LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057825.D
Acq On : 23 Jun 2023 2:32
Operator : CG/JU
Sample : 03320-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-12

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: BG057825.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.427	223	228	236	rVB	17861	25911	1.18%	0.207%
2	5.027	324	330	340	rVB	451930	667180	30.42%	5.337%
3	5.491	402	409	421	rBV	582056	908681	41.43%	7.269%
4	6.108	508	514	520	rBV	17650	27177	1.24%	0.217%
5	7.083	672	680	693	rBV	635932	1080287	49.26%	8.641%
6	7.923	816	823	830	rBV	155076	259383	11.83%	2.075%
7	9.081	1011	1020	1033	rBV	384280	665973	30.36%	5.327%
8	10.726	1292	1300	1307	rVB	223115	397051	18.10%	3.176%
9	13.176	1710	1717	1725	rBV	980484	1533910	69.94%	12.270%
10	14.557	1945	1952	1960	rBV	352377	555698	25.34%	4.445%
11	15.908	2176	2182	2193	rVB	217475	295214	13.46%	2.361%
12	16.037	2198	2204	2212	rBV	714700	1105906	50.42%	8.846%
13	16.472	2272	2278	2286	rVB	43116	59902	2.73%	0.479%
14	17.295	2412	2418	2425	rVB	447575	676999	30.87%	5.415%
15	18.188	2564	2570	2580	rBV2	105712	169385	7.72%	1.355%
16	19.463	2783	2787	2793	rBV4	30726	44172	2.01%	0.353%
17	19.915	2858	2864	2871	rBV	1706294	2193236	100.00%	17.544%
18	20.714	2997	3000	3005	rVB2	26207	32917	1.50%	0.263%
19	21.208	3079	3084	3092	rVB3	114551	191046	8.71%	1.528%
20	21.284	3093	3097	3102	rVB	53785	70167	3.20%	0.561%
21	21.549	3136	3142	3149	rBV	438113	692603	31.58%	5.540%
22	21.748	3173	3176	3181	rVB3	30575	38405	1.75%	0.307%
23	24.698	3670	3678	3694	rVB	279540	809996	36.93%	6.479%

