

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011724\
 Data File : BG060346.D
 Acq On : 17 Jan 2024 17:08
 Operator : MA/JU
 Sample : P1155-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BB-TESTPITS

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-BG010824.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060346.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.032	326	331	337	rBV2	116276	181006	1.08%	0.248%
2	5.502	404	411	429	rBV	3403504	5438803	32.32%	7.450%
3	7.094	674	682	699	rBV	3426813	6056319	35.99%	8.296%
4	7.928	816	824	834	rBV	726504	1243995	7.39%	1.704%
5	9.091	1013	1022	1041	rBV	2245389	4152346	24.67%	5.688%
6	10.731	1292	1301	1312	rBV	960531	1809249	10.75%	2.478%
7	13.187	1709	1719	1738	rBV	6769809	10686261	63.50%	14.638%
8	13.451	1757	1764	1769	rBV	286643	432551	2.57%	0.592%
9	14.562	1946	1953	1961	rBV	1823667	2811929	16.71%	3.852%
10	16.054	2198	2207	2220	rBV	5081789	8214414	48.81%	11.252%
11	17.311	2414	2421	2434	rBV	2483795	3868724	22.99%	5.299%
12	18.198	2566	2572	2584	rBV5	172281	416278	2.47%	0.570%
13	19.368	2766	2771	2777	rVB	168807	249370	1.48%	0.342%
14	19.726	2829	2832	2840	rVB	163099	243410	1.45%	0.333%
15	19.932	2861	2867	2882	rBV	12251049	16828633	100.00%	23.051%
16	21.218	3081	3086	3096	rBV	545499	859414	5.11%	1.177%
17	21.571	3139	3146	3153	rBV2	2586499	4558377	27.09%	6.244%
18	23.222	3422	3427	3433	rVB	102530	203002	1.21%	0.278%
19	24.738	3675	3685	3711	rBV	1456021	4750964	28.23%	6.508%

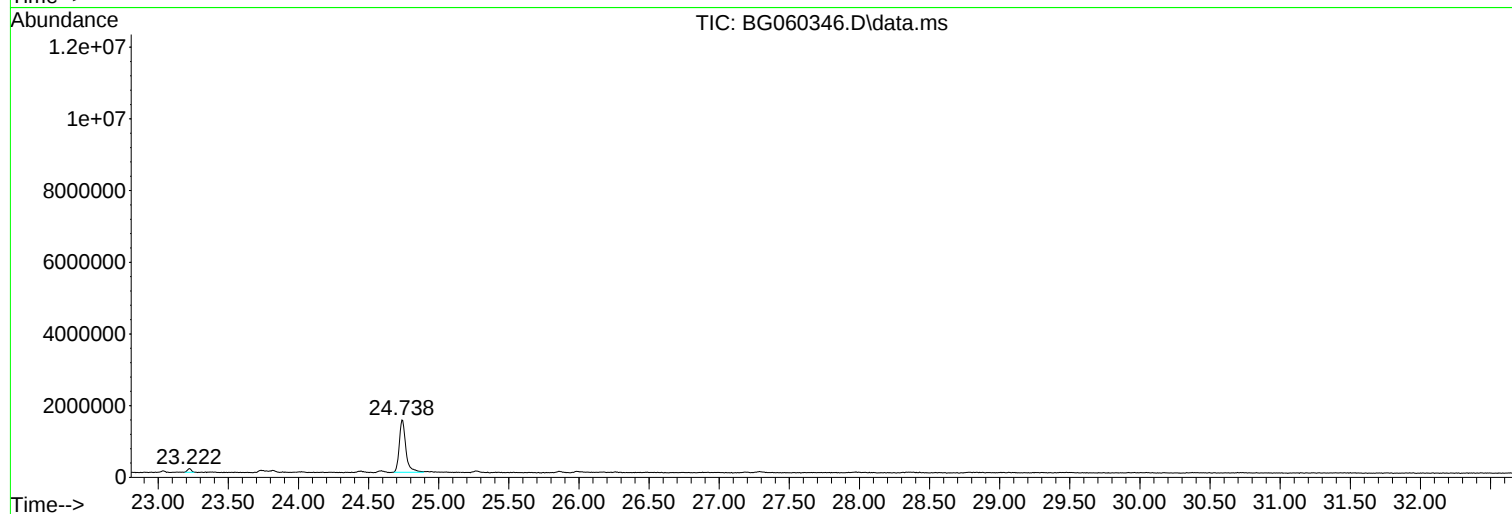
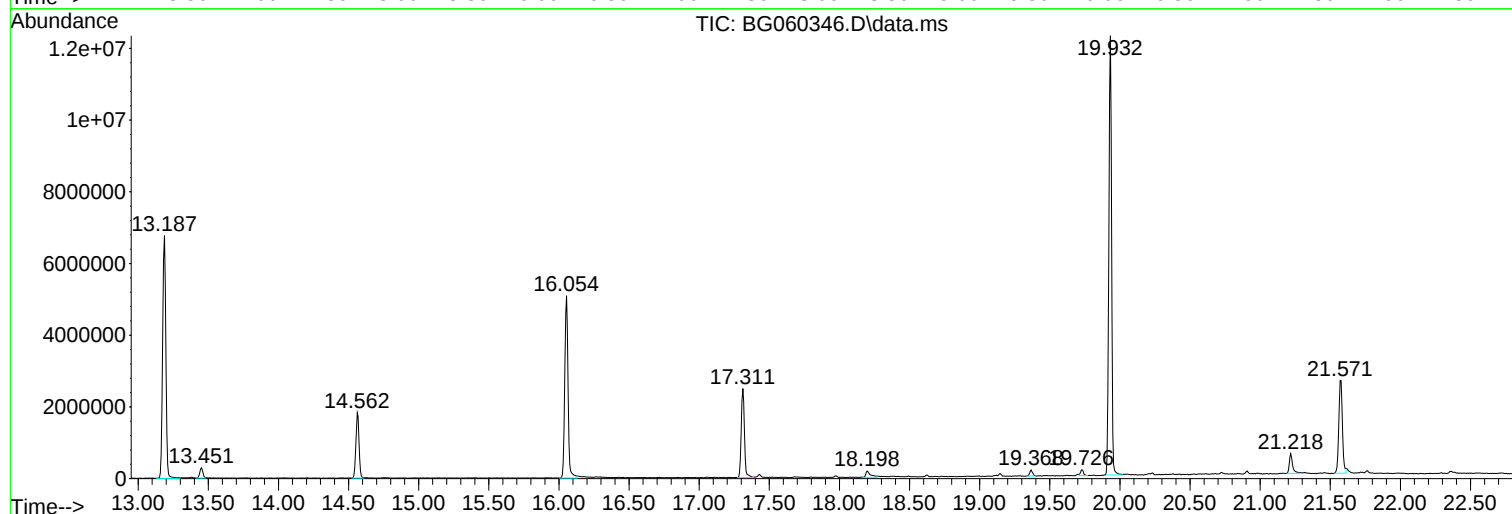
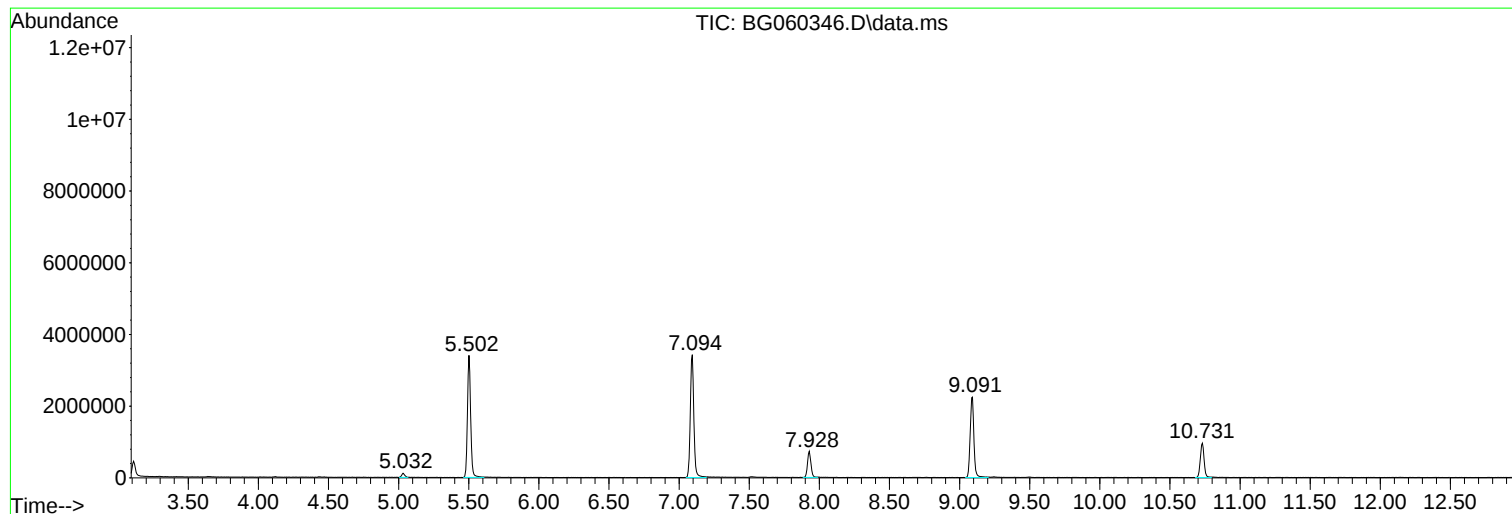
Sum of corrected areas: 73005045

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011724\
