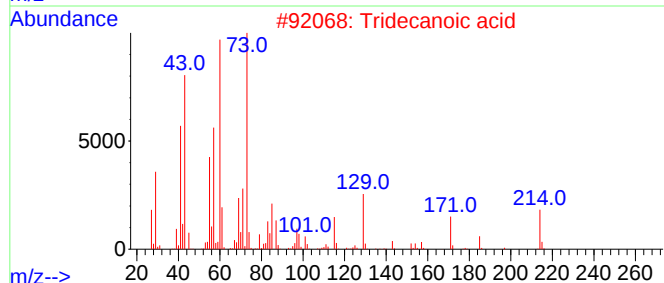
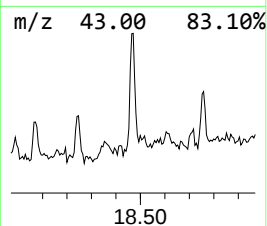
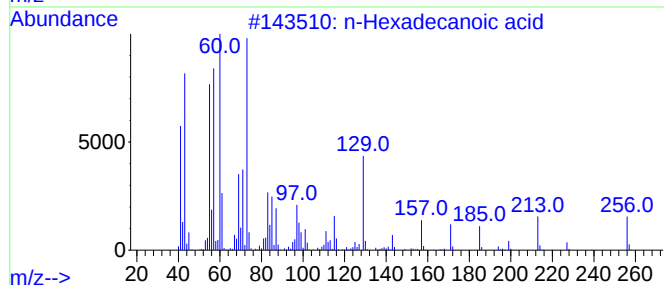
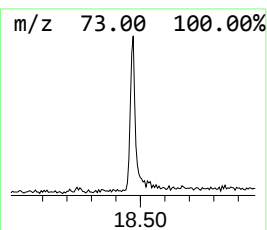
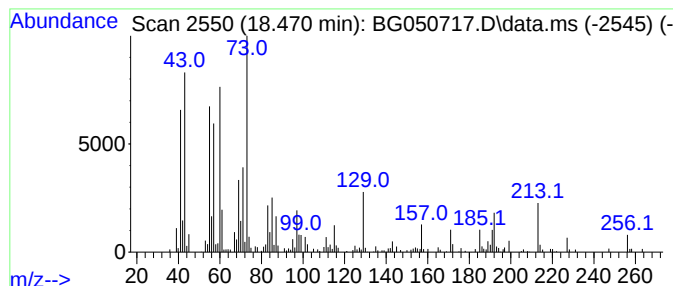
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.470	7.69 ng	215658	Phenanthrene-d10	17.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	62
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4			n-Decanoic acid	172	C10H20O2	000334-48-5	52
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	52



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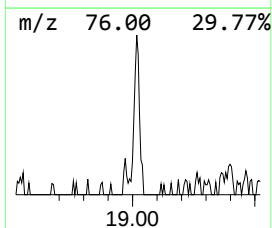
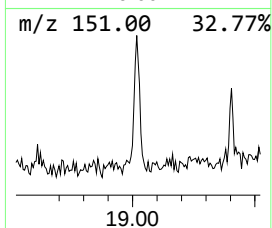
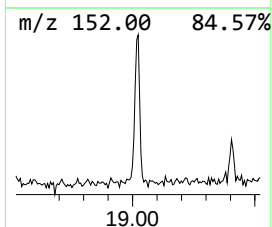
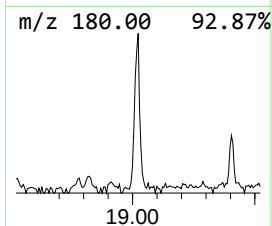
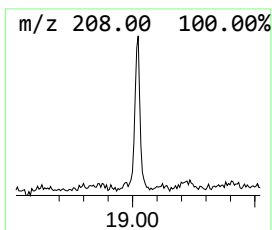
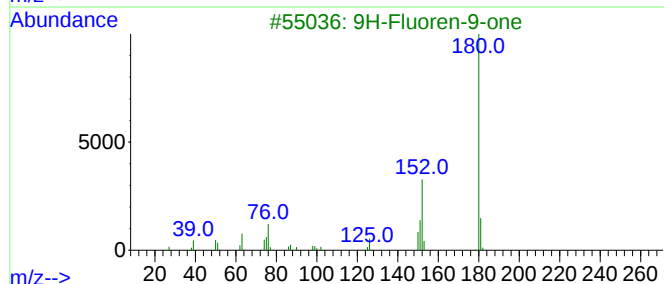
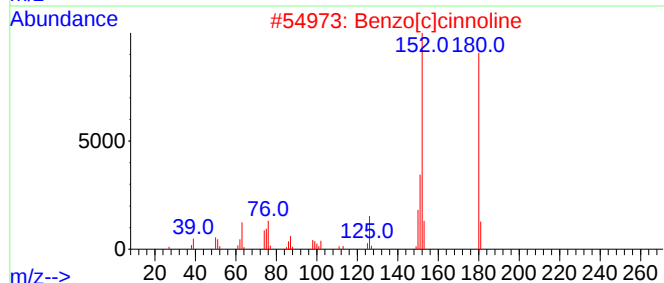
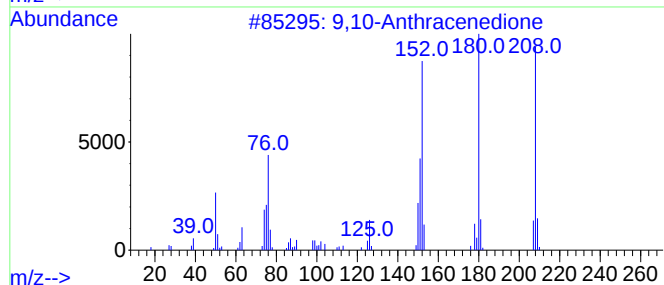
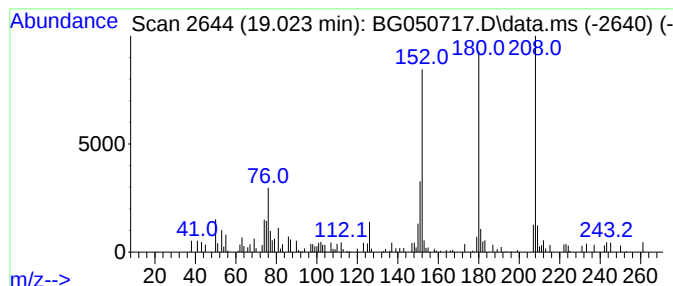
