LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
Data File : BG057928.D
Acq On : 30 Jun 2023 21:10
Operator : CG/JU
Sample : 03358-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1-(8-10)

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-BG062723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057928.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	323	328	335	rVB	41924	61227	1.44%	0.332%
2	5.486	401	408	419	rBV	916219	1418496	33.29%	7.697%
3	7.078	671	679	691	rBV	955728	1615237	37.91%	8.764%
4	7.912	814	821	828	rBV	129245	211957	4.97%	1.150%
5	9.076	1011	1019	1032	rBV	554863	980601	23.01%	5.321%
6	10.715	1289	1298	1307	rBV	183930	323465	7.59%	1.755%
7	13.171	1709	1716	1728	rVB	1593886	2447430	57.44%	13.279%
8	14.546	1944	1950	1959	rVB	347018	534684	12.55%	2.901%
9	15.903	2173	2181	2196	rVB	325932	444732	10.44%	2.413%
10	16.038	2197	2204	2221	rBV	1561517	2425127	56.91%	13.158%
11	16.467	2271	2277	2289	rVB	62899	91307	2.14%	0.495%
12	17.290	2410	2417	2426	rBV	490192	723757	16.99%	3.927%
13	18.177	2563	2568	2578	rBV	217160	355514	8.34%	1.929%
14	19.452	2781	2785	2795	rBV	63821	118145	2.77%	0.641%
15	19.910	2856	2863	2871	rBV	3220789	4261040	100.00%	23.120%
16	21.197	3077	3082	3092	rBV2	93306	154714	3.63%	0.839%
17	21.543	3135	3141	3148	rVB	443227	719876	16.89%	3.906%
18	21.731	3170	3173	3178	rVB2	32187	45668	1.07%	0.248%
19	22.325	3270	3274	3281	rVB	37976	56330	1.32%	0.306%
20	22.983	3379	3386	3400	rBV3	239546	569217	13.36%	3.089%
21	23.788	3519	3523	3529	rVB4	27596	53851	1.26%	0.292%
22	24.687	3666	3676	3687	rVB	285855	817766	19.19%	4.437%

