

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
 Data File : BG055893.D
 Acq On : 5 Dec 2022 20:33
 Operator : CG/JU
 Sample : N5870-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ML-1

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055893.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.218	321	328	338	rBV	187696	281744	13.99%	2.827%
2	5.706	404	411	422	rBV	423740	680187	33.76%	6.824%
3	7.327	680	687	707	rVB	469065	804855	39.95%	8.075%
4	8.173	824	831	837	rBV	103264	174474	8.66%	1.750%
5	9.342	1022	1030	1042	rVB	249677	453064	22.49%	4.545%
6	10.999	1305	1312	1320	rBV	152772	265299	13.17%	2.662%
7	13.426	1718	1725	1736	rBV	810317	1202639	59.70%	12.065%
8	14.801	1953	1959	1966	rBV	283423	422677	20.98%	4.240%
9	16.146	2183	2188	2196	rVB	90912	127299	6.32%	1.277%
10	16.287	2206	2212	2224	rBV	723293	1109044	55.05%	11.126%
11	16.710	2279	2284	2293	rVB	15716	24184	1.20%	0.243%
12	17.545	2420	2426	2432	rBV	391518	584528	29.02%	5.864%
13	18.402	2567	2572	2582	rBV	64576	106457	5.28%	1.068%
14	19.666	2782	2787	2793	rBV5	15559	27798	1.38%	0.279%
15	20.130	2860	2866	2872	rBV	1510712	2014476	100.00%	20.210%
16	20.406	2907	2913	2920	rBV	15517	27873	1.38%	0.280%
17	20.905	2994	2998	3002	rBV	23679	27703	1.38%	0.278%
18	21.428	3082	3087	3102	rBV2	75351	208395	10.34%	2.091%
19	21.828	3148	3155	3162	rBV	387969	644324	31.98%	6.464%
20	21.981	3177	3181	3184	rVB2	19818	24503	1.22%	0.246%
21	22.603	3283	3287	3292	rVB3	16953	26599	1.32%	0.267%
22	23.314	3405	3408	3414	rVB2	15401	25072	1.24%	0.252%
23	24.143	3546	3549	3556	rVB4	14630	29190	1.45%	0.293%
