

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
 Data File : BG055092.D
 Acq On : 6 Oct 2022 21:48
 Operator : CG/JU
 Sample : N5014-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-06-0-2.0

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-BG100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055092.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.373	9	14	30	rVB	245042	379692	24.11%	4.547%
2	5.382	346	356	363	rBV	101313	161475	10.25%	1.934%
3	5.852	429	436	444	rBV	321756	513315	32.60%	6.147%
4	7.462	701	710	719	rBV	332683	572988	36.39%	6.862%
5	8.332	852	858	864	rBV	88807	152906	9.71%	1.831%
6	9.501	1050	1057	1066	rBV	188965	344402	21.87%	4.124%
7	11.164	1332	1340	1348	rVB	126616	227580	14.45%	2.725%
8	13.573	1743	1750	1757	rVB	582278	881522	55.98%	10.557%
9	14.942	1976	1983	1989	rVB	251025	378965	24.07%	4.538%
10	16.416	2227	2234	2244	rVB	544669	828976	52.65%	9.927%
11	17.674	2442	2448	2454	rBV	344864	514757	32.69%	6.164%
12	18.473	2579	2584	2589	rBV2	17783	27563	1.75%	0.330%
13	18.526	2589	2593	2603	rVV	66771	103234	6.56%	1.236%
14	19.701	2789	2793	2798	rVB	35863	48703	3.09%	0.583%
15	19.783	2800	2807	2814	rBV5	23828	43056	2.73%	0.516%
16	20.065	2850	2855	2860	rVB	29665	43979	2.79%	0.527%
17	20.247	2880	2886	2892	rBV	1161512	1574607	100.00%	18.857%
18	21.034	3015	3020	3026	rBV3	11454	21382	1.36%	0.256%
19	21.569	3106	3111	3124	rBV3	41934	76688	4.87%	0.918%
20	21.969	3170	3179	3185	rBV	347443	614475	39.02%	7.359%
21	22.815	3318	3323	3332	rBV7	10816	28471	1.81%	0.341%