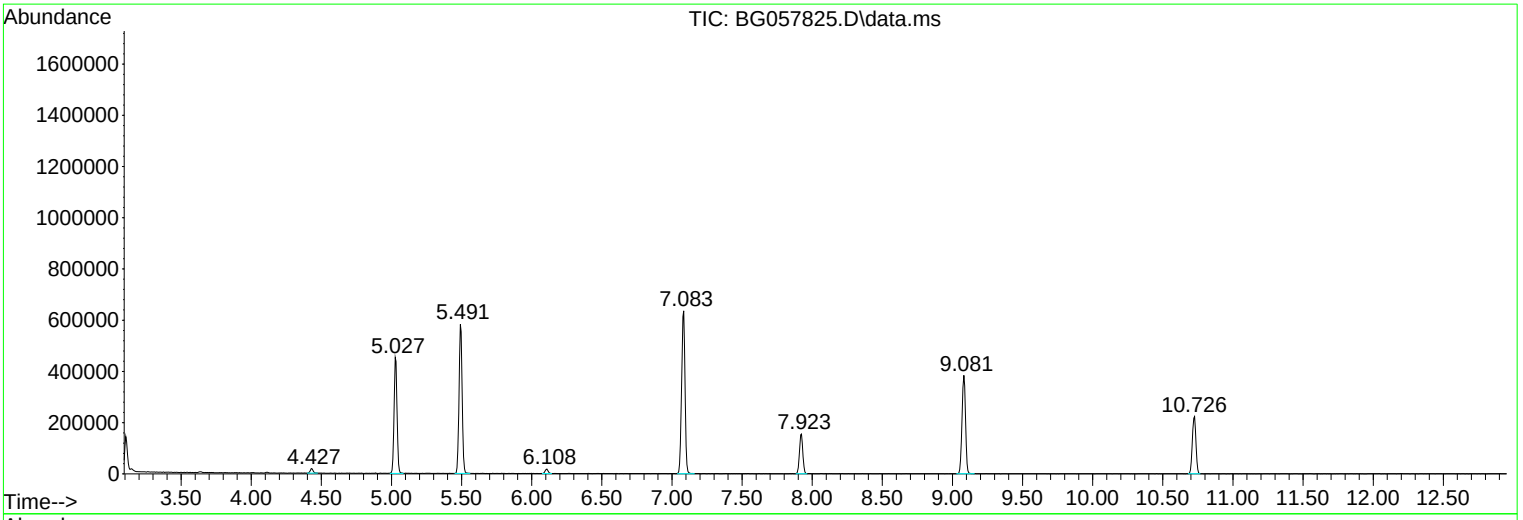
Sum of corrected areas: 12501199

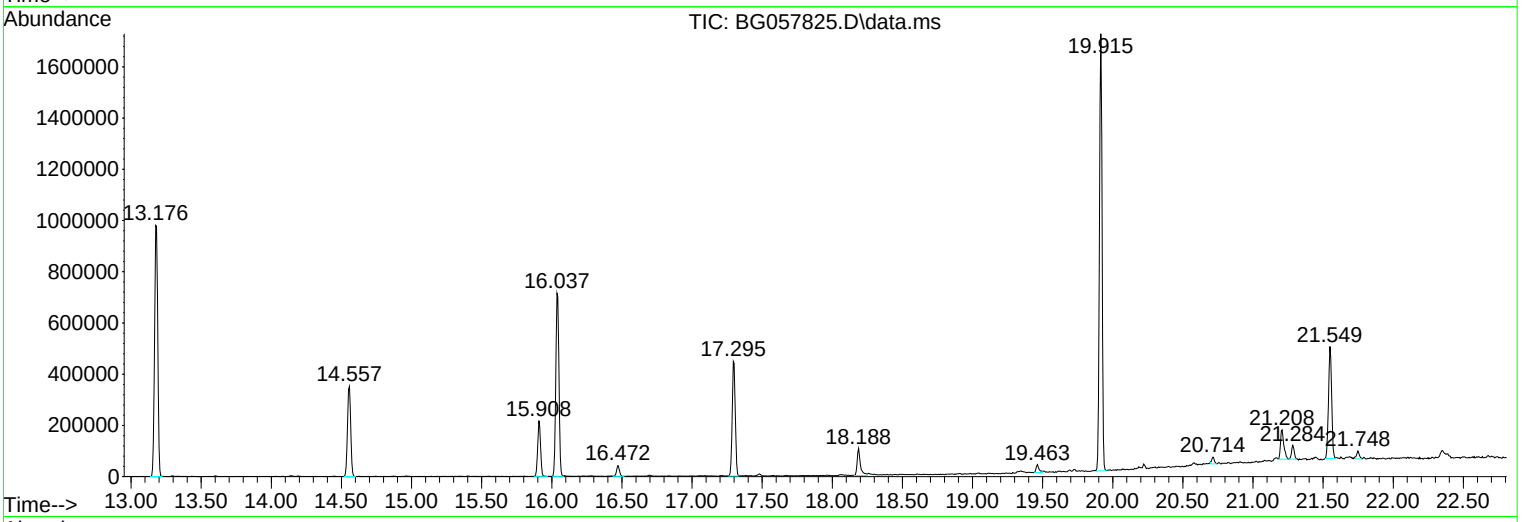
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057825.D
Acq On : 23 Jun 2023 2:32
Operator : CG/JU
Sample : 03320-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

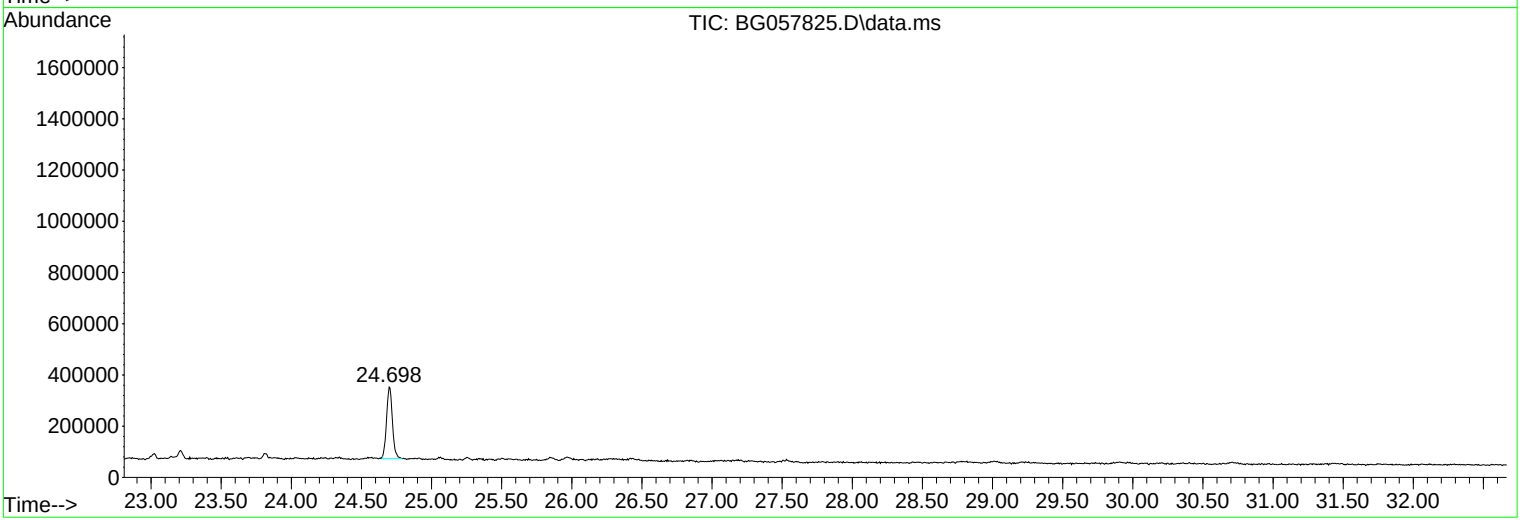
Instrument :
BNA_G
ClientSampleId :
WC-12