Sum of corrected areas: 18430141

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
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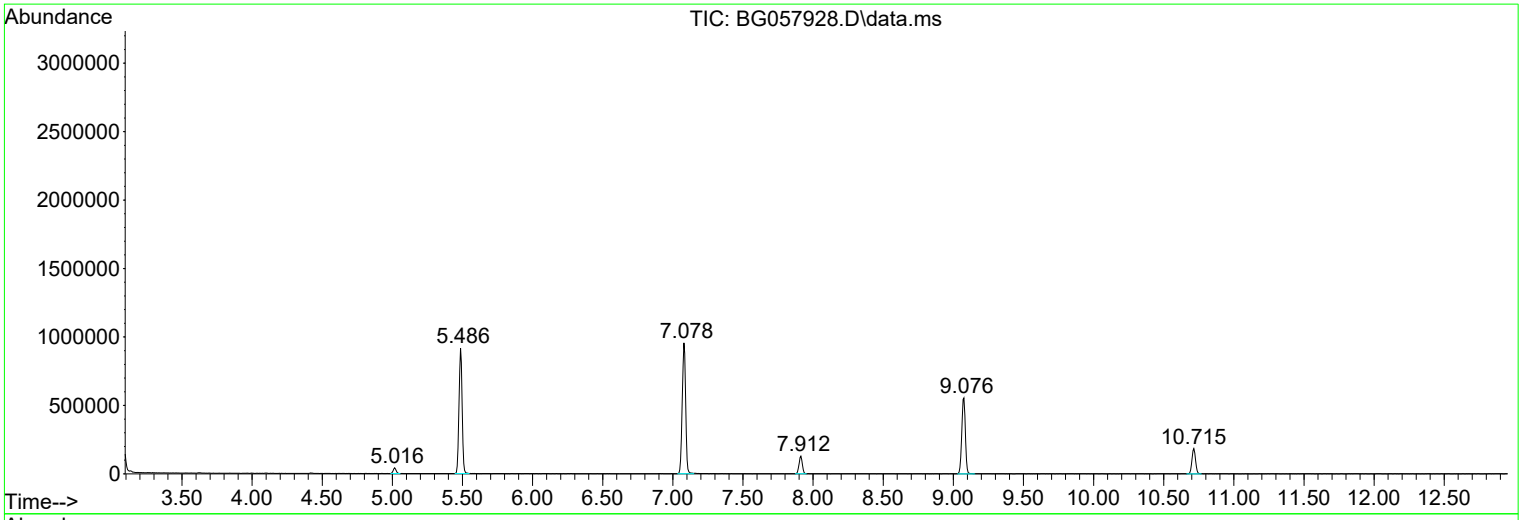
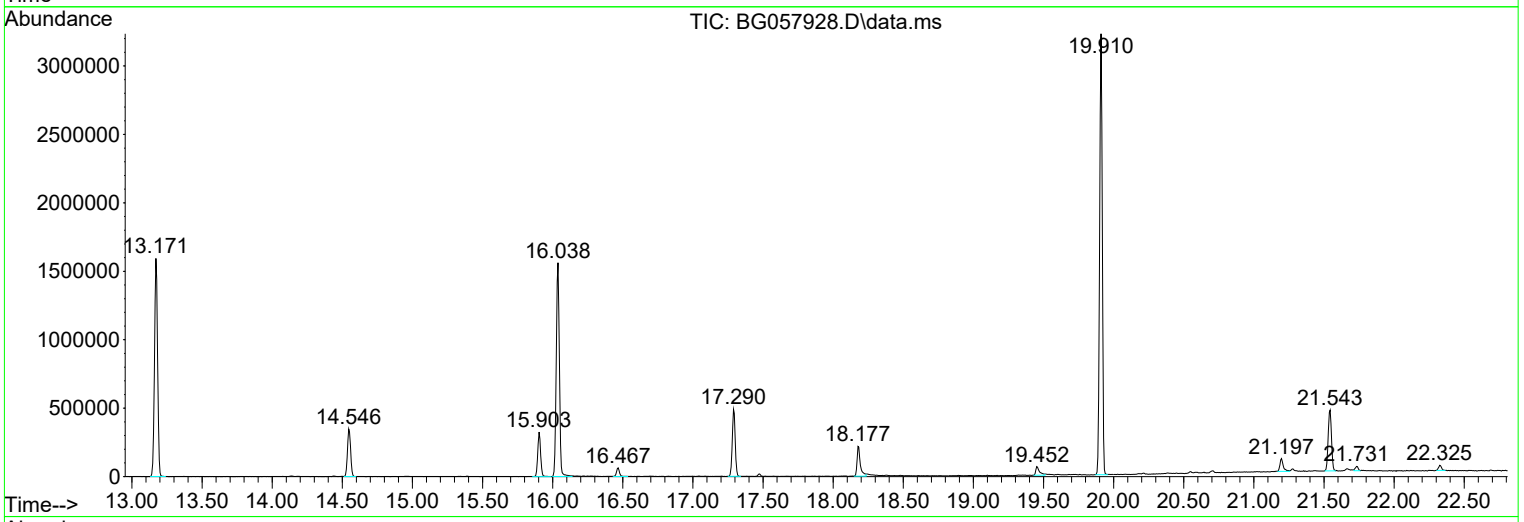
Misc :
ALS Vial : 11 Sample Multiplier: 1