22	23.931	3506	3513	3521	rBV5	26260	56716	3.60%	0.679%
23	24.430	3594	3598	3603	rVV3	9479	16375	1.04%	0.196%
24	24.489	3603	3608	3618	rVB8	15546	38622	2.45%	0.463%
25	25.094	3703	3711	3712	rBV4	8913	17017	1.08%	0.204%
26	25.247	3730	3737	3745	rVB3	10529	31379	1.99%	0.376%
27	25.412	3754	3765	3777	rBV3	186122	575361	36.54%	6.890%
28	26.023	3860	3869	3879	rBV3	11200	36979	2.35%	0.443%
29	26.710	3979	3986	3993	rVB4	14679	39250	2.49%	0.470%

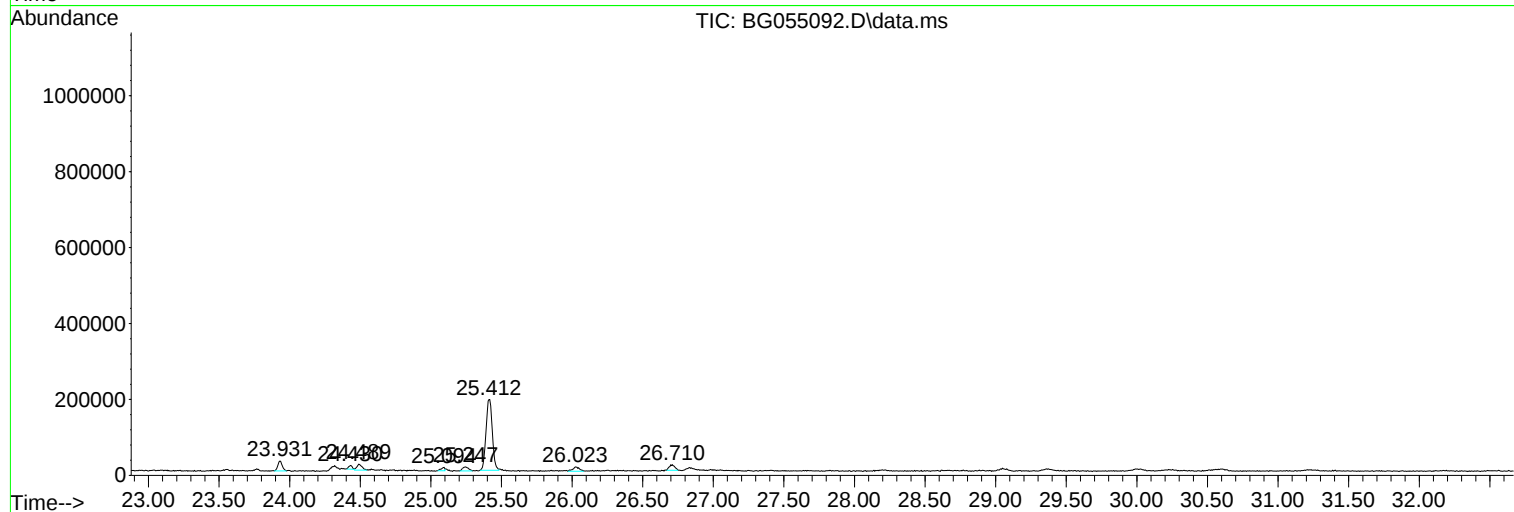
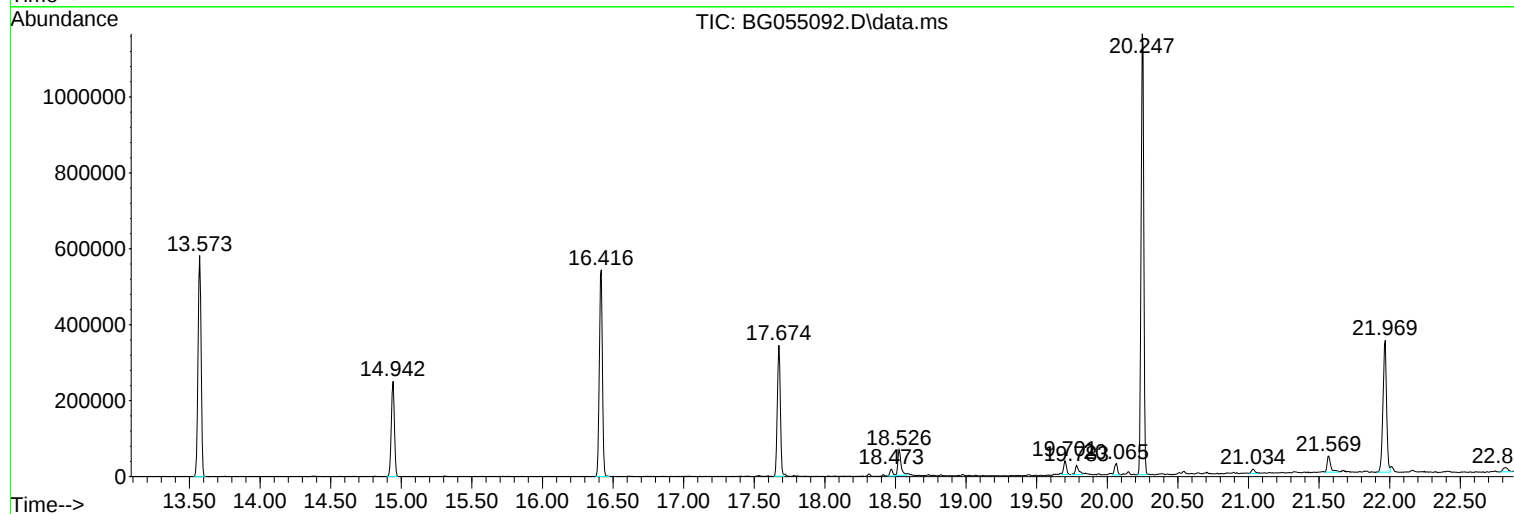
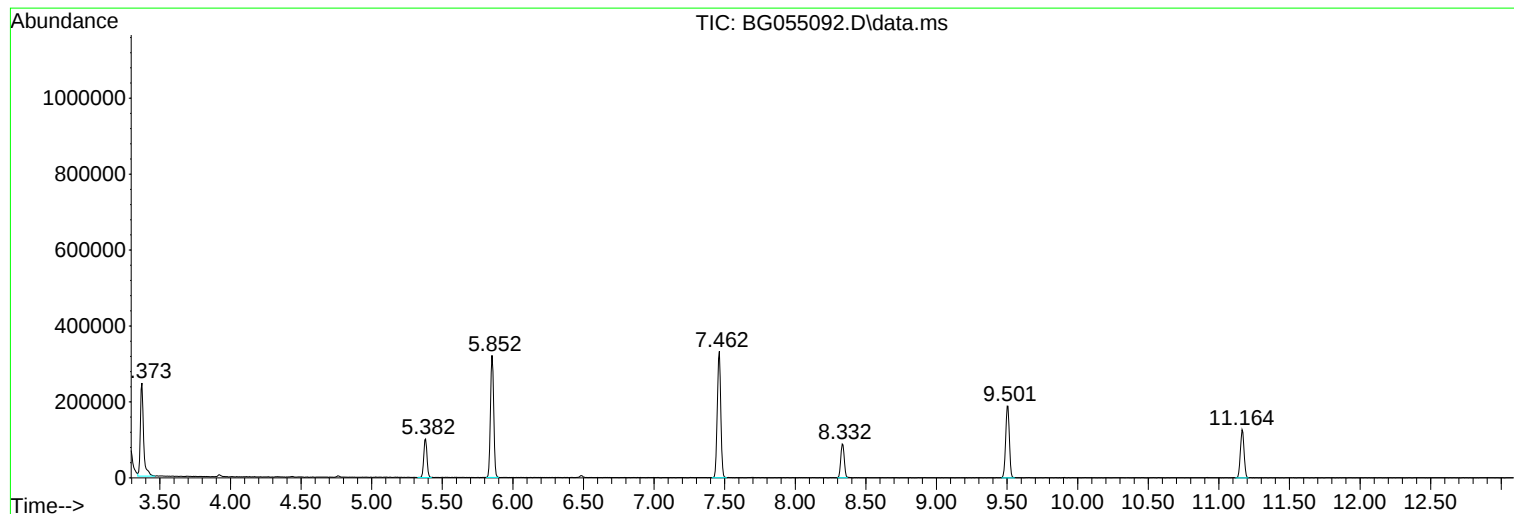
Sum of corrected areas: 8350435

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055092.D
Acq On : 6 Oct 2022 21:48
Operator : CG/JU