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,10-Anthracenedione Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.023	2.40 ng	67310	Phenanthrene-d10	17.612

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,10-Anthracenedione	208	C14H8O2	000084-65-1	93
2		Benzo[c]cinnoline	180	C12H8N2	000230-17-1	78
3		9H-Fluoren-9-one	180	C13H8O	000486-25-9	64
4		Benzo[h]cinnoline	180	C12H8N2	000230-31-9	64
5		1,4-Anthracenedione	208	C14H8O2	000635-12-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102521\
Data File : BG050717.D
Acq On : 25 Oct 2021 19:26
Operator : CG/JU
Sample : M4295-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

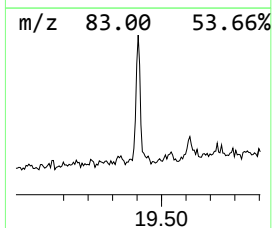
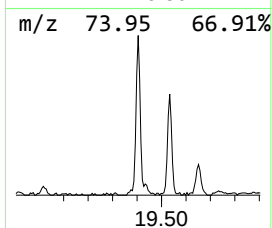
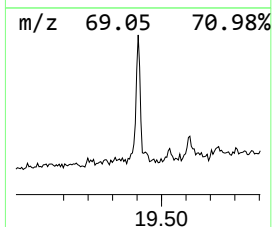
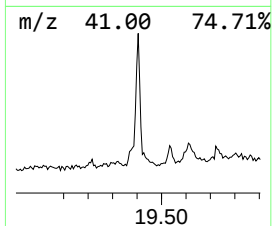
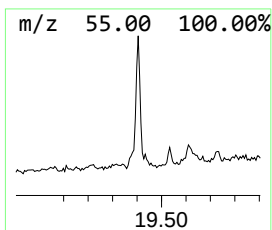
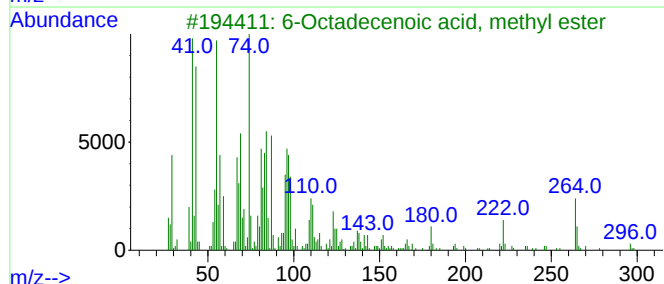
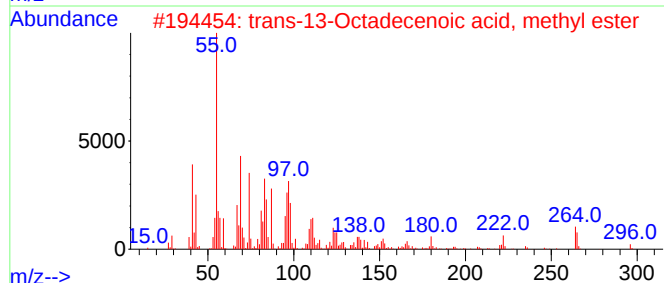
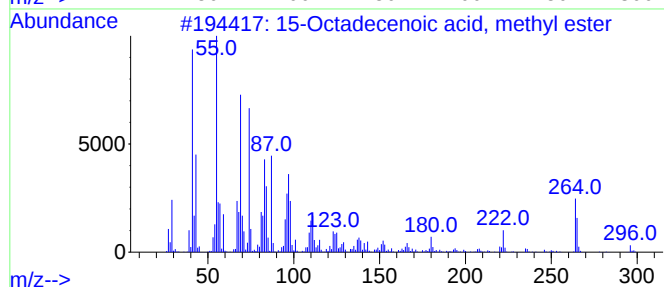
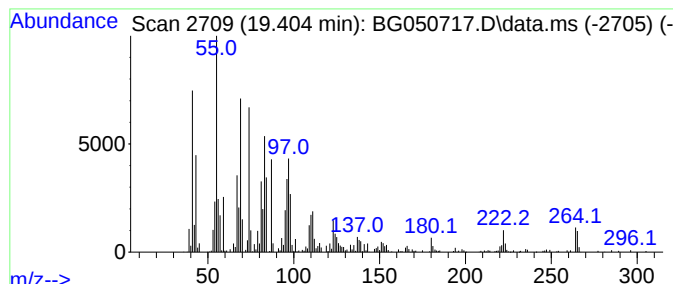
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BNA_G
