LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057845.D
Acq On : 23 Jun 2023 16:45
Operator : CG/JU
Sample : 03336-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

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-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057845.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.024	324	329	339	rVB	39461	60022	2.17%	0.397%
2	5.494	402	409	420	rBV	846848	1300832	46.94%	8.605%
3	7.086	672	680	693	rBV	837433	1412881	50.98%	9.346%
4	7.920	814	822	829	rBV	157738	258676	9.33%	1.711%
5	9.084	1011	1020	1028	rBV	480499	846607	30.55%	5.600%
6	10.723	1290	1299	1308	rVB	247547	412626	14.89%	2.730%
7	13.179	1710	1717	1724	rBV	1279732	1951557	70.42%	12.910%
8	14.554	1945	1951	1963	rVB2	386292	596012	21.51%	3.943%
9	15.911	2176	2182	2190	rVB	138079	192919	6.96%	1.276%
10	16.040	2197	2204	2211	rBV	1076510	1645389	59.37%	10.885%
11	17.298	2411	2418	2424	rBV	510026	729859	26.34%	4.828%
12	18.185	2564	2569	2586	rBV	173832	272954	9.85%	1.806%
13	19.460	2782	2786	2799	rBV2	52305	84081	3.03%	0.556%
14	19.918	2858	2864	2869	rBV	2101299	2771297	100.00%	18.333%
15	20.711	2995	2999	3008	rBV5	16740	29065	1.05%	0.192%
16	21.205	3078	3083	3094	rBV2	115586	200906	7.25%	1.329%
17	21.551	3136	3142	3148	rBV	485459	784145	28.30%	5.187%
18	21.663	3148	3161	3162	rBV5	135639	397475	14.34%	2.629%
19	22.350	3273	3278	3288	rBV4	24872	61326	2.21%	0.406%
20	22.997	3382	3388	3401	rBV4	84887	203078	7.33%	1.343%
21	23.808	3522	3526	3534	rVB4	20614	38863	1.40%	0.257%
22	24.701	3669	3678	3691	rVB	307985	866176	31.26%	5.730%