Sample : N5014-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055092.D
Acq On : 6 Oct 2022 21:48
Operator : CG/JU
Sample : N5014-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

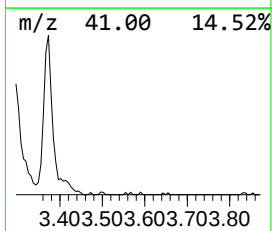
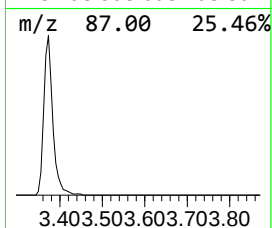
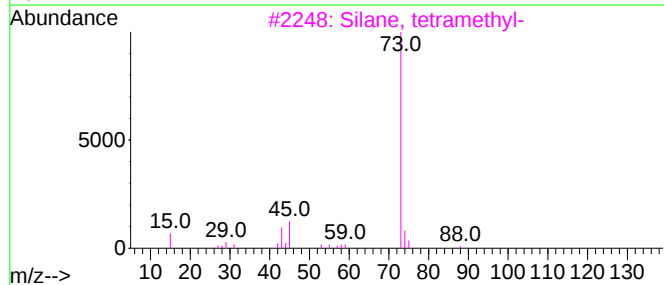
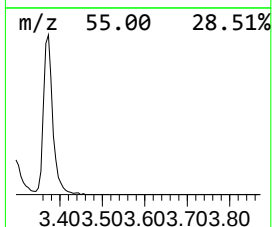
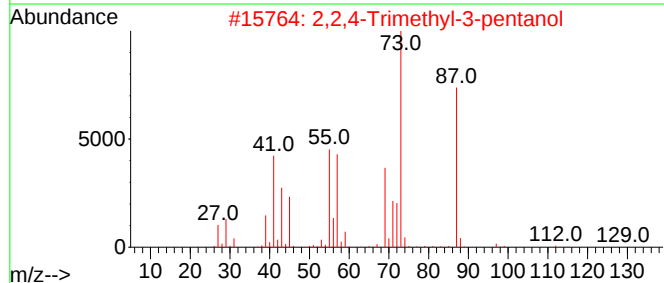
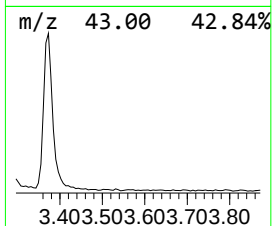
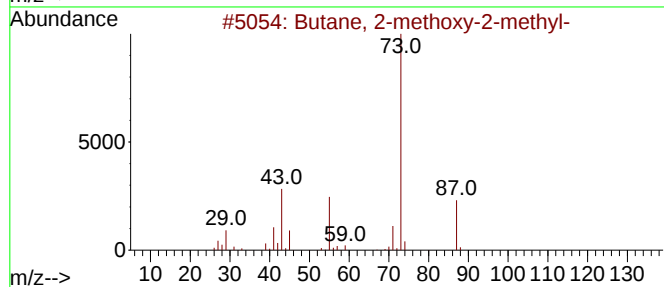
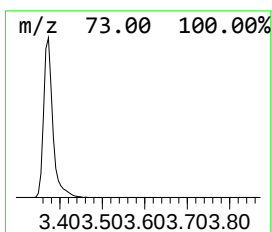
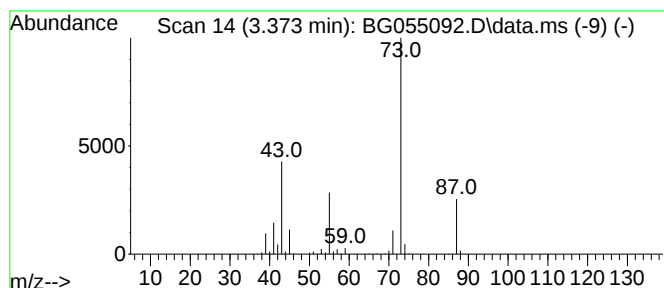
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.373	49.66 ng	379692	1,4-Dichlorobenzene-d4	8.332

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055092.D
Acq On : 6 Oct 2022 21:48
Operator : CG/JU