ClientSampleId :
RBR-251686

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 7 15-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.404	14.19 ng	398072	Phenanthrene-d10	17.612	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	98
3	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	97
4	10-Octadecenoic acid, methyl est...	296	C19H36O2	013038-45-4	95
5	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102521\
Data File : BG050717.D
Acq On : 25 Oct 2021 19:26
Operator : CG/JU
Sample : M4295-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-251686

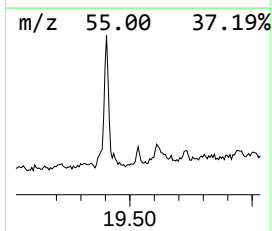
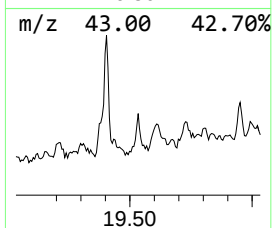
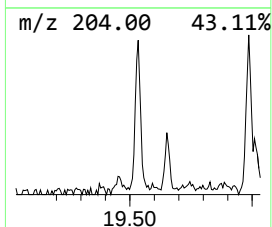
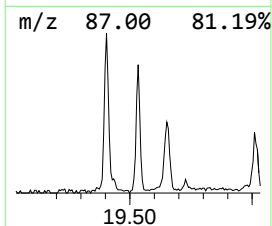
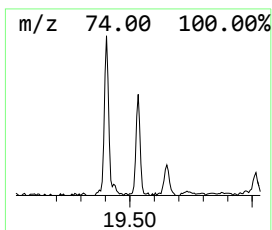
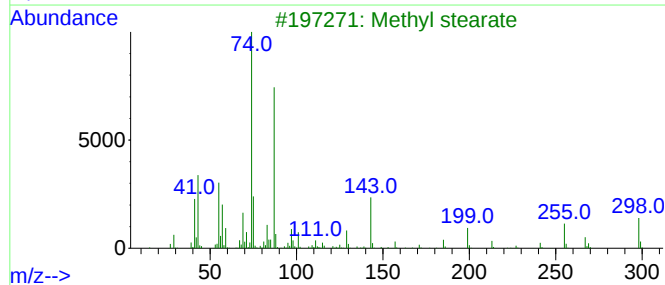
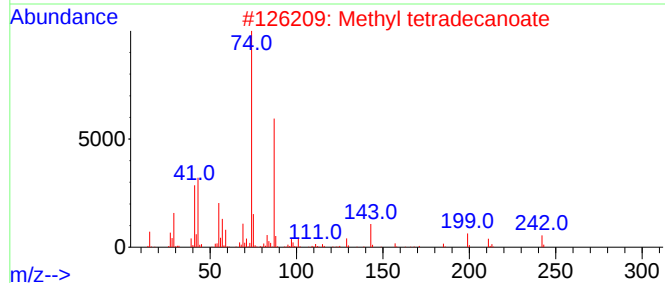
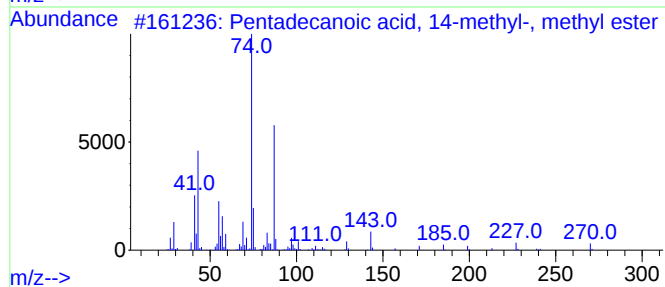
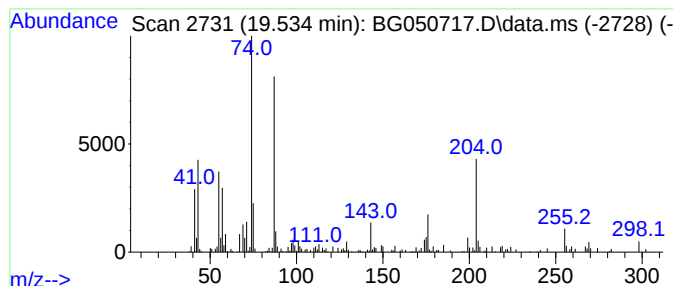