24	25.177	3712	3725	3736	rVB2	219950	675368	33.53%	6.776%

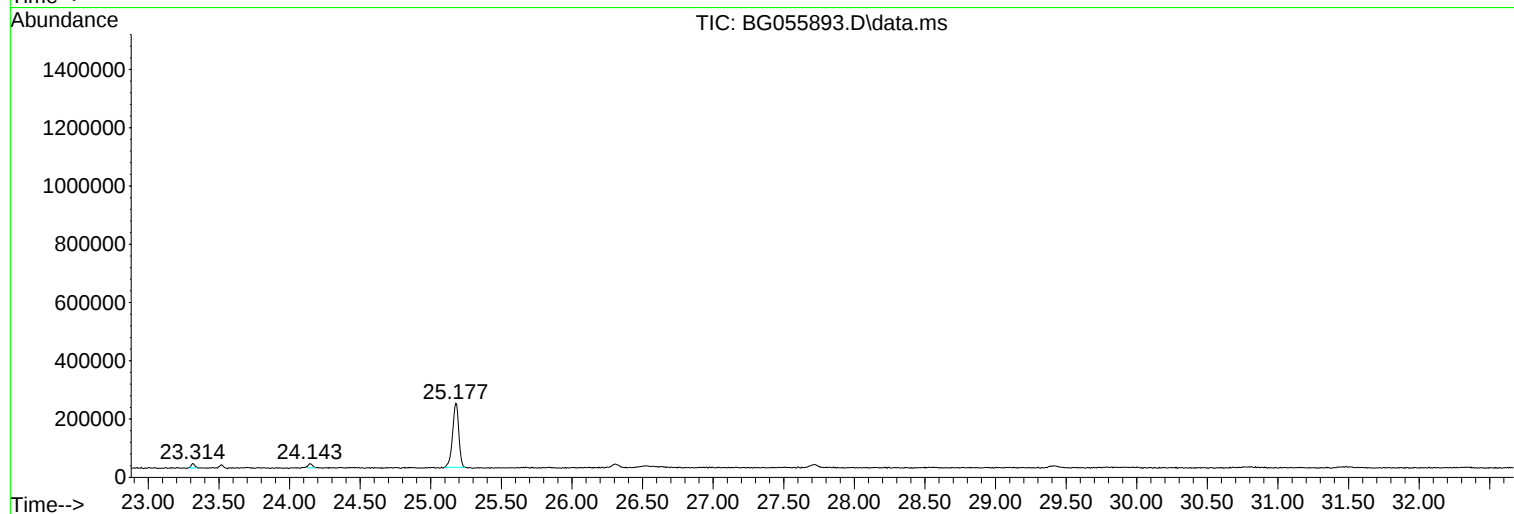
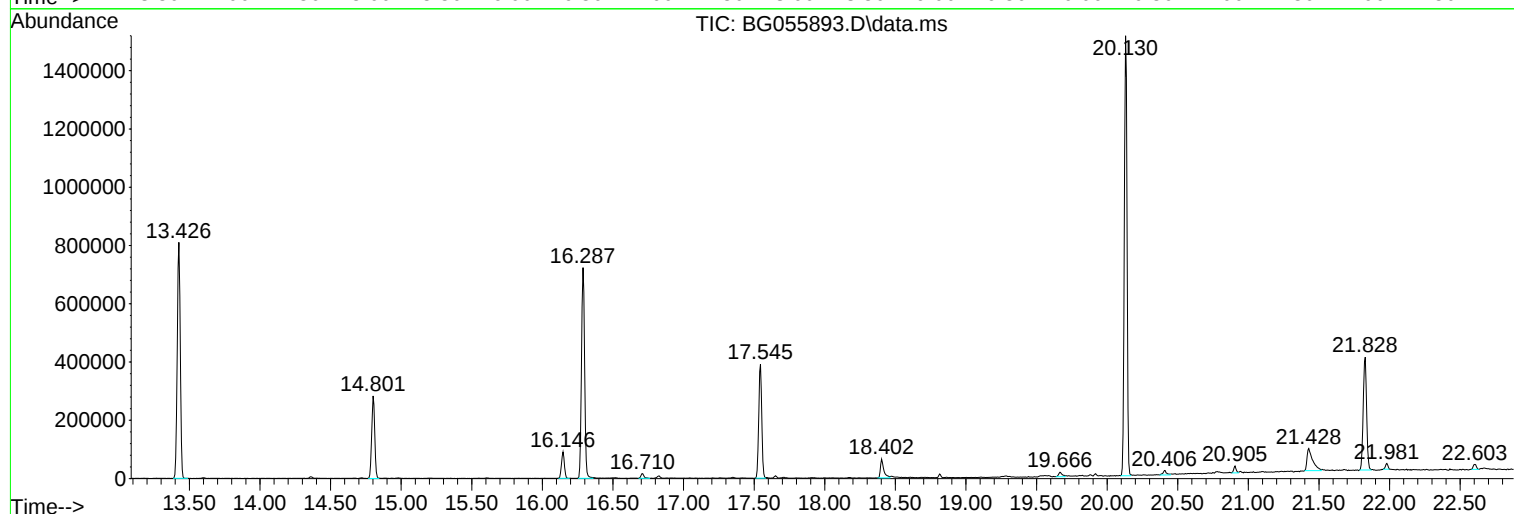
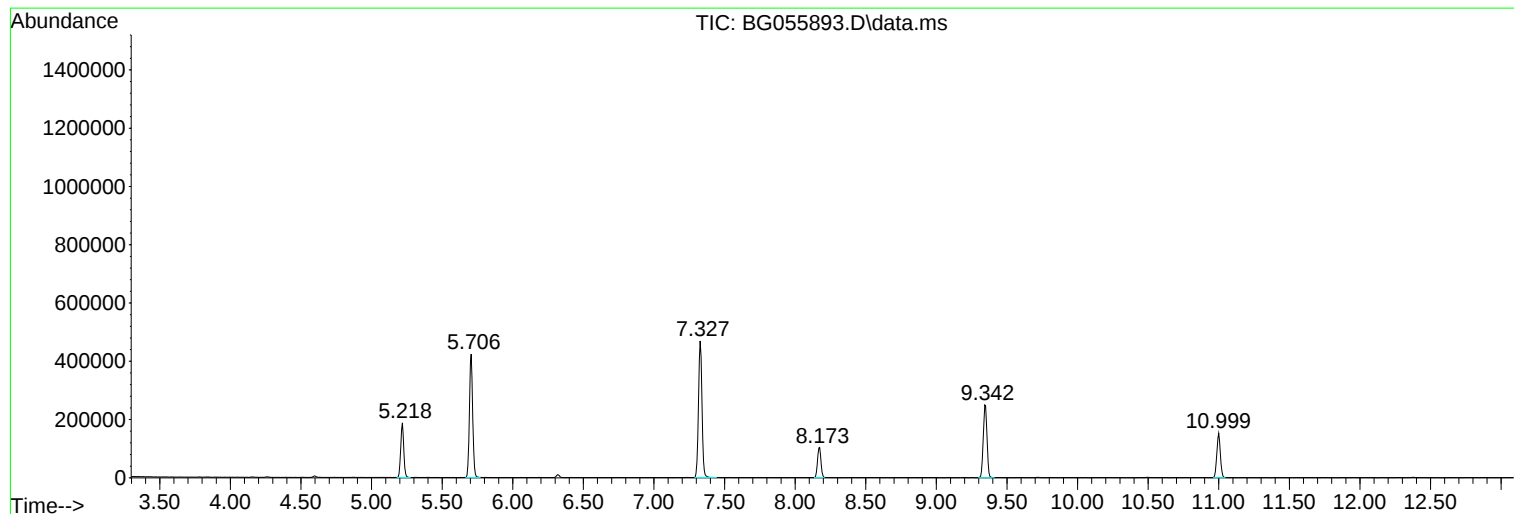
Sum of corrected areas: 9967752

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055893.D
Acq On : 5 Dec 2022 20:33
Operator : CG/JU
Sample : N5870-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ML-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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\BG120522\
Data File : BG055893.D
Acq On : 5 Dec 2022 20:33
Operator : CG/JU
Sample : N5870-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ML-1

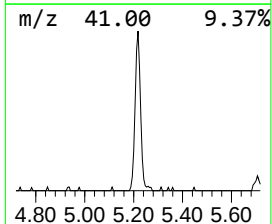
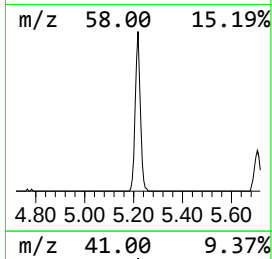
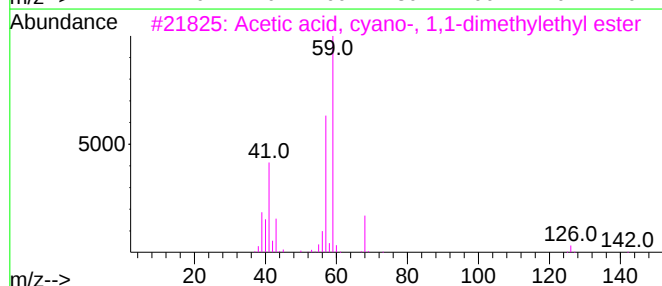