Sum of corrected areas: 15116746

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
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Misc :
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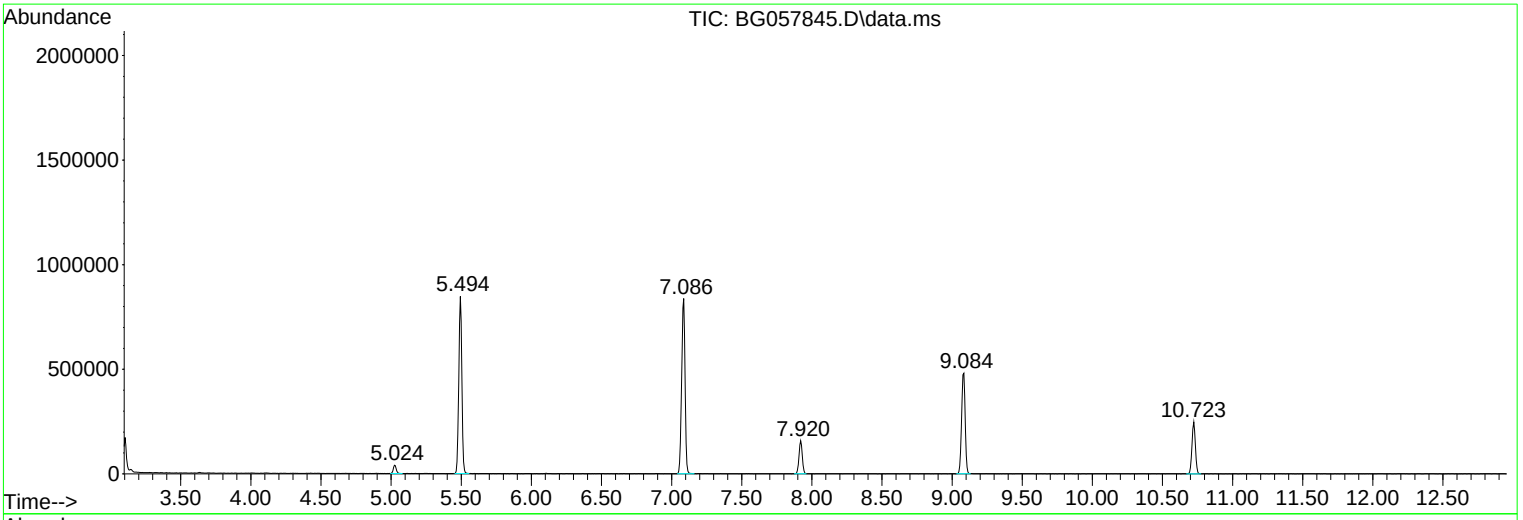
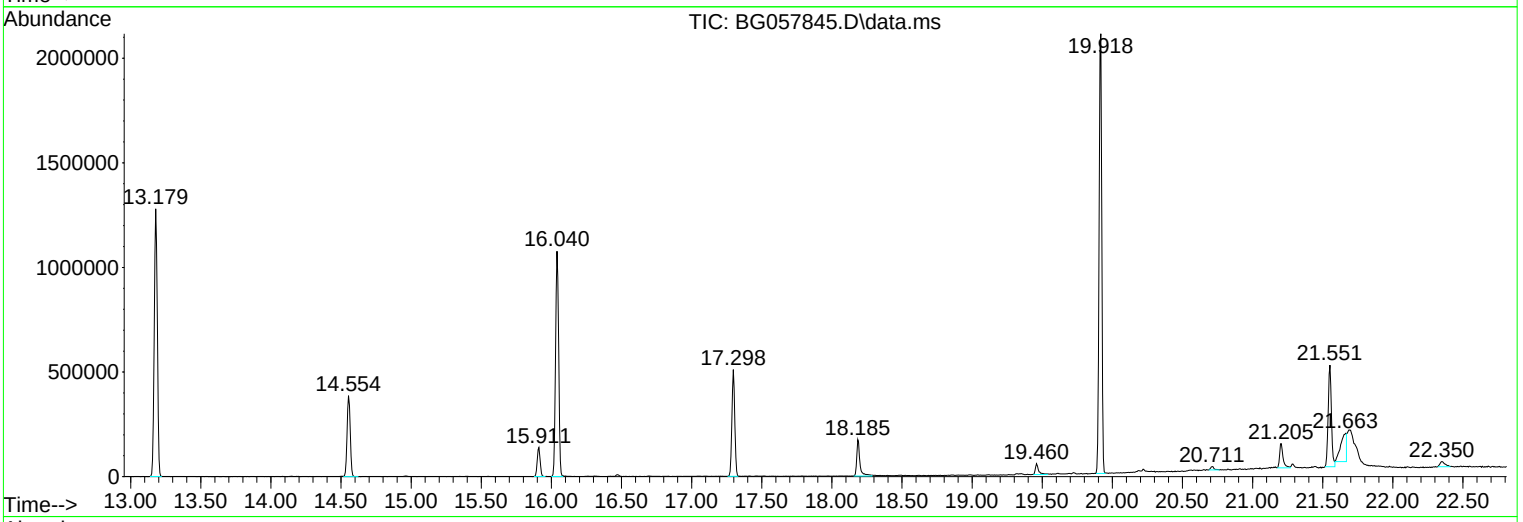
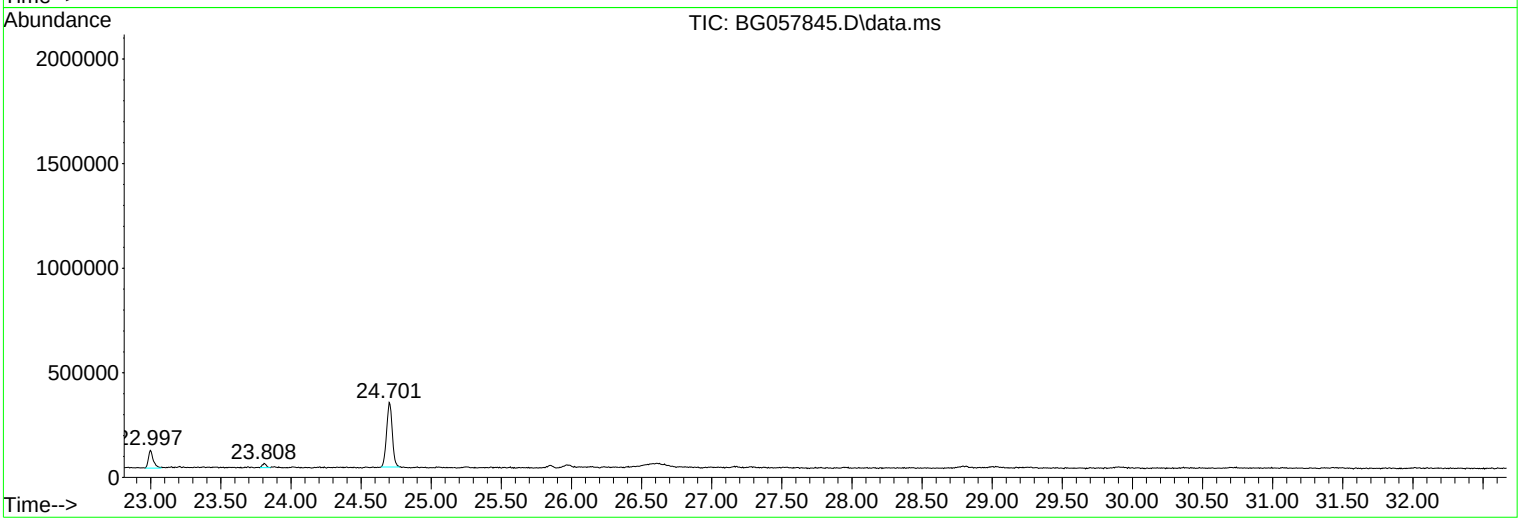
Instrument :
BNA_G
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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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Operator : CG/JU
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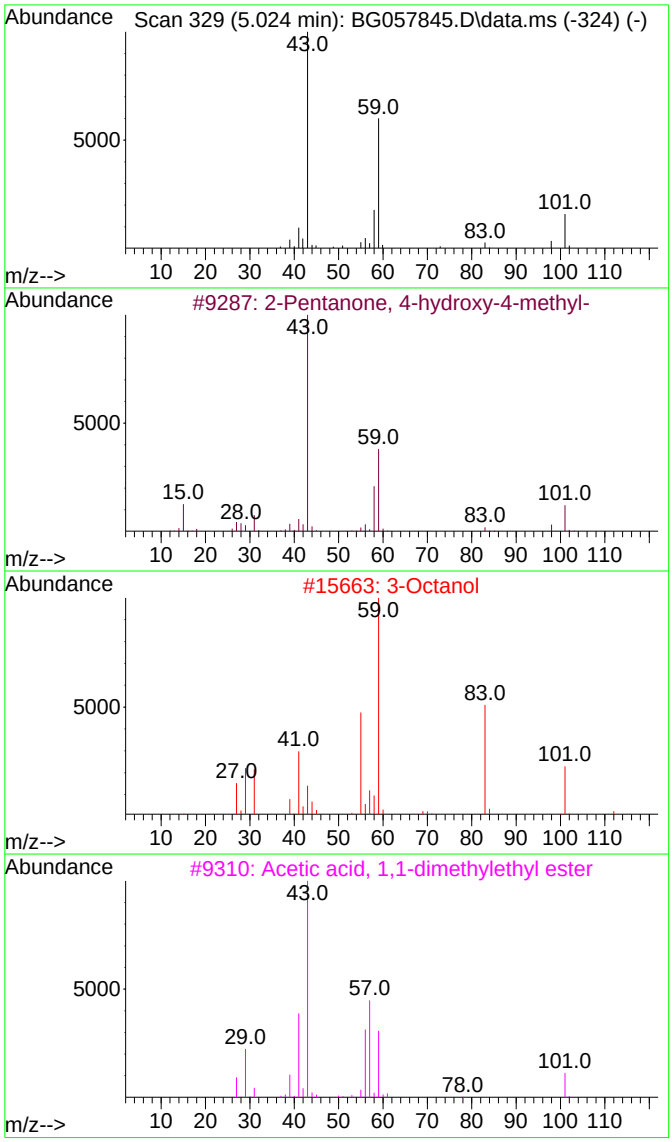
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