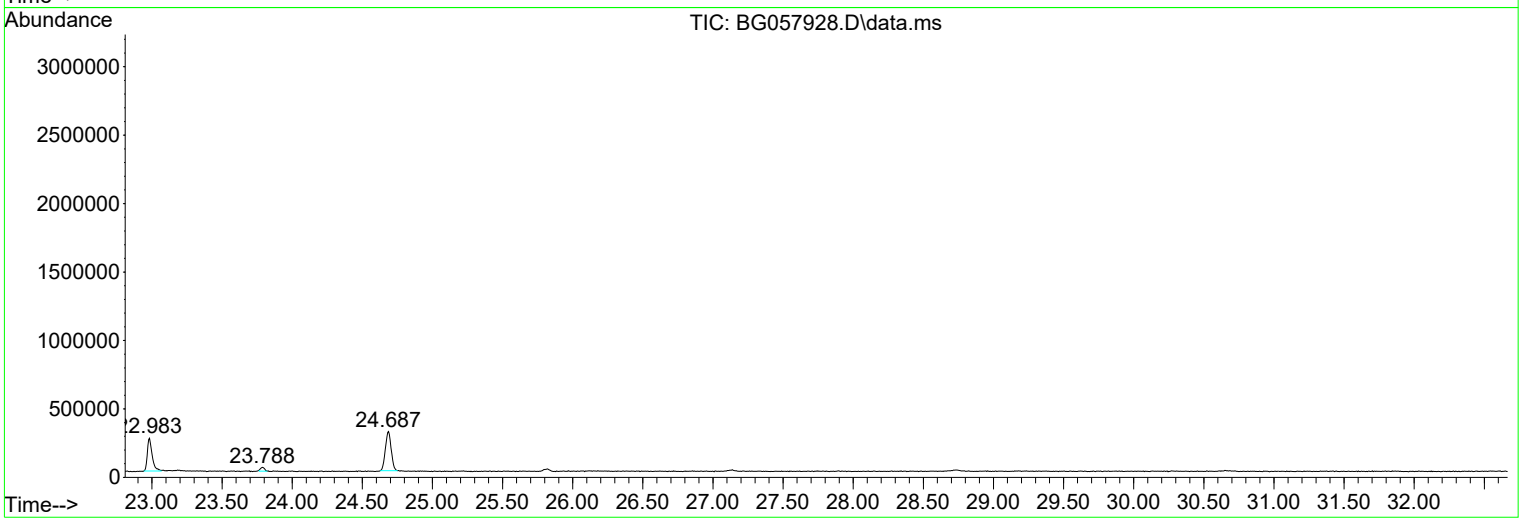
Instrument :
BNA_G
ClientSampleId :
SB-1-(8-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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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Data File : BG057928.D
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Sample : 03358-02
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Instrument :
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ClientSampleId :
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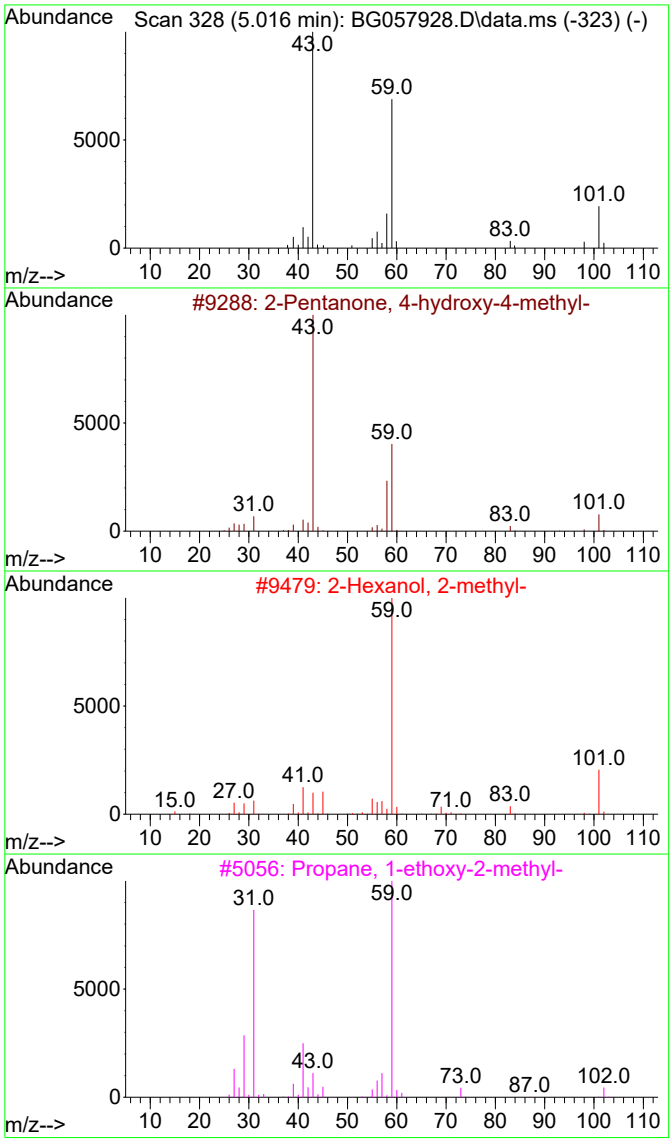
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

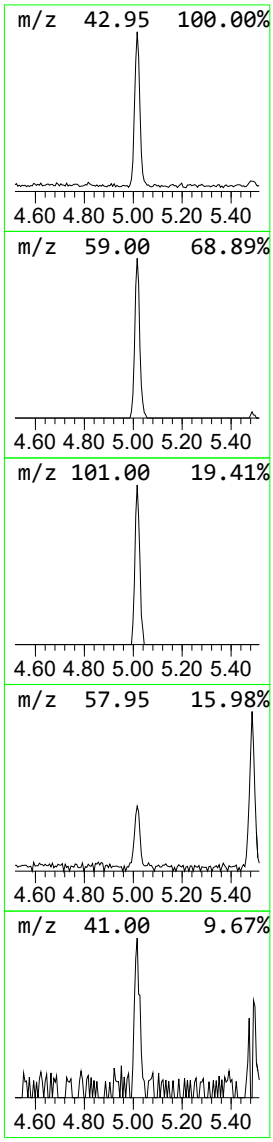
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	5.78 ng	61227	1,4-Dichlorobenzene-d4	7.912

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32
4	3-Pentanol	88	C5H12O	000584-02-1	25
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	23