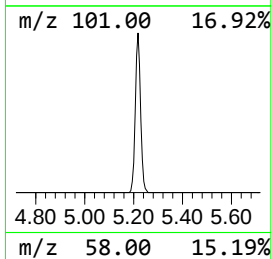
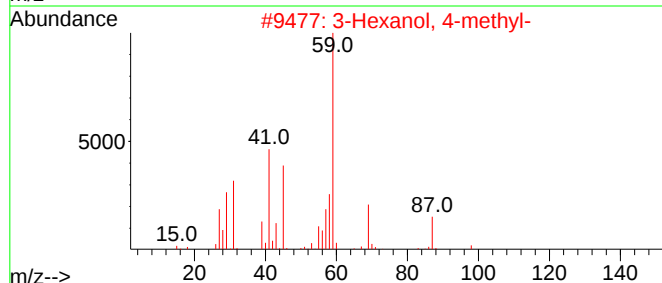
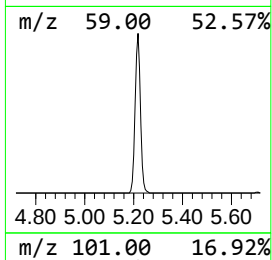
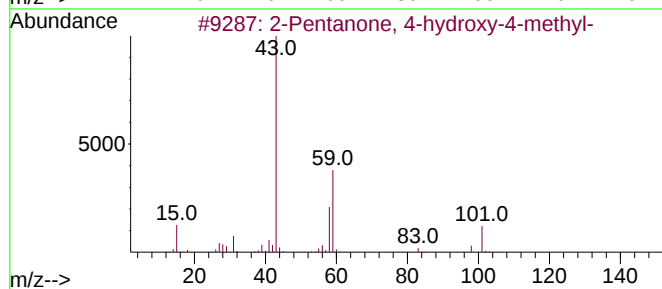
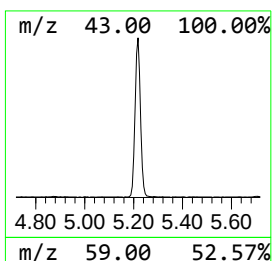
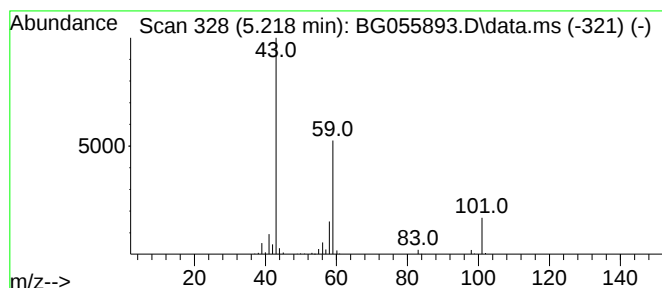
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.218	32.30 ng	281744	1,4-Dichlorobenzene-d4	8.173

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055893.D
Acq On : 5 Dec 2022 20:33
Operator : CG/JU
Sample : N5870-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ML-1

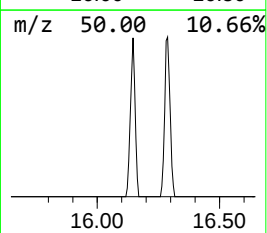
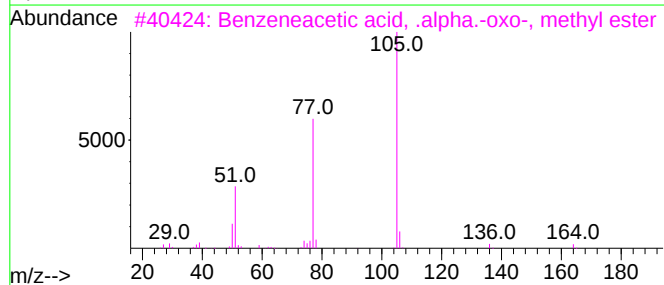
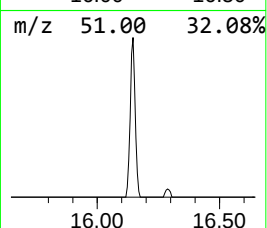
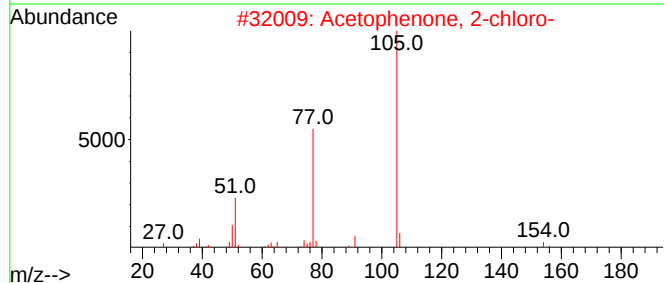
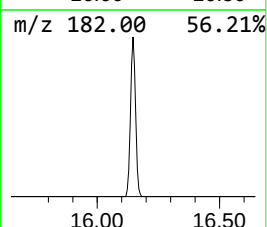
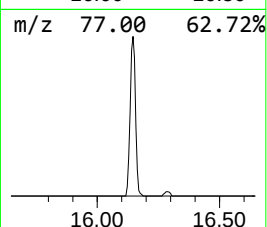
