

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
 Data File : BG060137.D
 Acq On : 22 Dec 2023 14:10
 Operator : MA/JU
 Sample : 05898-10
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-74a

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-BG122123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060137.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	3	5	21	rVB	311226	530742	4.24%	0.930%
2	5.514	406	413	432	rBV	2045348	3567966	28.52%	6.250%
3	7.101	674	683	698	rBV	2478715	4339403	34.69%	7.601%
4	7.941	818	826	842	rBV	522000	944557	7.55%	1.655%
5	9.098	1015	1023	1037	rBV	1381809	2501394	20.00%	4.382%
6	10.744	1295	1303	1314	rBV	849177	1522225	12.17%	2.666%
7	13.199	1712	1721	1734	rBV	4576544	6972509	55.74%	12.213%
8	14.574	1949	1955	1964	rBV	1797422	2853870	22.82%	4.999%
9	16.067	2199	2209	2223	rBV2	4258757	6539746	52.28%	11.455%
10	17.324	2415	2423	2435	rBV	2746563	4201584	33.59%	7.360%
11	18.217	2570	2575	2582	rBV	306300	476046	3.81%	0.834%
12	19.945	2863	2869	2881	rBV	9252115	12508658	100.00%	21.911%
13	20.250	2917	2921	2928	rVB	107266	141777	1.13%	0.248%
14	21.237	3084	3089	3095	rBV2	475949	736714	5.89%	1.290%
15	21.590	3142	3149	3162	rVB	2572217	4113510	32.89%	7.205%
16	22.395	3281	3286	3295	rVB4	128760	316007	2.53%	0.554%
17	23.922	3542	3546	3551	rVB7	79117	148673	1.19%	0.260%
18	24.768	3680	3690	3704	rVB2	1222222	3514083	28.09%	6.155%
19	30.697	4690	4699	4716	rVB2	244254	1159861	9.27%	2.032%

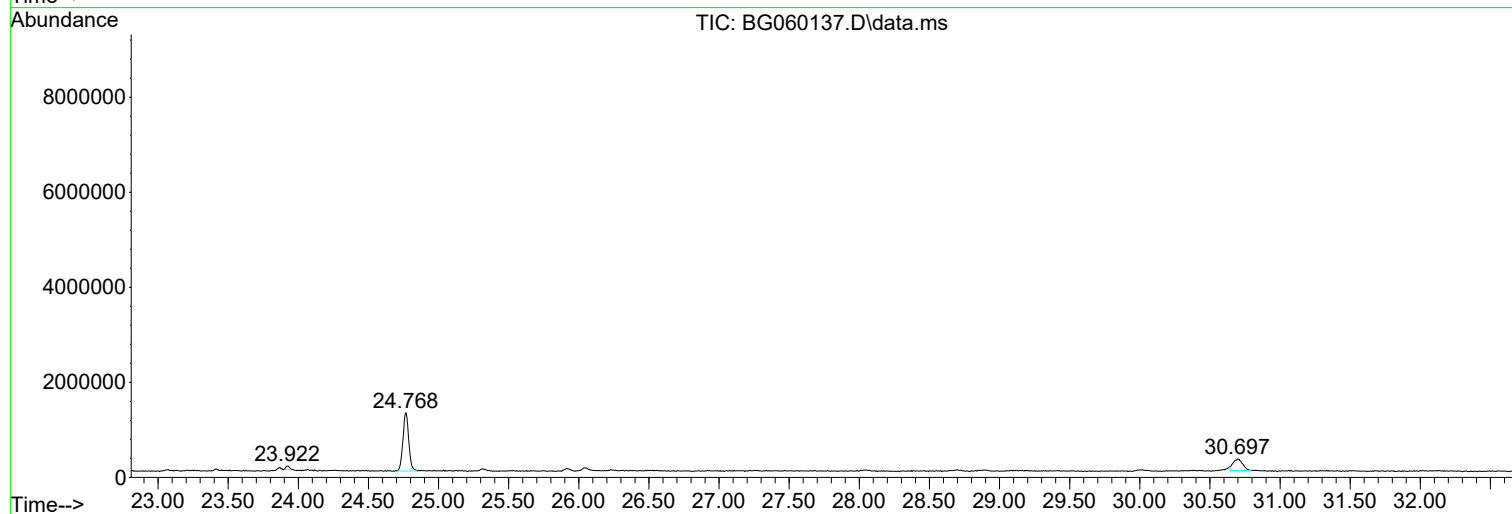
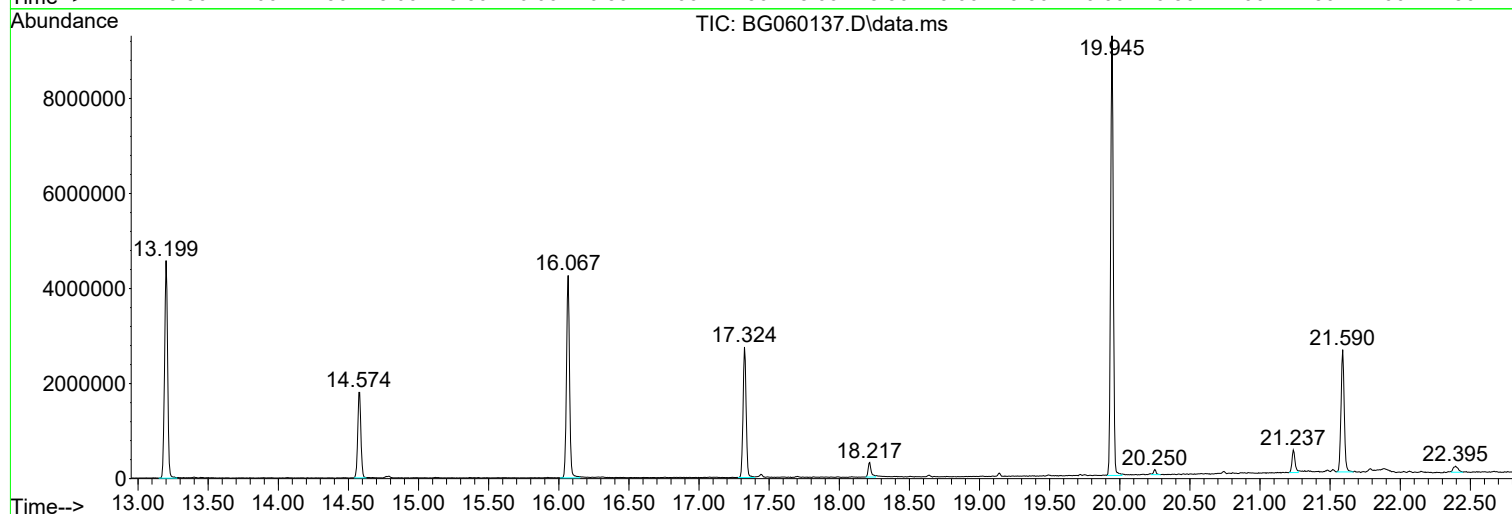
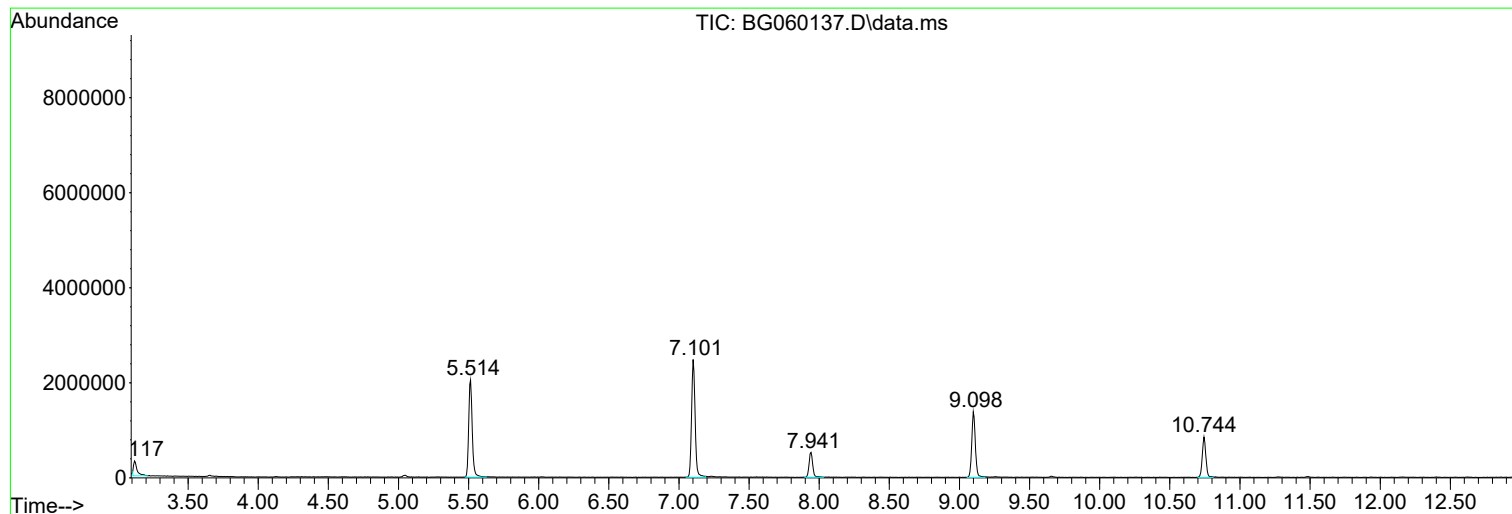
Sum of corrected areas: 57089325

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060137.D