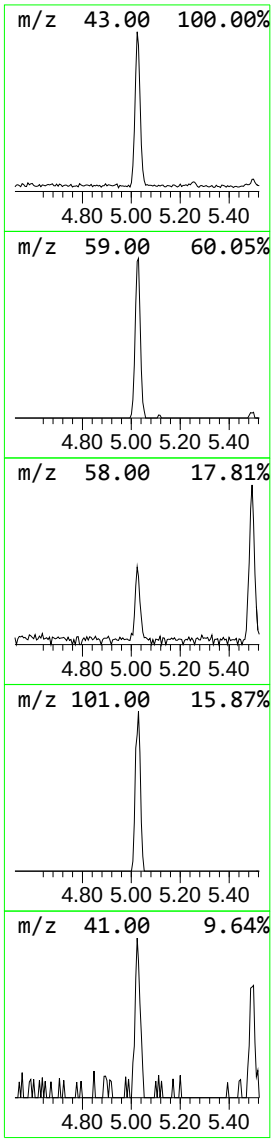
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.024	4.64 ng	60022	1,4-Dichlorobenzene-d4	7.920

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Octanol	130	C8H18O	000589-98-0	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057845.D
Acq On : 23 Jun 2023 16:45
Operator : CG/JU
Sample : 03336-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