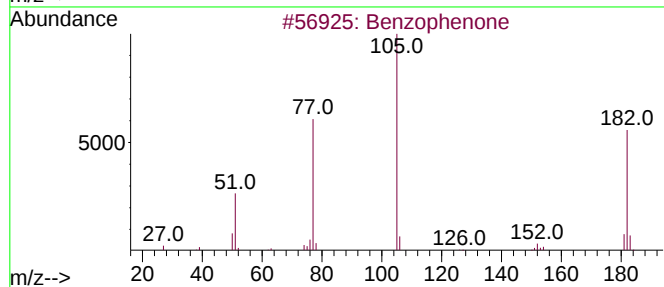
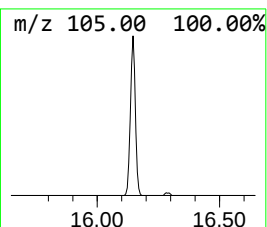
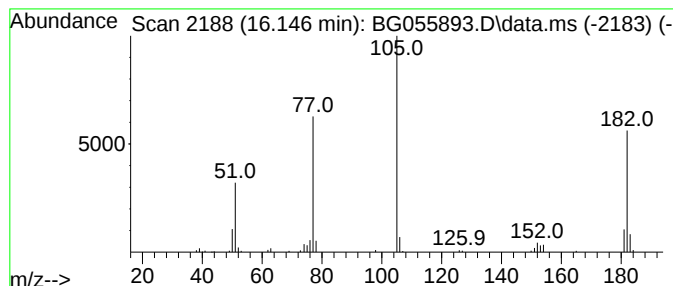
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.146	6.02 ng	127299	Acenaphthene-d10	14.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Benzenecetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5			1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055893.D
Acq On : 5 Dec 2022 20:33
Operator : CG/JU
Sample : N5870-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ML-1

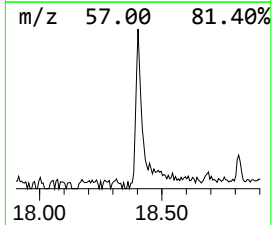
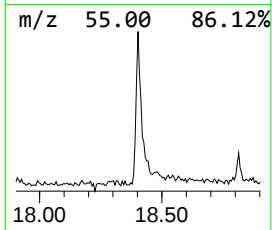
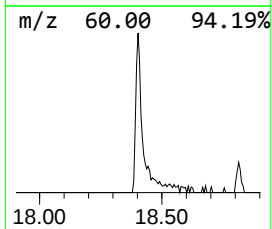
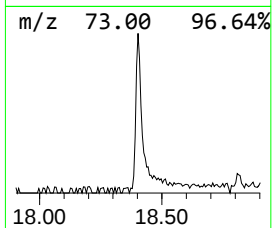
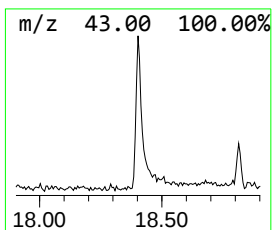
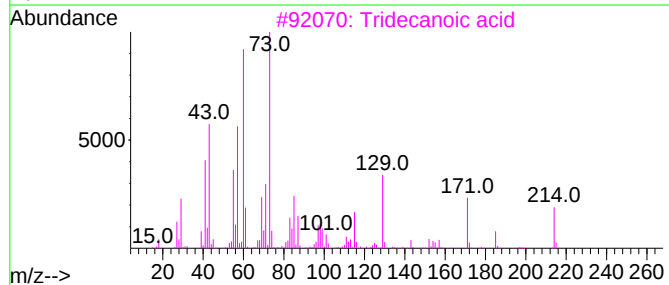
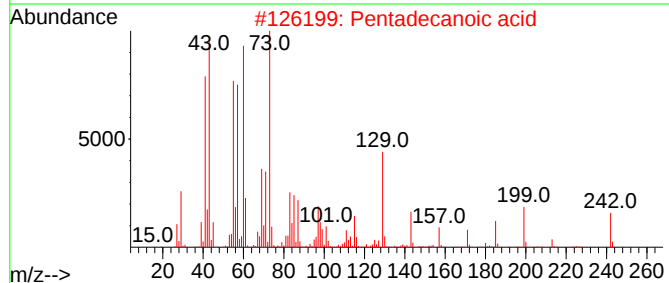