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Data File : BG057928.D
Acq On : 30 Jun 2023 21:10
Operator : CG/JU
Sample : 03358-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-1-(8-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

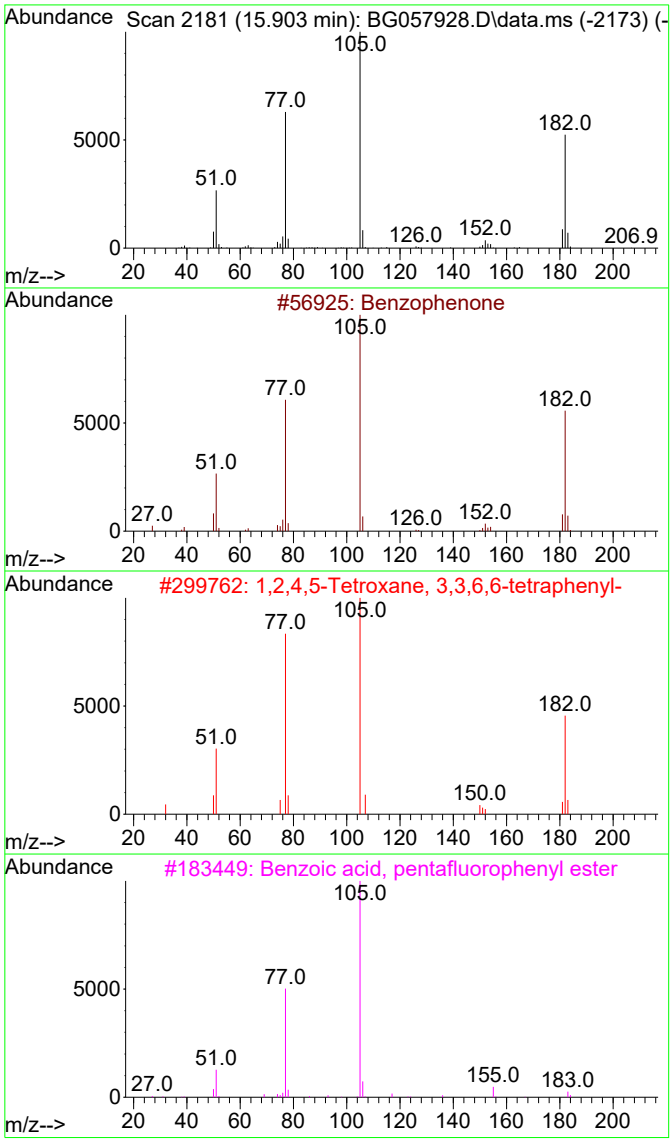
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

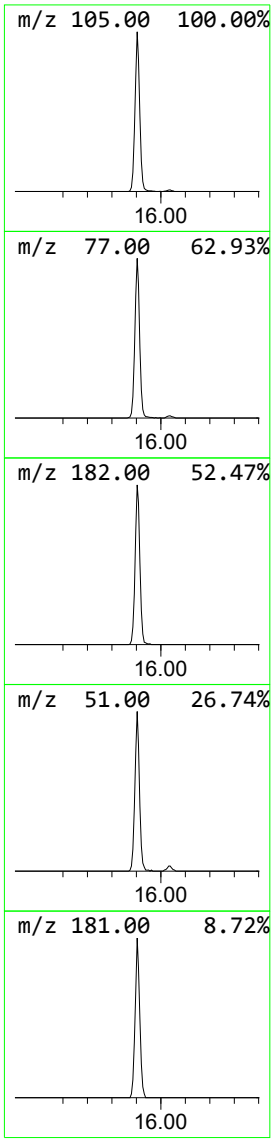
****

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.903	16.64 ng	444732	Acenaphthene-d10	14.546

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	Methyl hippurate, N-trifluoroace...	289	C12H10F3NO4	073749-76-5	47





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Acq On : 30 Jun 2023 21:10
Operator : CG/JU
Sample : 03358-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1-(8-10)