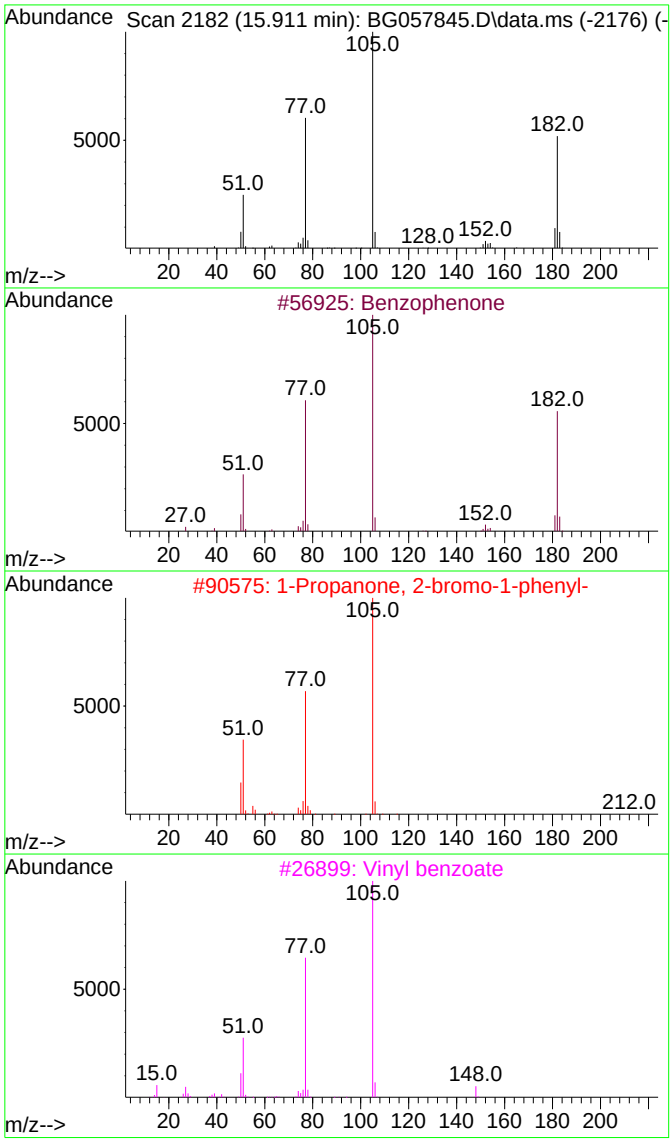
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

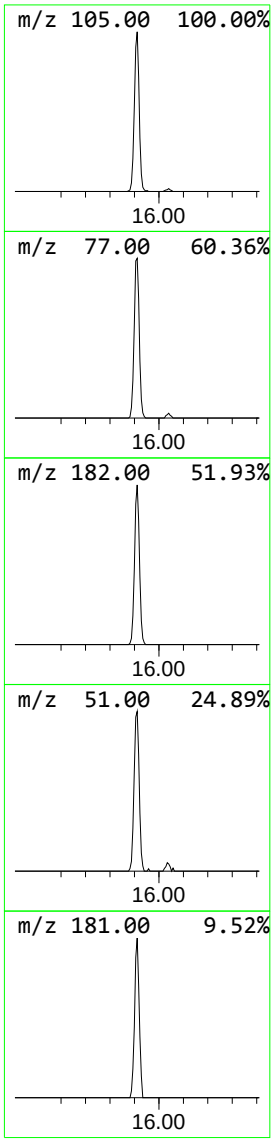
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.911	6.47 ng	192919	Acenaphthene-d10	14.554

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
5	N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057845.D
Acq On : 23 Jun 2023 16:45
Operator : CG/JU
Sample : 03336-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