Acq On : 22 Dec 2023 14:10
Operator : MA/JU
Sample : 05898-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-74a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.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\BG122223\
Data File : BG060137.D
Acq On : 22 Dec 2023 14:10
Operator : MA/JU
Sample : 05898-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-74a

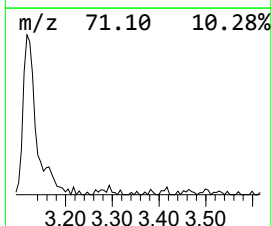
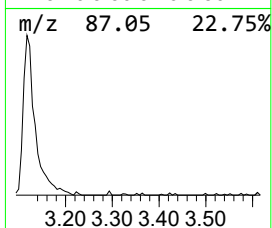
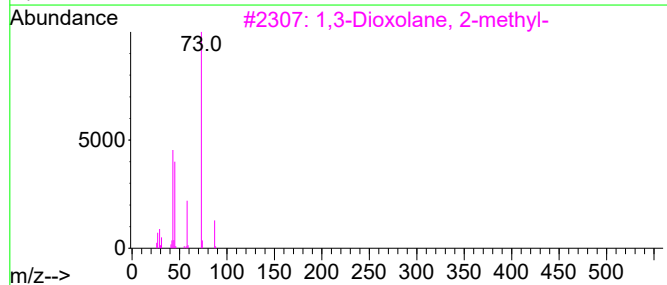
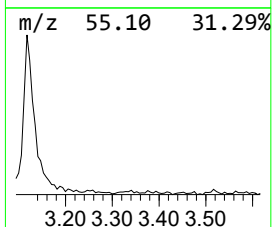
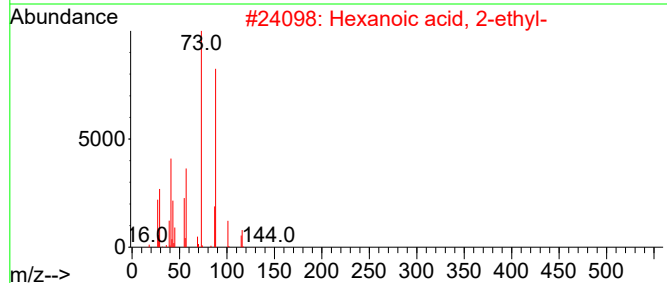
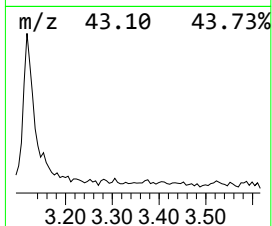
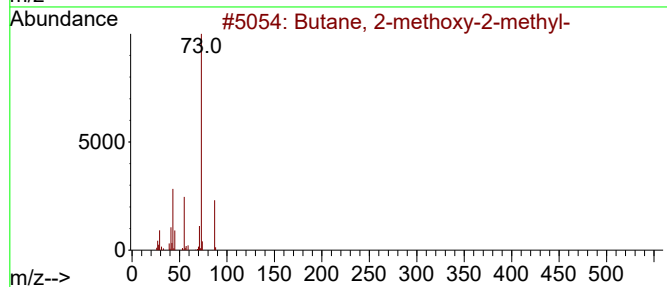
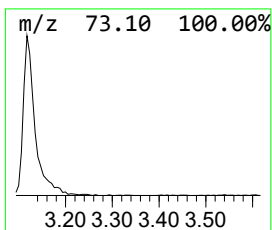
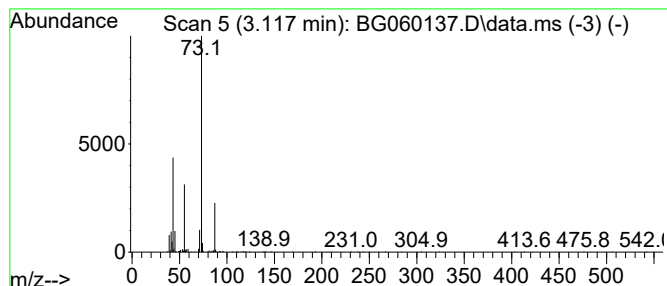
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.117	11.24 ng	530742	1,4-Dichlorobenzene-d4	7.941