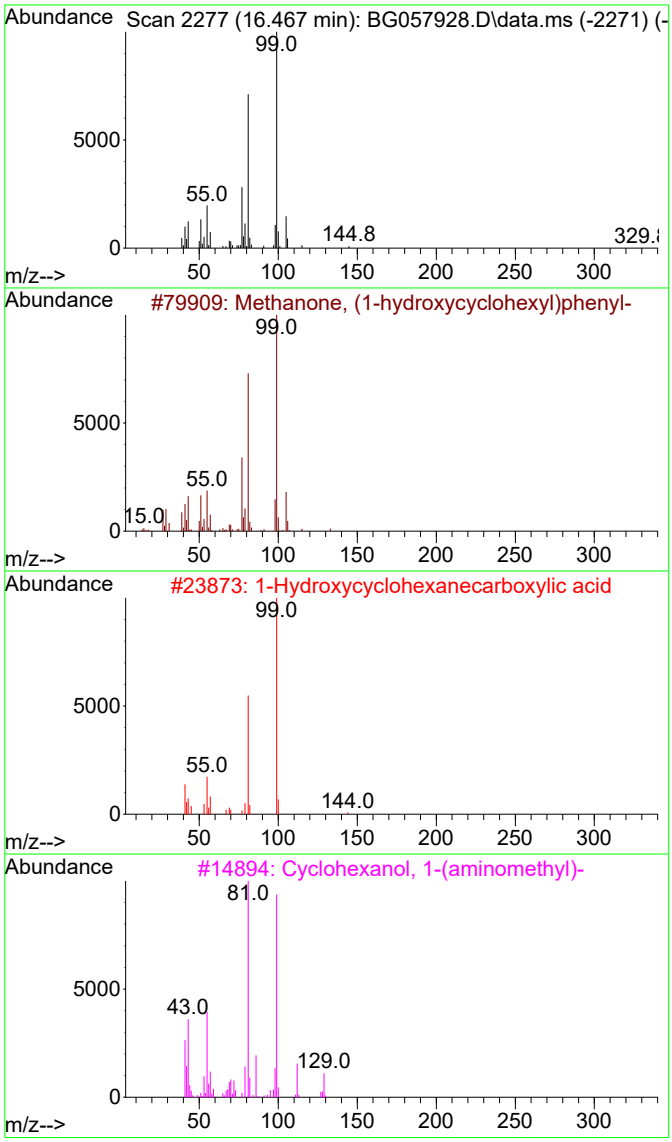
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

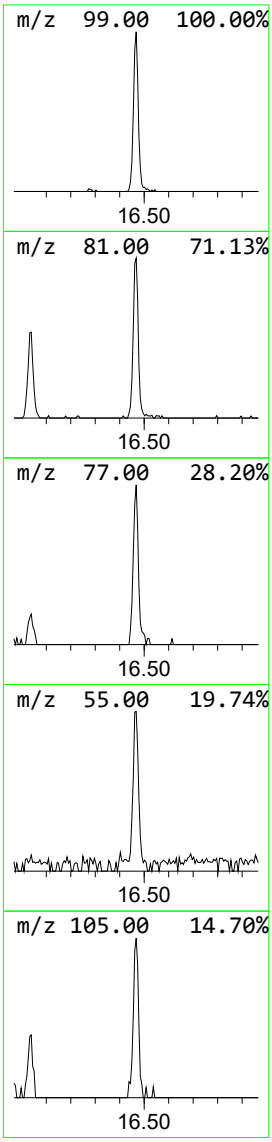
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Methanone, (1-hydroxycycloh... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.467	2.52 ng	91307	Phenanthrene-d10	17.290

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	50
3	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	42
4	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	38
5	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	33





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Acq On : 30 Jun 2023 21:10
Operator : CG/JU
Sample : 03358-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1-(8-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

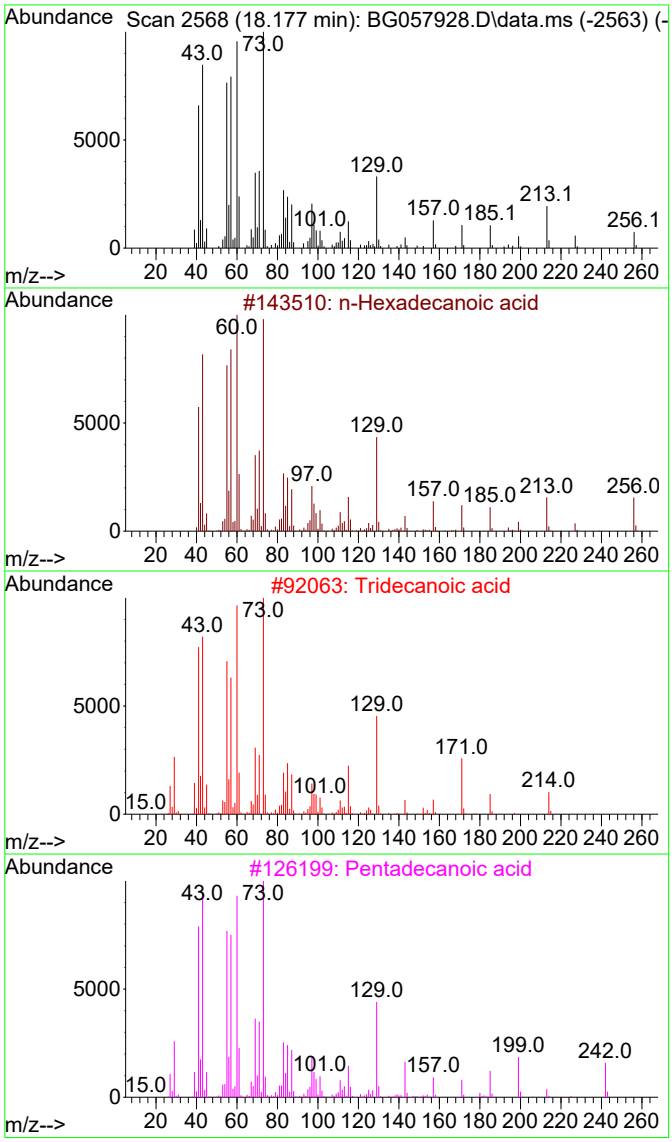
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