Sample : N5014-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

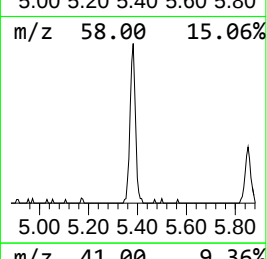
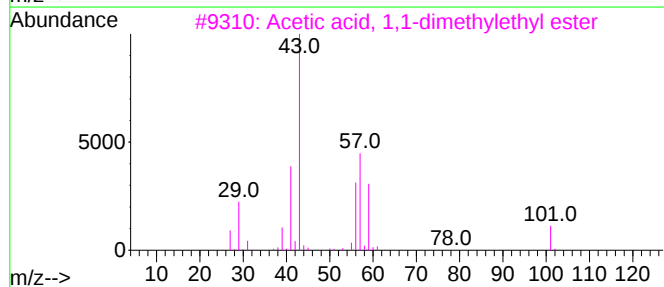
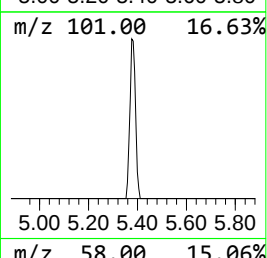
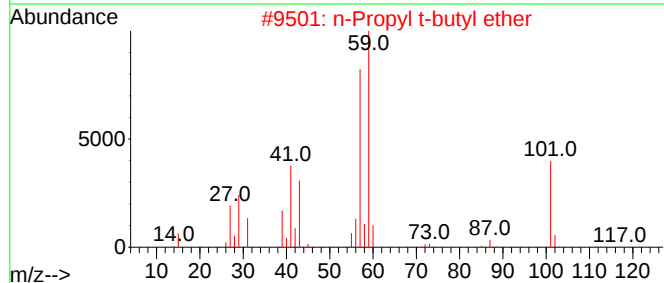
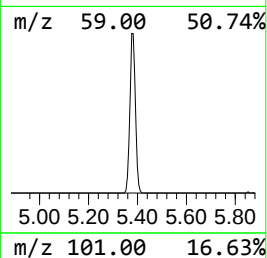
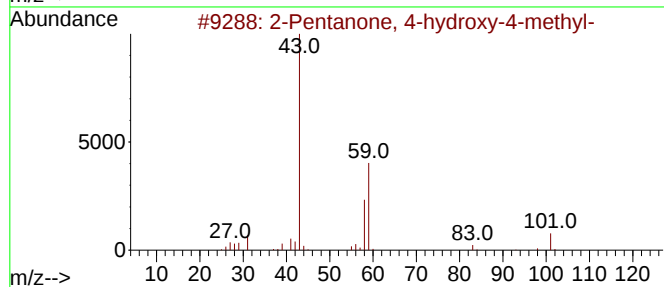
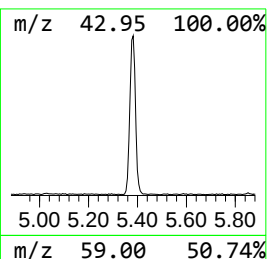
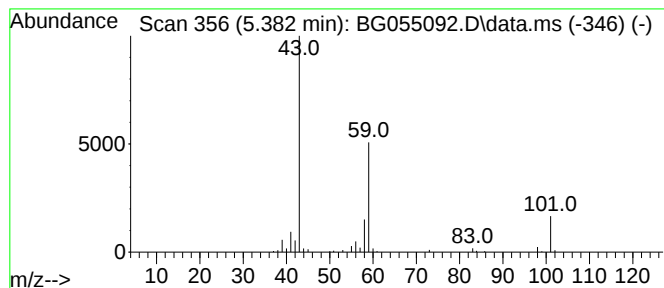
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.382	21.12 ng	161475	1,4-Dichlorobenzene-d4	8.332

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055092.D
Acq On : 6 Oct 2022 21:48
Operator : CG/JU
Sample : N5014-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

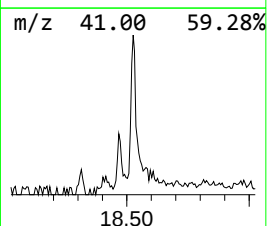
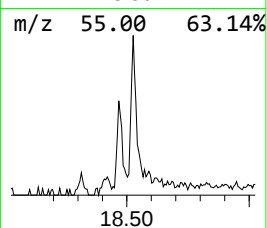