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	33
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	25
5			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060137.D
Acq On : 22 Dec 2023 14:10
Operator : MA/JU
Sample : 05898-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-74a

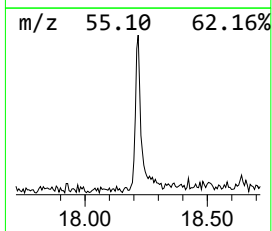
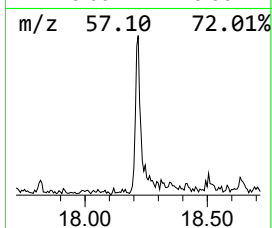
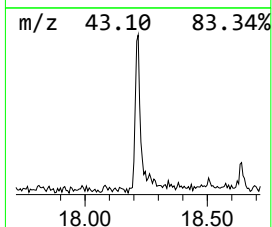
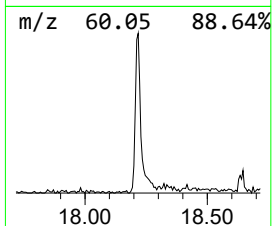
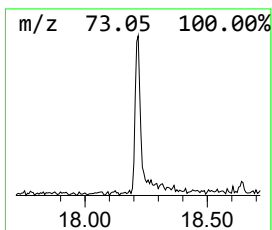
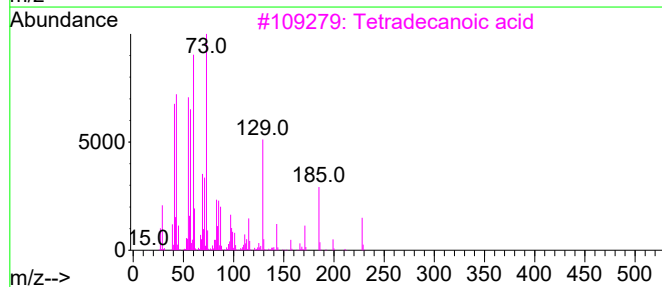
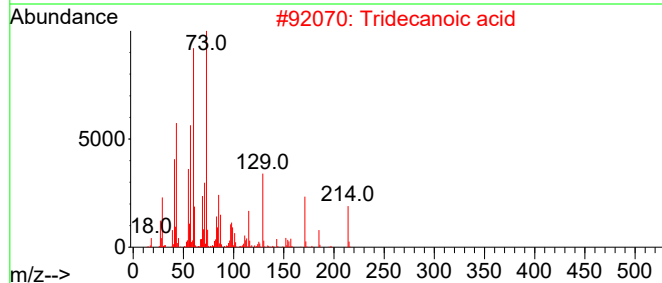
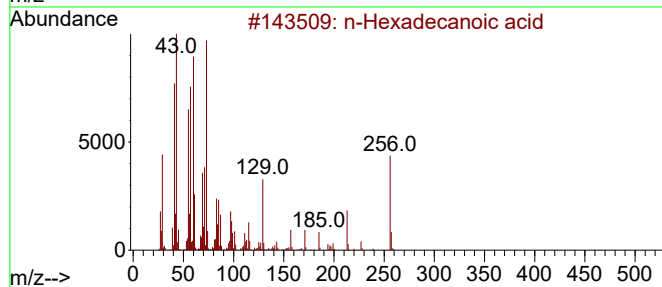
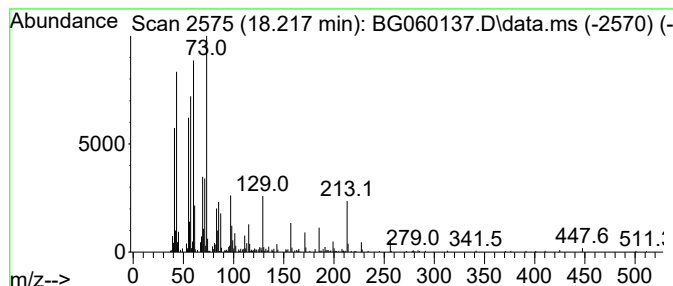
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.217	2.27 ng	476046	Phenanthrene-d10	17.324

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060137.D