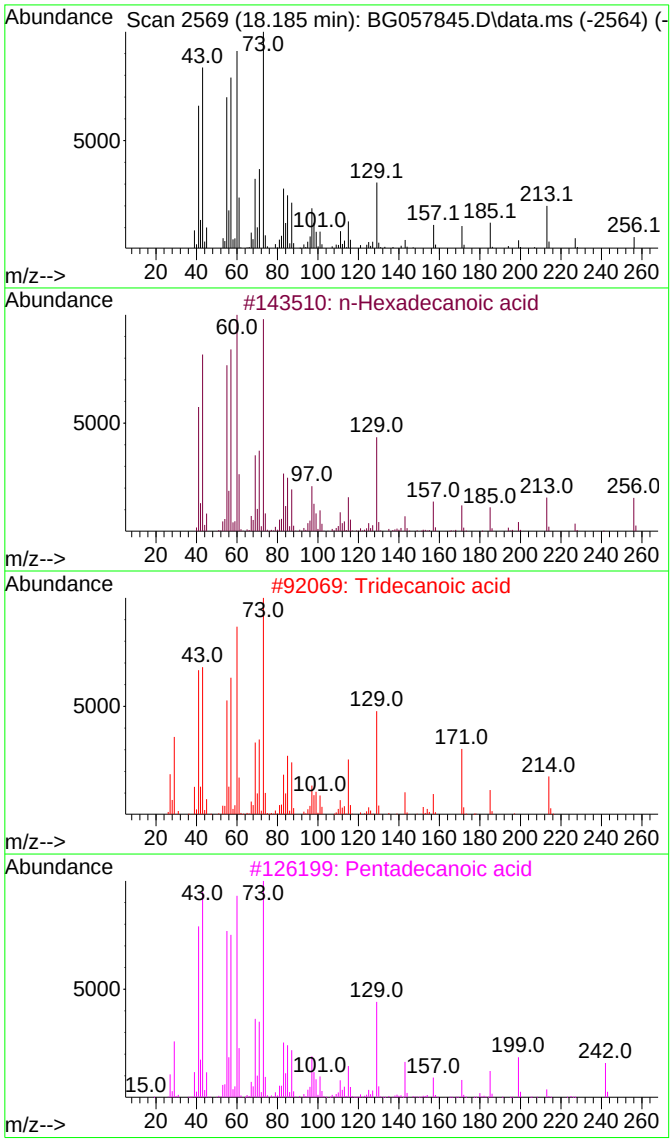
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

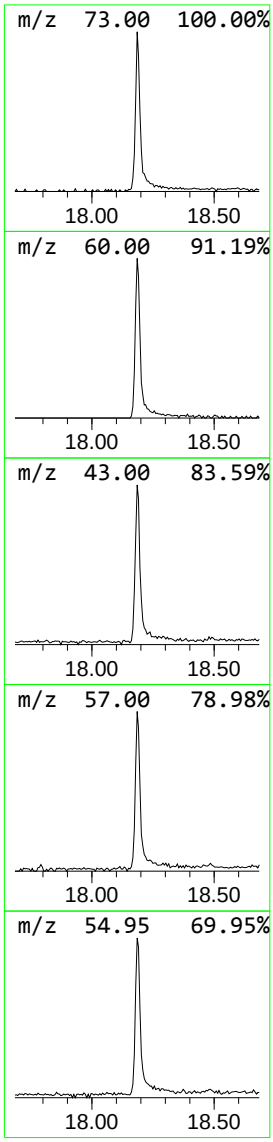
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.185	7.48 ng	272954	Phenanthrene-d10	17.297

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057845.D
Acq On : 23 Jun 2023 16:45
Operator : CG/JU
Sample : 03336-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
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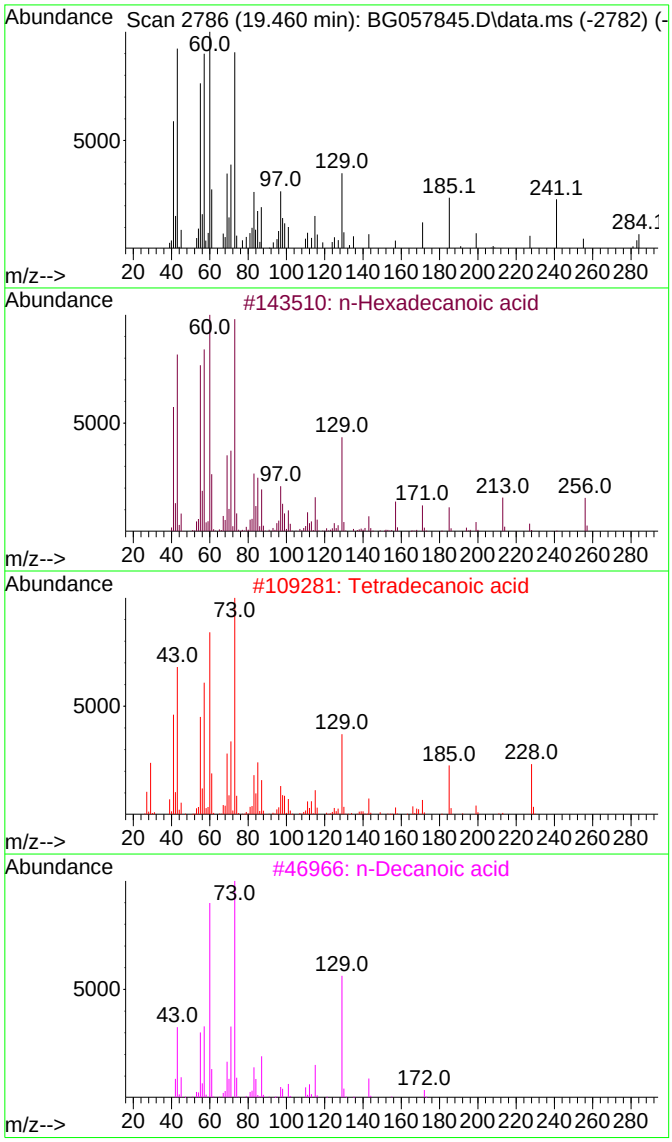
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