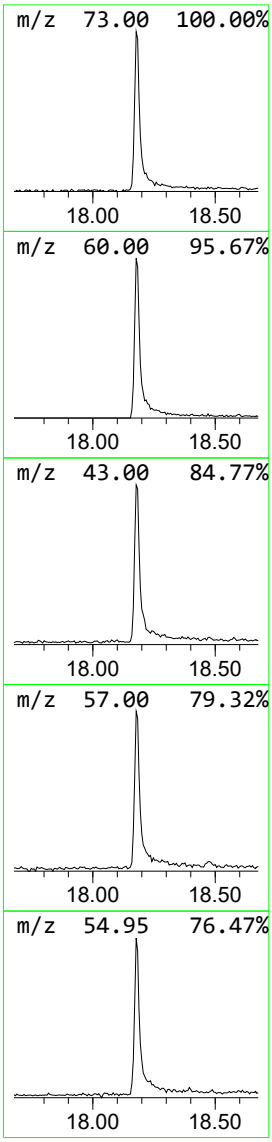
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.177	9.82 ng	355514	Phenanthrene-d10	17.290

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Octanoic acid	144	C8H16O2	000124-07-2	49





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Instrument :
BNA_G
ClientSampleId :
SB-1-(8-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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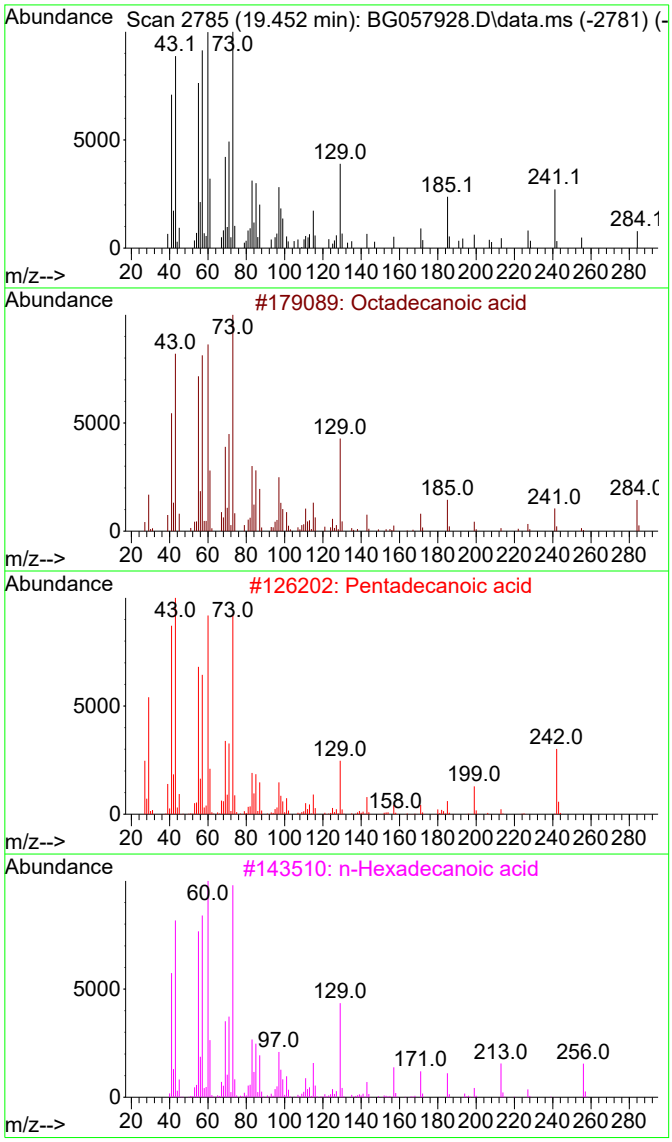
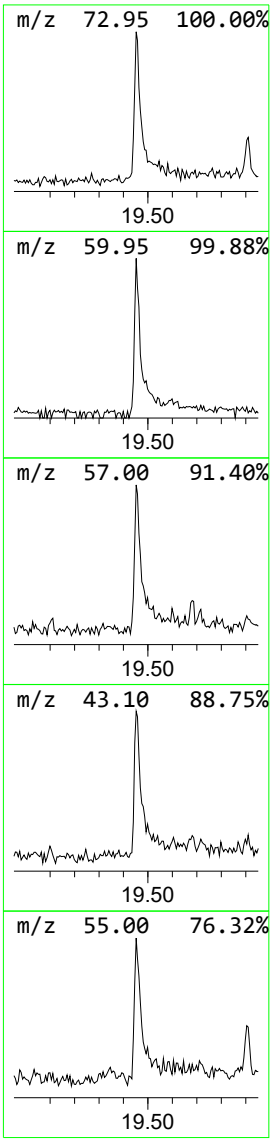
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.452	3.28 ng	118145	Chrysene-d12	21.543