Acq On : 22 Dec 2023 14:10
Operator : MA/JU
Sample : 05898-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-74a

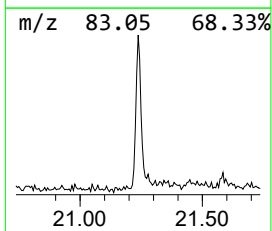
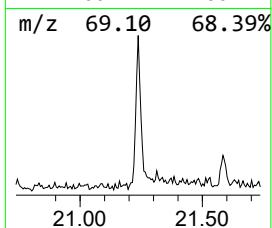
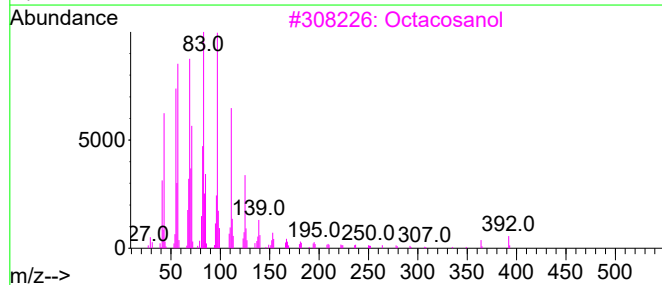
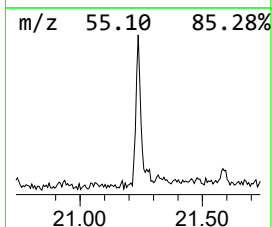
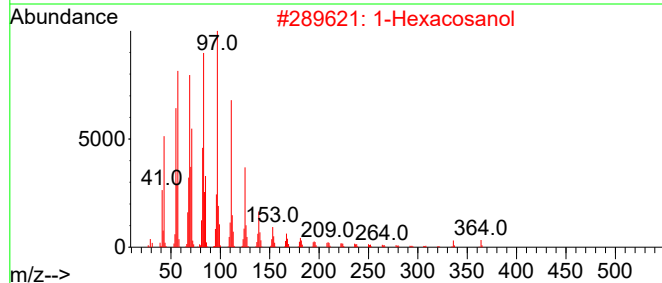
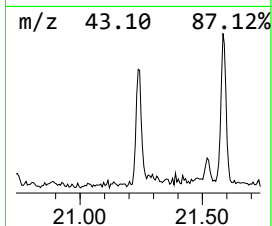
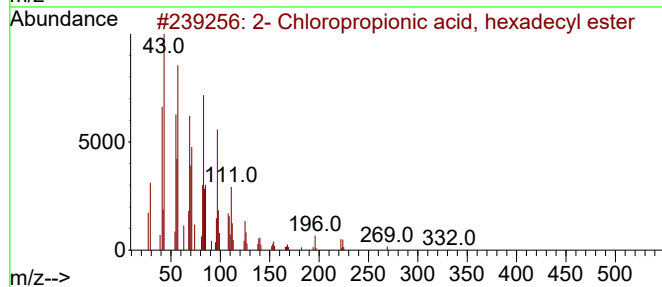
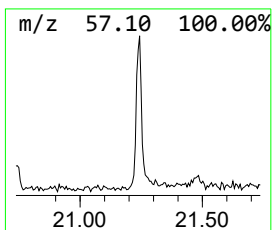
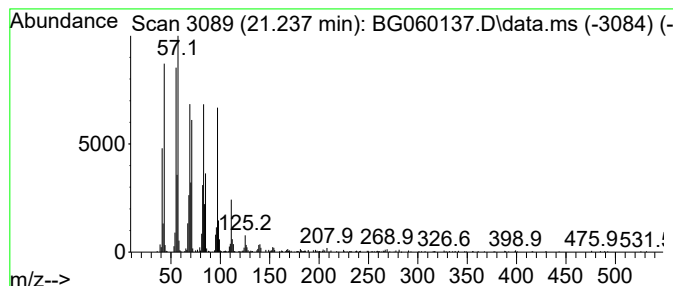
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2- Chloropropionic acid, he... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	3.58 ng	736714	Chrysene-d12	21.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91	
2	1-	Hexacosanol	382	C26H54O	000506-52-5	91	
3	Octacosanol	410	C28H58O	000557-61-9	90		
4	17-	Pentatriacontene	491	C35H70	006971-40-0	87	