Data File : BG060346.D
Acq On : 17 Jan 2024 17:08
Operator : MA/JU
Sample : P1155-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BB-TESTPITS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.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\BG011724\
Data File : BG060346.D
Acq On : 17 Jan 2024 17:08
Operator : MA/JU
Sample : P1155-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BB-TESTPITS

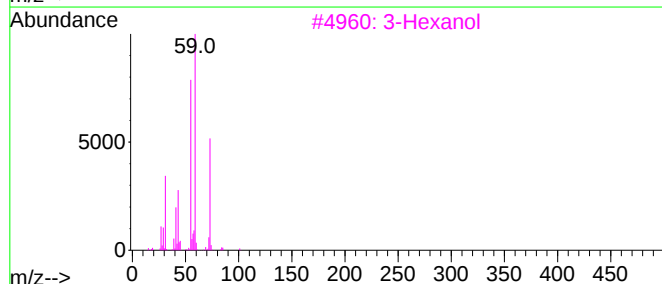
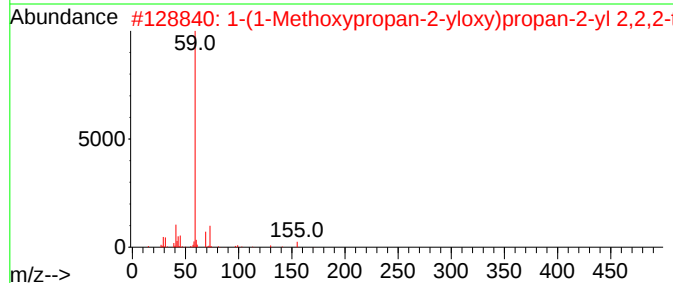
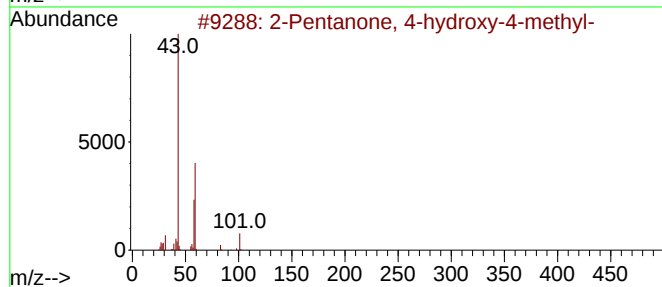
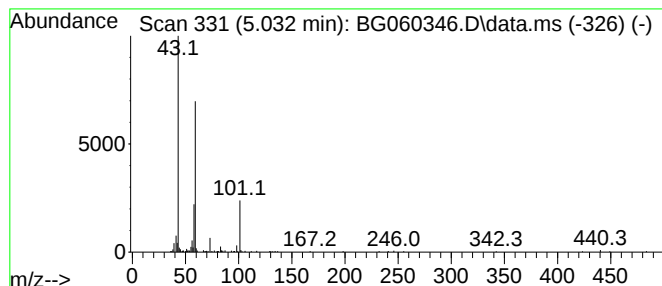
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.032	2.91 ng	181006	1,4-Dichlorobenzene-d4	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	1-(1-Methoxypropan-2-yloxy)propa...	244	C9H15F3O4	1010367-08-7	17		
3	3-Hexanol	102	C6H14O	000623-37-0	17		