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057825.D
Acq On : 23 Jun 2023 2:32
Operator : CG/JU
Sample : 03320-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-12

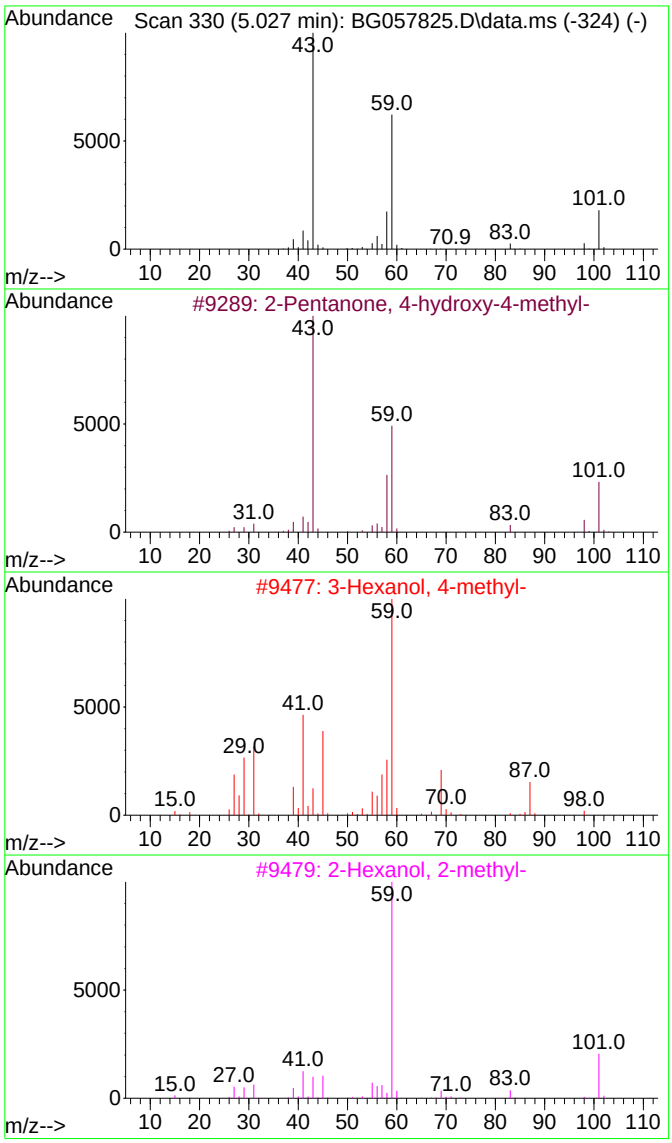
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

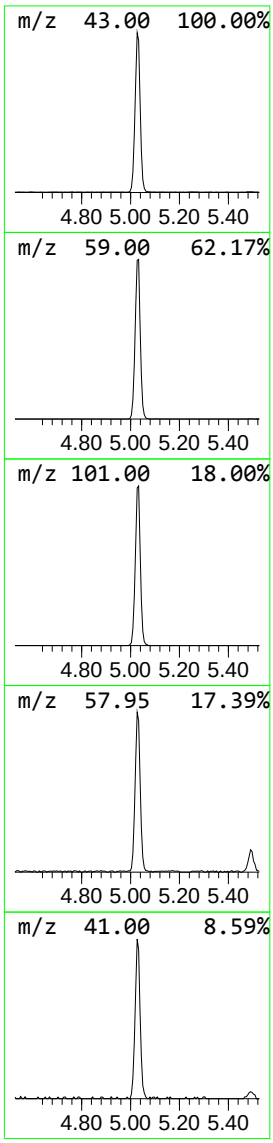
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.027	51.44 ng	667180	1,4-Dichlorobenzene-d4	7.923