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1-(8-10)

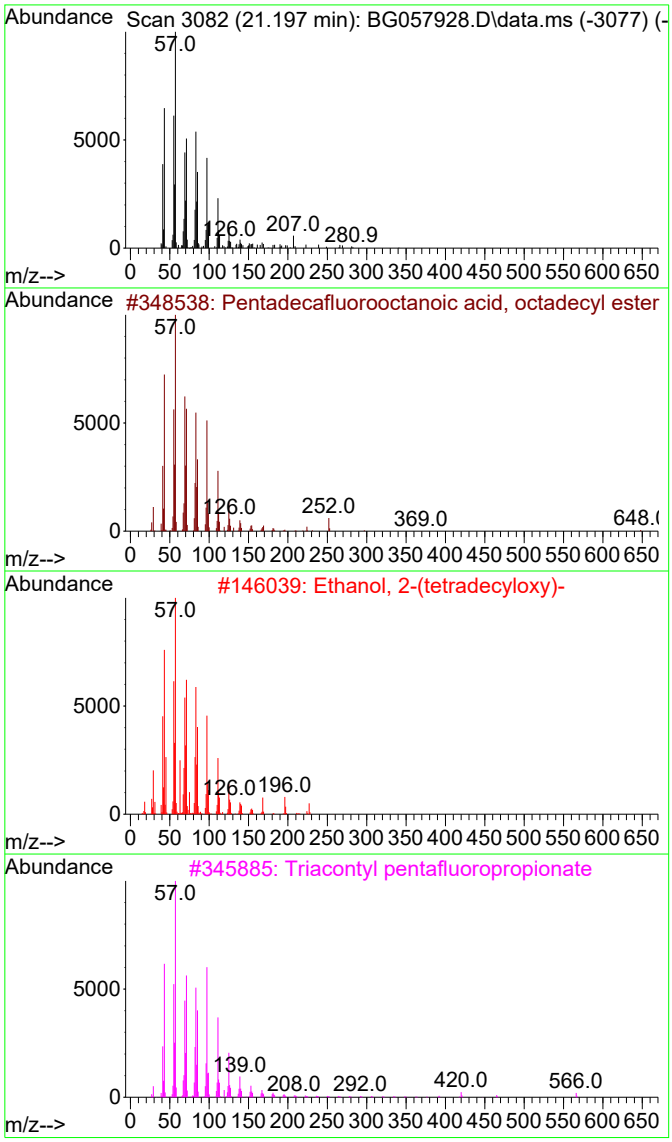
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

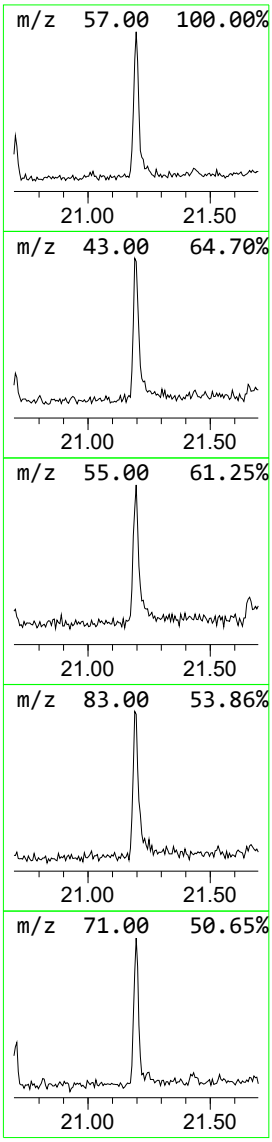
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.197	4.30 ng	154714	Chrysene-d12	21.543