4	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011724\
Data File : BG060346.D
Acq On : 17 Jan 2024 17:08
Operator : MA/JU
Sample : P1155-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

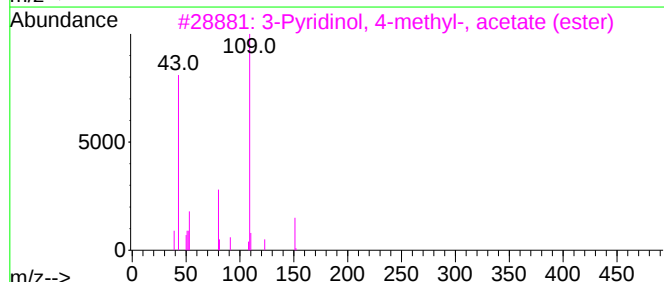
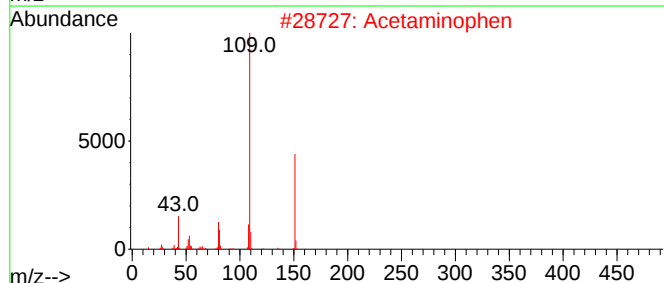
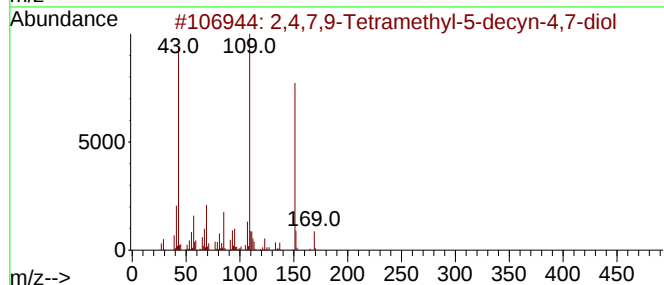
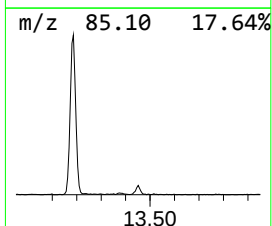
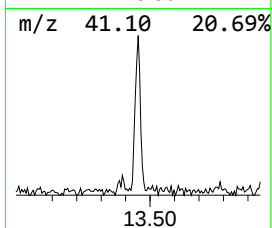
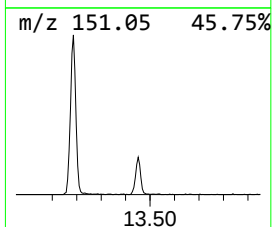
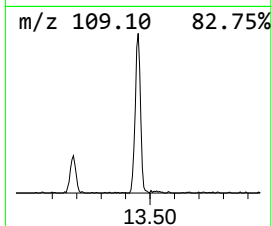
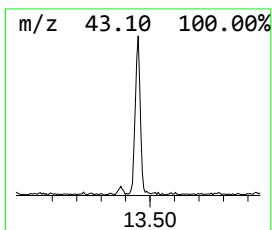
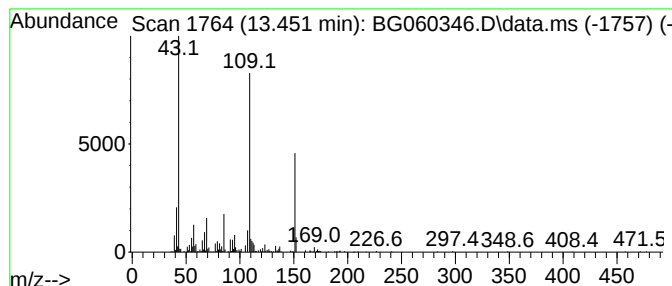
Instrument :
BNA_G
ClientSampleId :
BB-TESTPITS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.451	3.08 ng	432551	Acenaphthene-d10		14.562
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	Acetaminophen	151	C8H9NO2	000103-90-2	59
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