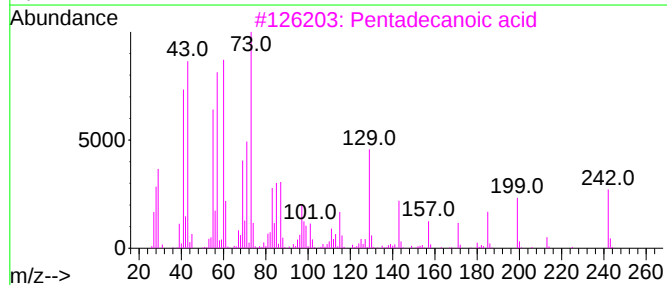
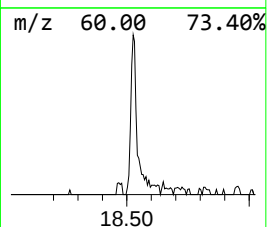
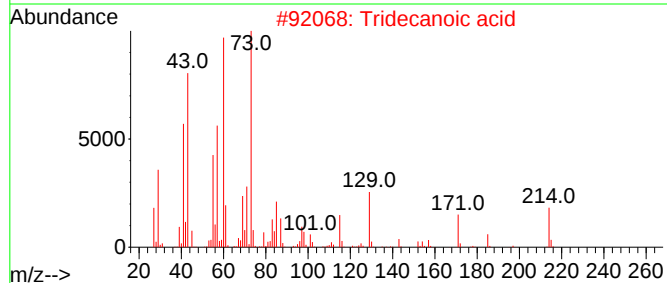
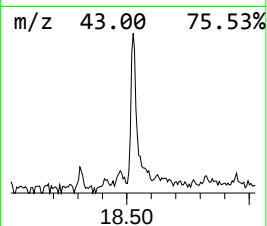
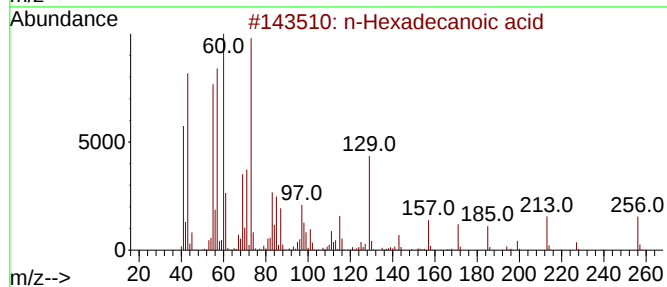
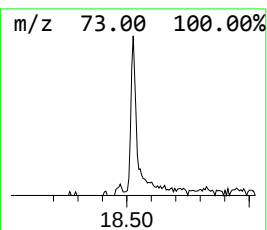
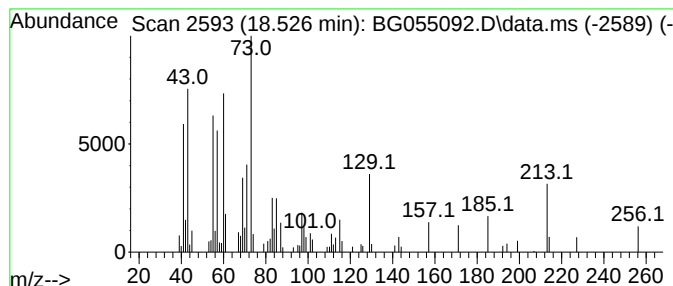
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.526	4.01 ng	103234	Phenanthrene-d10	17.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Hexadecane	226	C16H34	000544-76-3	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055092.D
Acq On : 6 Oct 2022 21:48
Operator : CG/JU
Sample : N5014-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

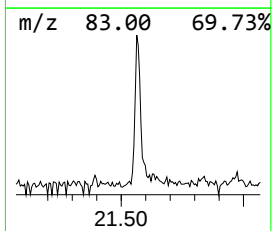
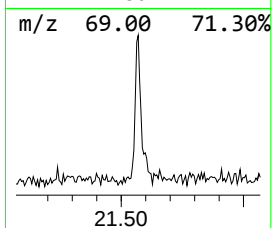