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecanoic acid, 14-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.534	3.29 ng	92269	Phenanthrene-d10	17.612

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	76
2		Methyl tetradecanoate	242	C15H30O2	000124-10-7	68
3		Methyl stearate	298	C19H38O2	000112-61-8	64
4		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	60
5		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102521\
Data File : BG050717.D
Acq On : 25 Oct 2021 19:26
Operator : CG/JU
Sample : M4295-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

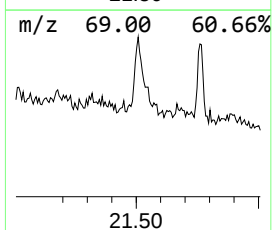
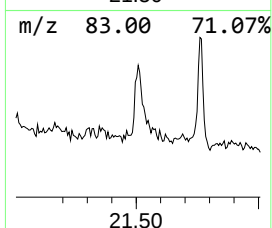
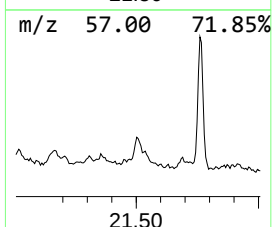
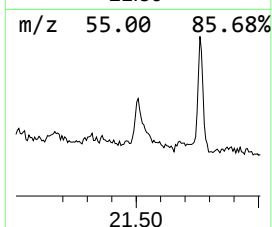
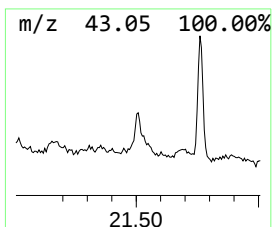
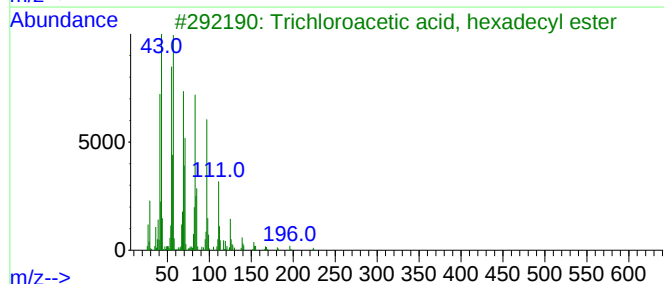
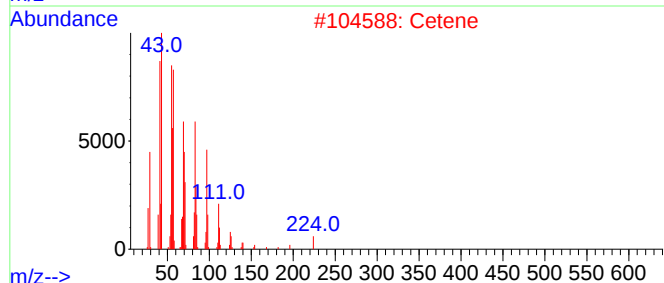
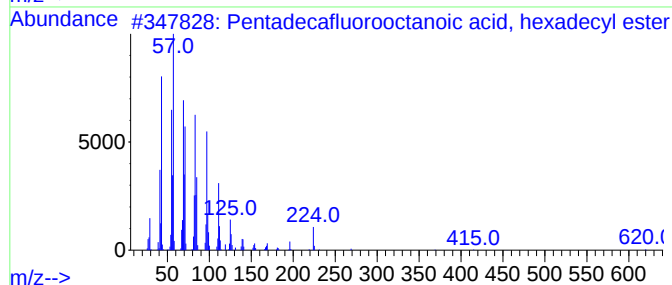
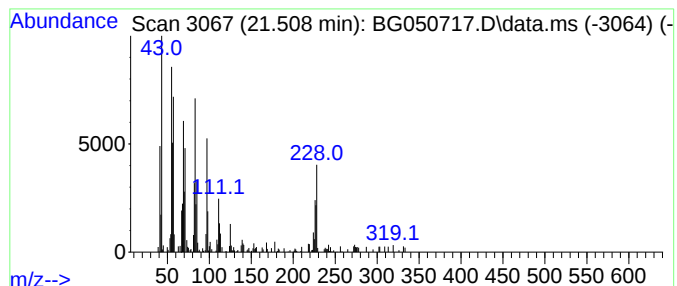
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.508	3.79 ng	150575	Chrysene-d12	21.913	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	70
2	Cetene	224	C16H32	000629-73-2	70
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64
4	Cyclopentadecane	210	C15H30	000295-48-7	64
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102521\
Data File : BG050717.D
Acq On : 25 Oct 2021 19:26
Operator : CG/JU
Sample : M4295-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-251686

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...	10.815	9.8	ng	186053	2	11.073	379387	20.0
Benzenesulfonam...	16.543	4.0	ng	112565	4	17.612	561030	20.0
Nonadecane	17.330	3.1	ng	86608	4	17.612	561030	20.0
Hexadecanoic ac...	18.241	2.6	ng	72303	4	17.612	561030	20.0
n-Hexadecanoic ...	18.470	7.7	ng	215658	4	17.612	561030	20.0
9,10-Anthracene...	19.023	2.4	ng	67310	4	17.612	561030	20.0
15-Octadecenoic...	19.404	14.2	ng	398072	4	17.612	561030	20.0
Pentadecanoic a...	19.534	3.3	ng	92269	4	17.612	561030	20.0
Pentadecafluoro...	21.508	3.8	ng	150575	5	21.913	794639	20.0