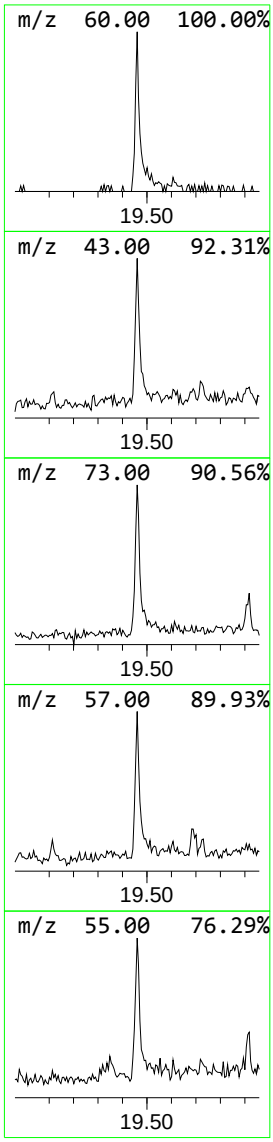
****

Peak Number 4 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.460	2.14 ng	84081	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	Tridecanoic acid	214	C13H26O2	000638-53-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
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Operator : CG/JU
Sample : 03336-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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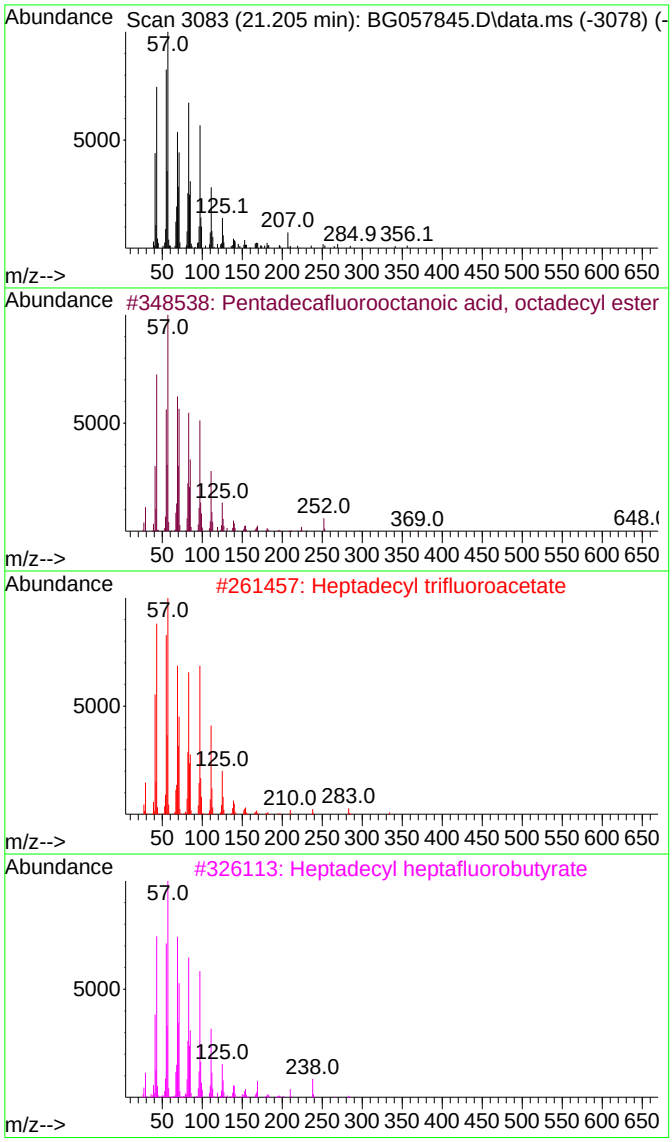
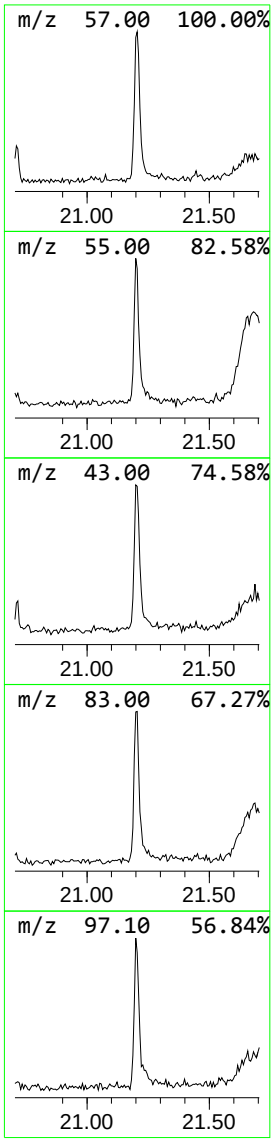
****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.205	5.12 ng	200906	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93