4	benzenamine, 3-[(tetrahydro-2H-p...	193	C11H15NO2	1010400-28-1	46
5	Metacetamol	151	C8H9NO2	000621-42-1	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011724\
Data File : BG060346.D
Acq On : 17 Jan 2024 17:08
Operator : MA/JU
Sample : P1155-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

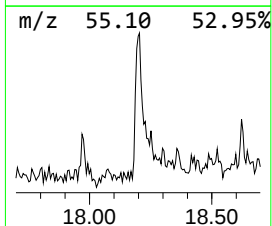
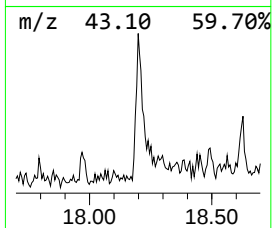
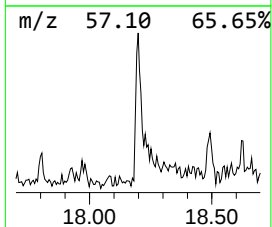
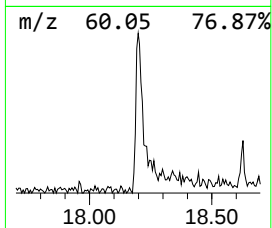
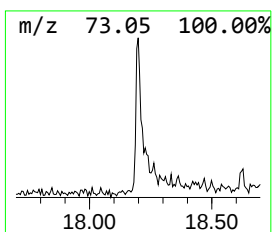
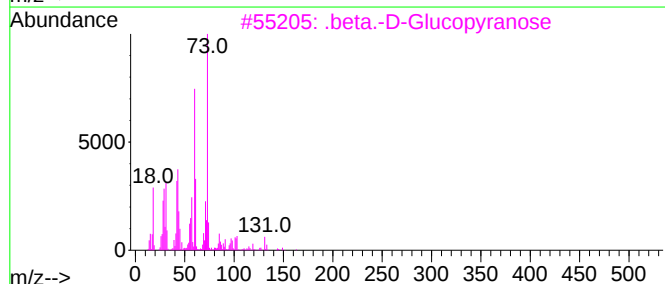
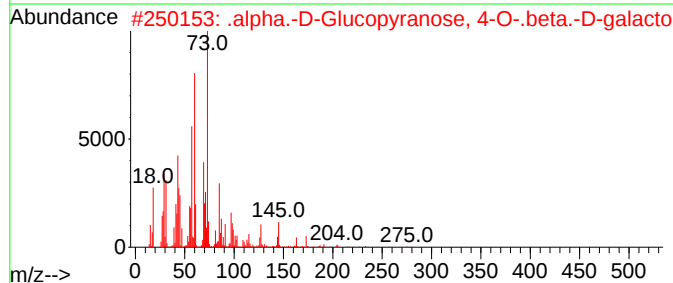
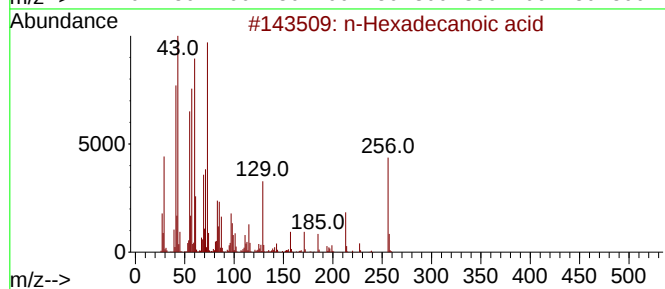
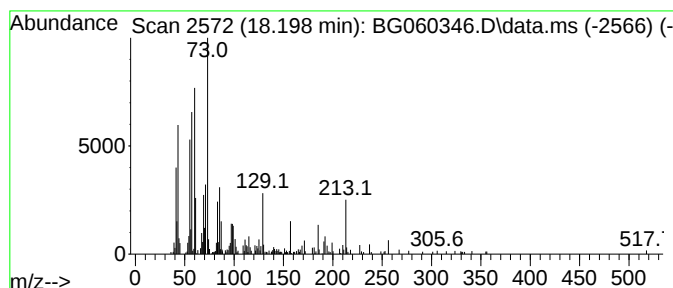
Instrument :
BNA_G
ClientSampleId :
BB-TESTPITS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.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.	