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91
4	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91
5	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91





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ClientSampleId :
SB-1-(8-10)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

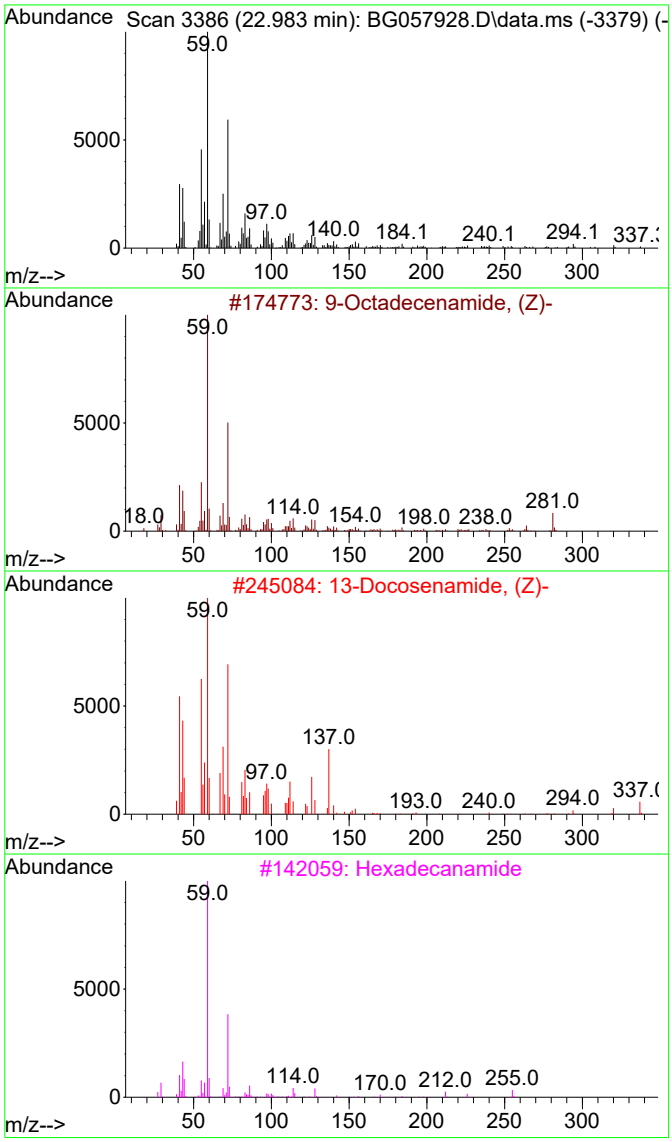
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

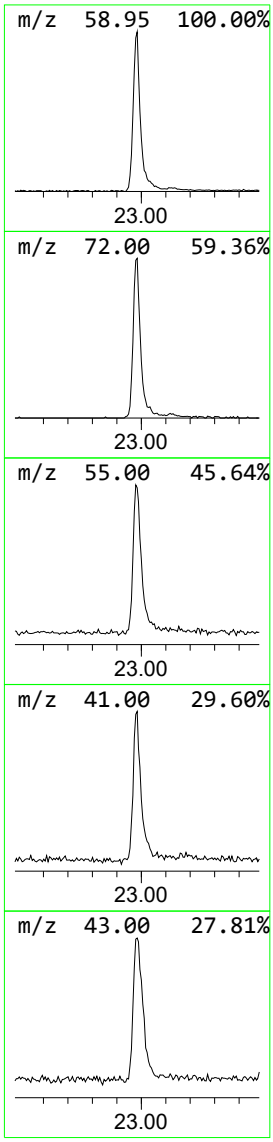
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.983	15.81 ng	569217	Chrysene-d12	21.543

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
3	Hexadecanamide	255	C16H33NO	000629-54-9	78
4	Tetradecanamide	227	C14H29NO	000638-58-4	78
5	Palmitoleamide	253	C16H31NO	106010-22-4	64





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.016	5.8	ng	61227	1	7.912	211957	20.0
Benzophenone	15.903	16.6	ng	444732	3	14.546	534684	20.0
Methanone, (1-h...	16.467	2.5	ng	91307	4	17.290	723757	20.0
n-Hexadecanoic ...	18.177	9.8	ng	355514	4	17.290	723757	20.0
Octadecanoic acid	19.452	3.3	ng	118145	5	21.543	719876	20.0
Pentadecafluoro...	21.197	4.3	ng	154714	5	21.543	719876	20.0
9-Octadecenamid...	22.983	15.8	ng	569217	5	21.543	719876	20.0