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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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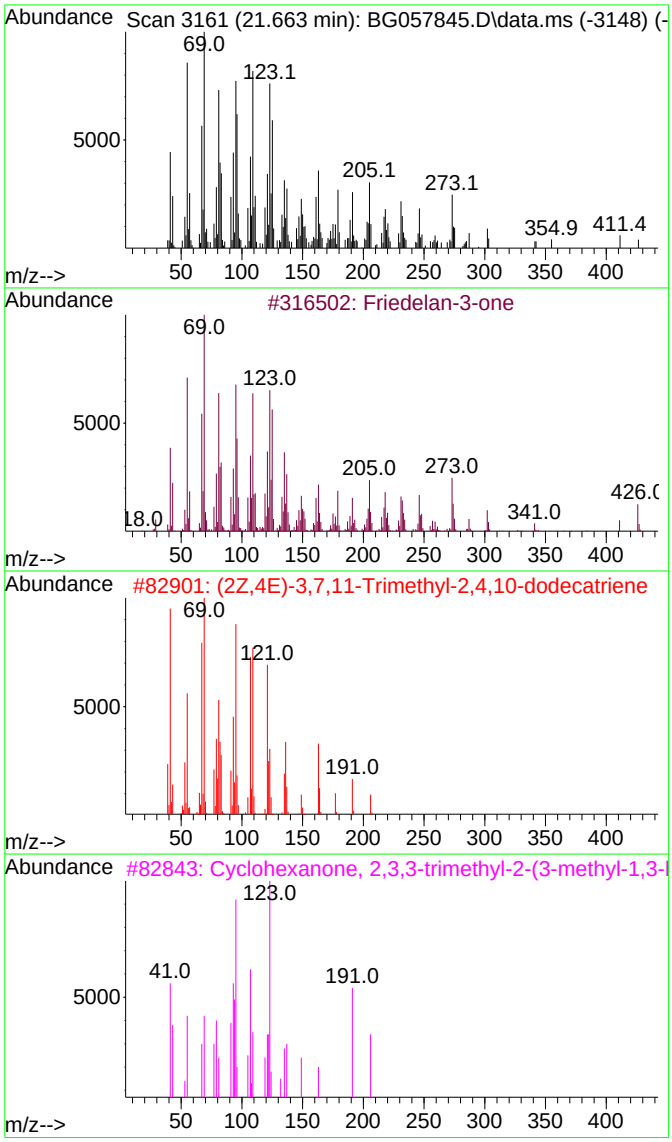
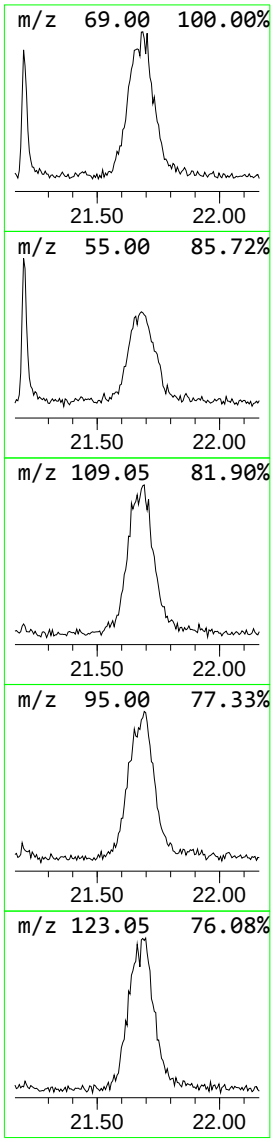
****