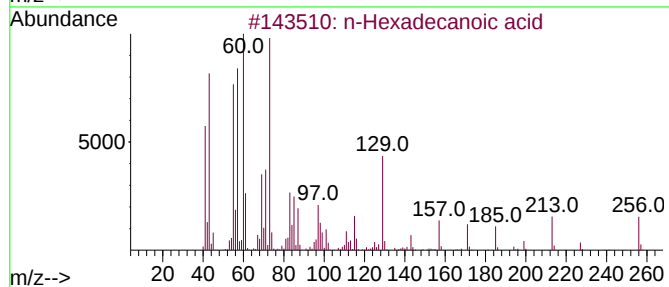
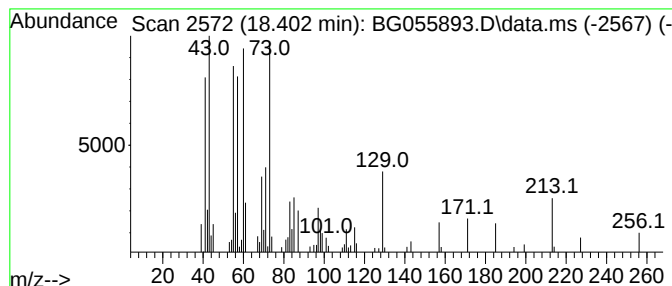
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.402	3.64 ng	106457	Phenanthrene-d10	17.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055893.D
Acq On : 5 Dec 2022 20:33
Operator : CG/JU
Sample : N5870-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ML-1

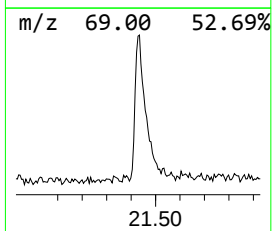
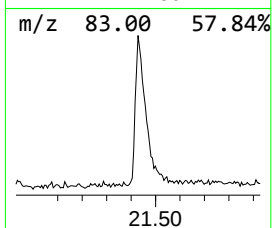
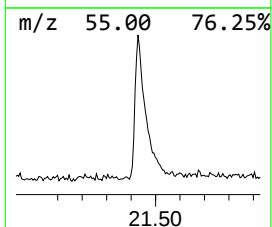
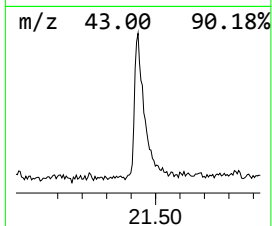
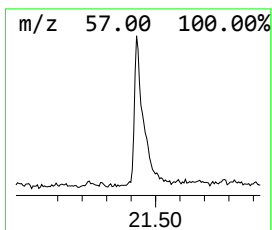
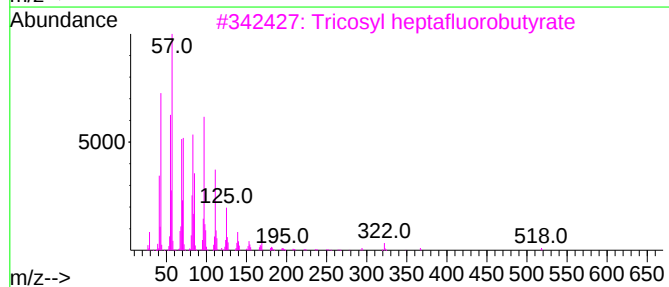
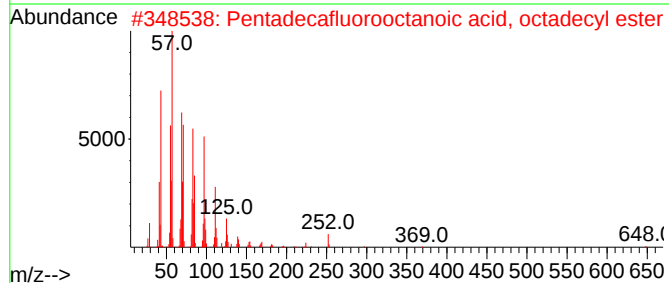
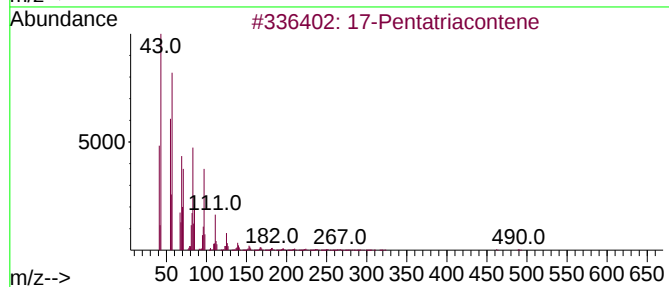
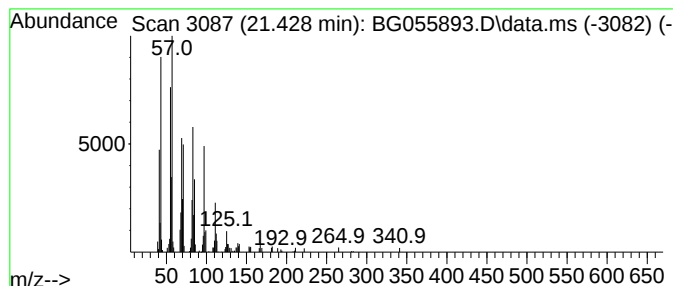
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 17-Pentatriacontene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.428	6.47 ng	208395	Chrysene-d12	21.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
4			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5			Hexadecyl propyl ether	284	C19H40O	1000406-27-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055893.D
Acq On : 5 Dec 2022 20:33
Operator : CG/JU
Sample : N5870-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ML-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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
2-Pentanone, 4-...	5.218	32.3	ng	281744	1	8.173	174474	20.0
Benzophenone	16.146	6.0	ng	127299	3	14.801	422677	20.0
n-Hexadecanoic ...	18.402	3.6	ng	106457	4	17.545	584528	20.0
17-Pentatriacon...	21.428	6.5	ng	208395	5	21.828	644324	20.0