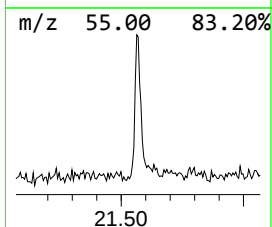
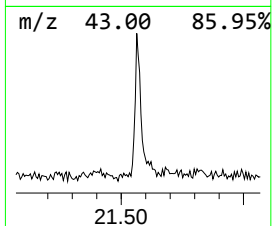
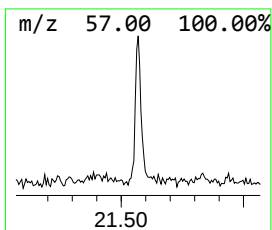
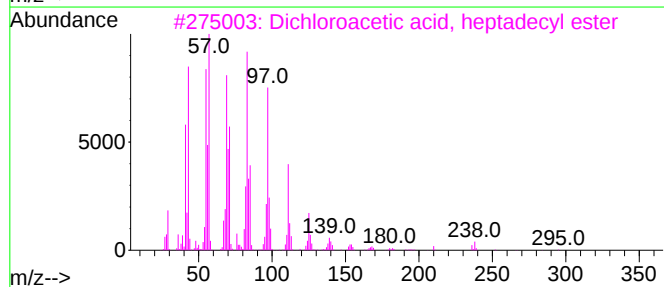
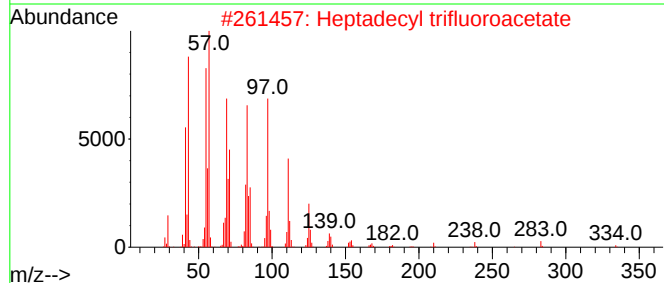
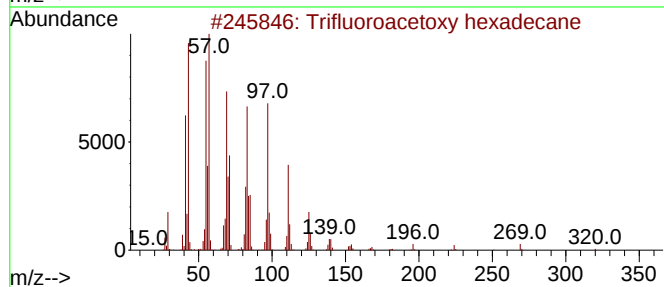
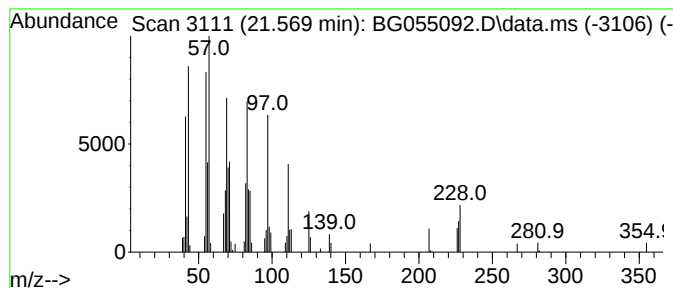
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.569	2.50 ng	76688	Chrysene-d12	21.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055092.D
Acq On : 6 Oct 2022 21:48
Operator : CG/JU
Sample : N5014-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.373	49.7	ng	379692	1	8.332	152906	20.0
2-Pentanone, 4-...	5.382	21.1	ng	161475	1	8.332	152906	20.0
n-Hexadecanoic ...	18.526	4.0	ng	103234	4	17.674	514757	20.0
Trifluoroacetox...	21.569	2.5	ng	76688	5	21.969	614475	20.0