18.198	2.15 ng	416278	Phenanthrene-d10	17.311	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	53
3	.beta.-D-Glucopyranose	180	C6H12O6	000492-61-5	47
4	Tridecanoic acid	214	C13H26O2	000638-53-9	45
5	Cyclohexanebutanoic acid	170	C10H18O2	004441-63-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011724\
Data File : BG060346.D
Acq On : 17 Jan 2024 17:08
Operator : MA/JU
Sample : P1155-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BB-TESTPITS

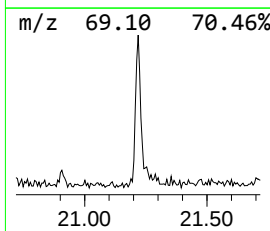
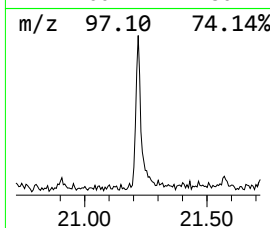
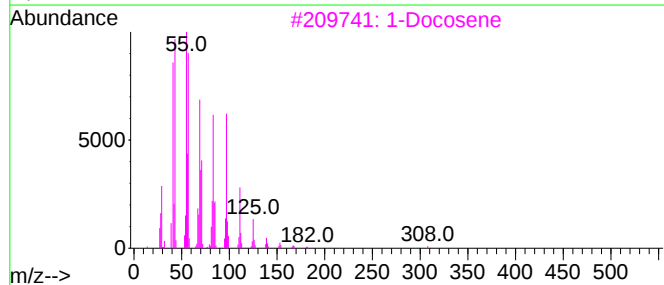
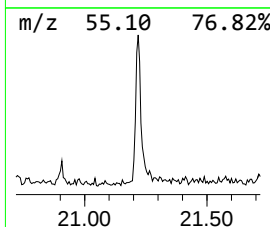
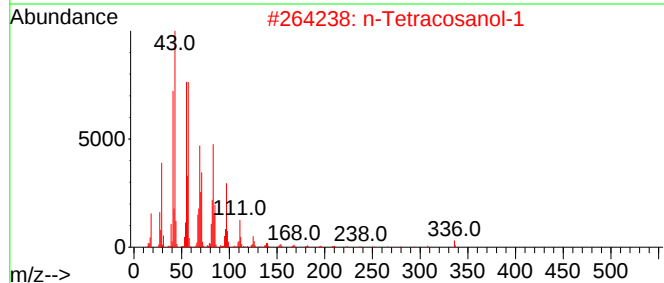
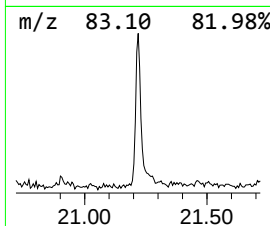
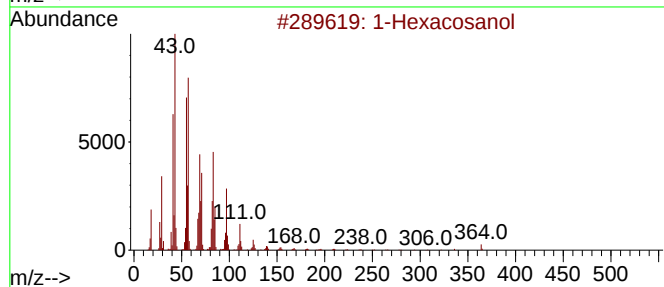
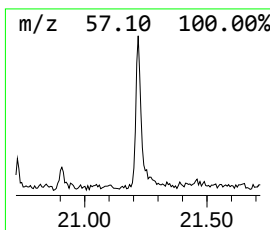
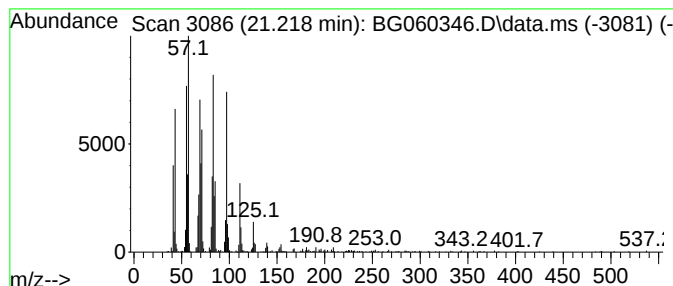
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Hexacosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.218	3.77 ng	859414	Chrysene-d12	21.577

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosanol	382	C26H54O	000506-52-5	91
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			1-Docosene	308	C22H44	001599-67-3	91
4			Behenic alcohol	326	C22H46O	000661-19-8	90
5			2-Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011724\
Data File : BG060346.D
Acq On : 17 Jan 2024 17:08
Operator : MA/JU
Sample : P1155-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BB-TESTPITS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.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-...	5.032	2.9	ng	181006	1	7.928	1244000	20.0
2,4,7,9-Tetrame...	13.451	3.1	ng	432551	3	14.562	2811930	20.0
n-Hexadecanoic ...	18.198	2.1	ng	416278	4	17.311	3868720	20.0
1-Hexacosanol	21.218	3.8	ng	859414	5	21.577	4558380	20.0