Peak Number 6 Friedelan-3-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.663	10.14 ng	397475	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Friedelan-3-one	426	C30H50O	000559-74-0	99
2	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	55
3	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	52
4	2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	52
5	7-Tetradecyne	194	C14H26	035216-11-6	38





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

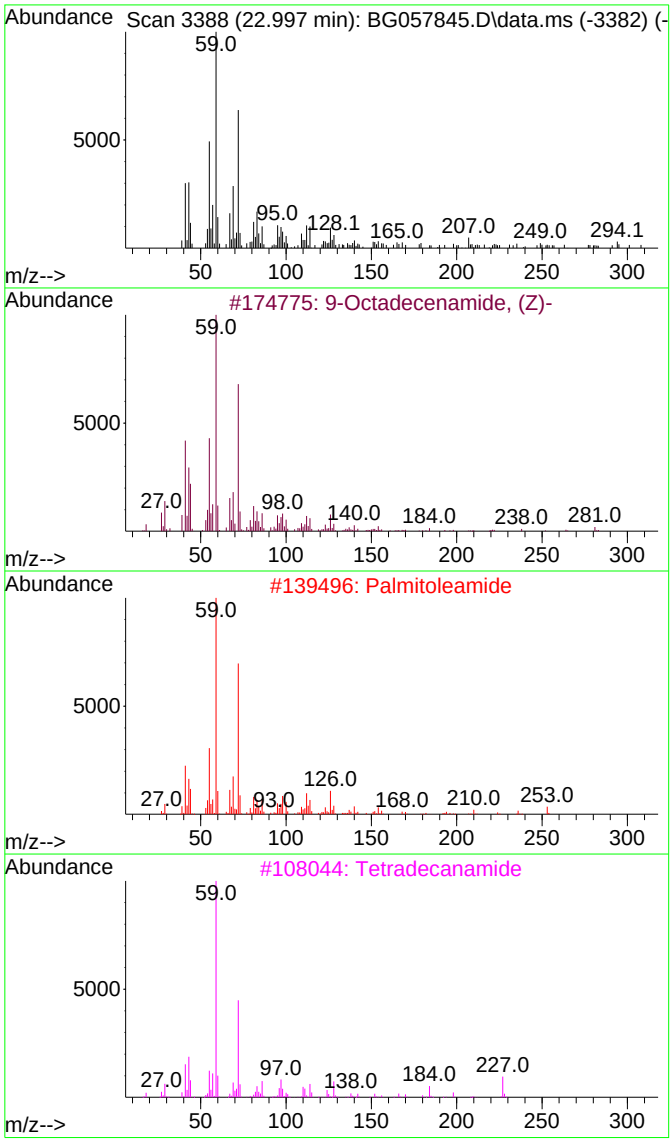
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

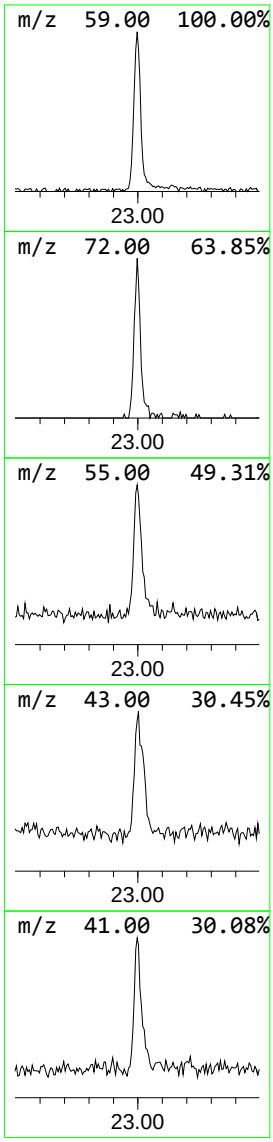
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.997	5.18 ng	203078	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	Palmitoleamide	253	C16H31NO	106010-22-4	87
3	Tetradecanamide	227	C14H29NO	000638-58-4	53
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	50
5	Dodecanamide	199	C12H25NO	001120-16-7	47





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.024	4.6	ng	60022	1	7.920	258676	20.0
Benzophenone	15.911	6.5	ng	192919	3	14.554	596012	20.0
n-Hexadecanoic ...	18.185	7.5	ng	272954	4	17.297	729859	20.0
Tetradecanoic acid	19.460	2.1	ng	84081	5	21.551	784145	20.0
Pentadecafluoro...	21.205	5.1	ng	200906	5	21.551	784145	20.0
Friedelan-3-one	21.663	10.1	ng	397475	5	21.551	784145	20.0
9-Octadecenamid...	22.997	5.2	ng	203078	5	21.551	784145	20.0