5	3-	Eicosene, (E)-	280	C20H40	074685-33-9	74	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060137.D
Acq On : 22 Dec 2023 14:10
Operator : MA/JU
Sample : 05898-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-74a

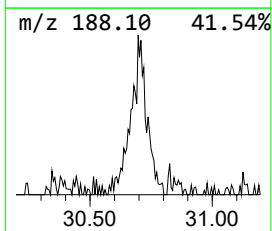
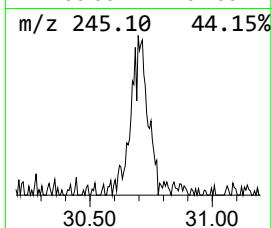
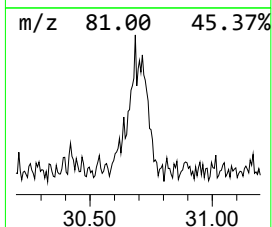
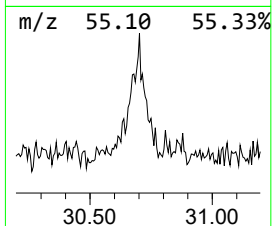
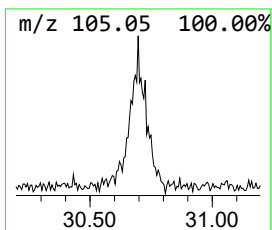
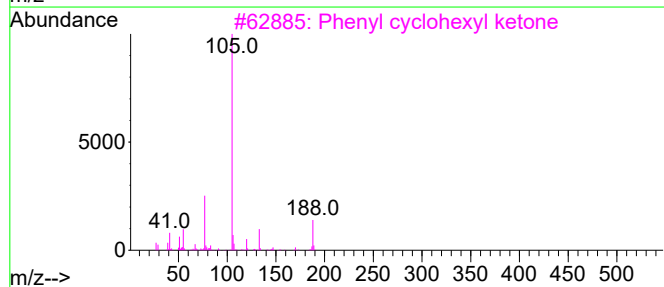
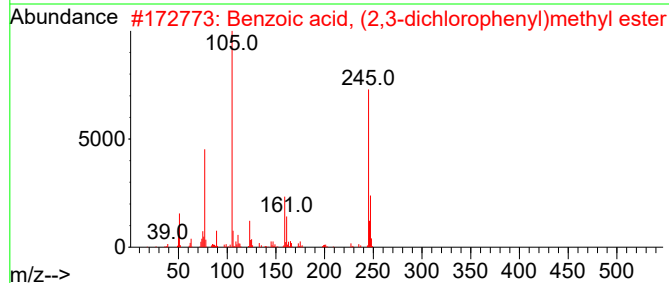
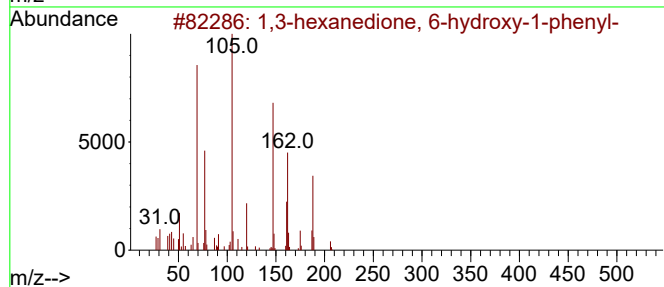
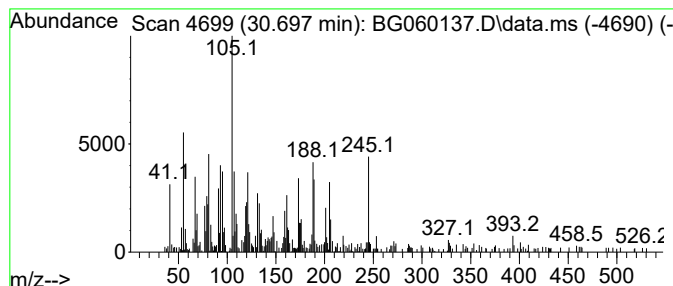
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown30.697 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.697	6.60 ng	1159860	Perylene-d12	24.768

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-hexanedione, 6-hydroxy-1-phe...	206	C12H14O3	1000400-50-6	10		
2	Benzoic acid, (2,3-dichloropheny...	280	C14H10Cl2O2	1000368-89-2	10		
3	Phenyl cyclohexyl ketone	188	C13H16O	000712-50-5	10		
4	2-Methoxy-4-methyl-3-(2-oxopyrro...	273	C16H19NO3	1000105-06-9	9		
5	Succinic acid, di(2,6-dichloroph...	406	C16H10Cl4O4	1000389-87-5	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060137.D
Acq On : 22 Dec 2023 14:10
Operator : MA/JU
Sample : 05898-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-74a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.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...	3.117	11.2	ng	530742	1	7.941	944557	20.0
n-Hexadecanoic ...	18.217	2.3	ng	476046	4	17.324	4201580	20.0
2-Chloropropio...	21.237	3.6	ng	736714	5	21.590	4113510	20.0
unknown30.697	30.697	6.6	ng	1159860	6	24.768	3514080	20.0