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057825.D
Acq On : 23 Jun 2023 2:32
Operator : CG/JU
Sample : 03320-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-12

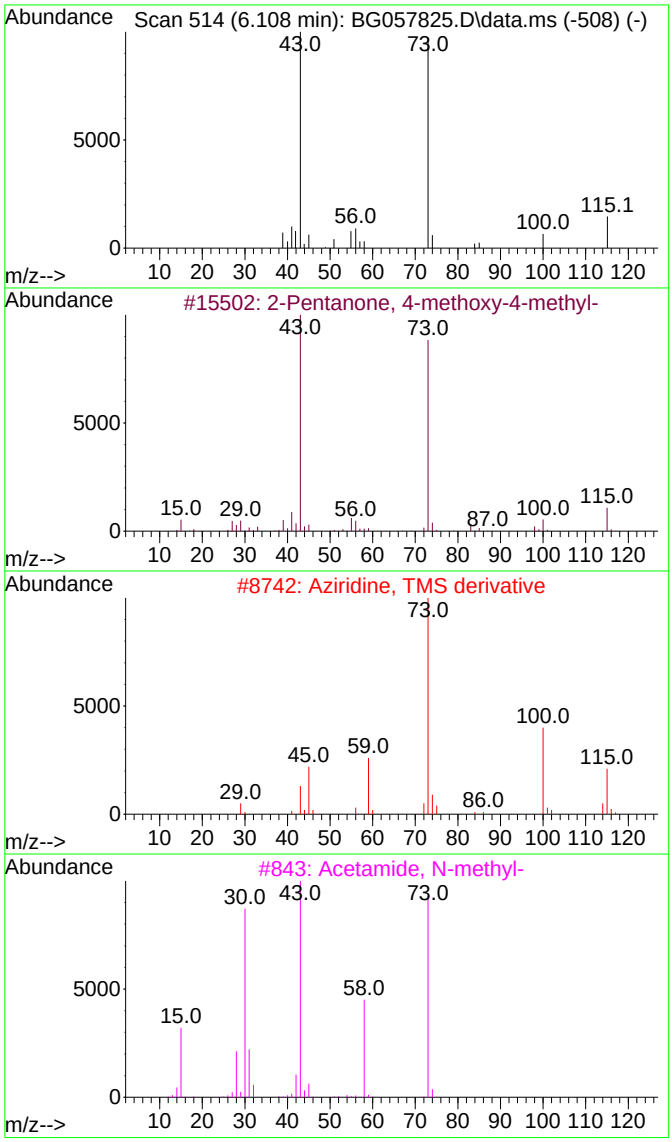
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

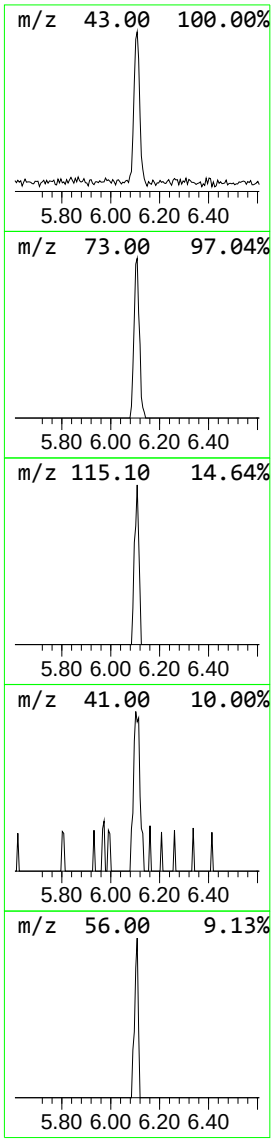
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.108	2.10 ng	27177	1,4-Dichlorobenzene-d4	7.923

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	Aziridine, TMS derivative	115	C5H13NSi	002116-90-7	9
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Propanone, oxime	73	C3H7NO	000127-06-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057825.D
Acq On : 23 Jun 2023 2:32
Operator : CG/JU
Sample : 03320-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-12

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

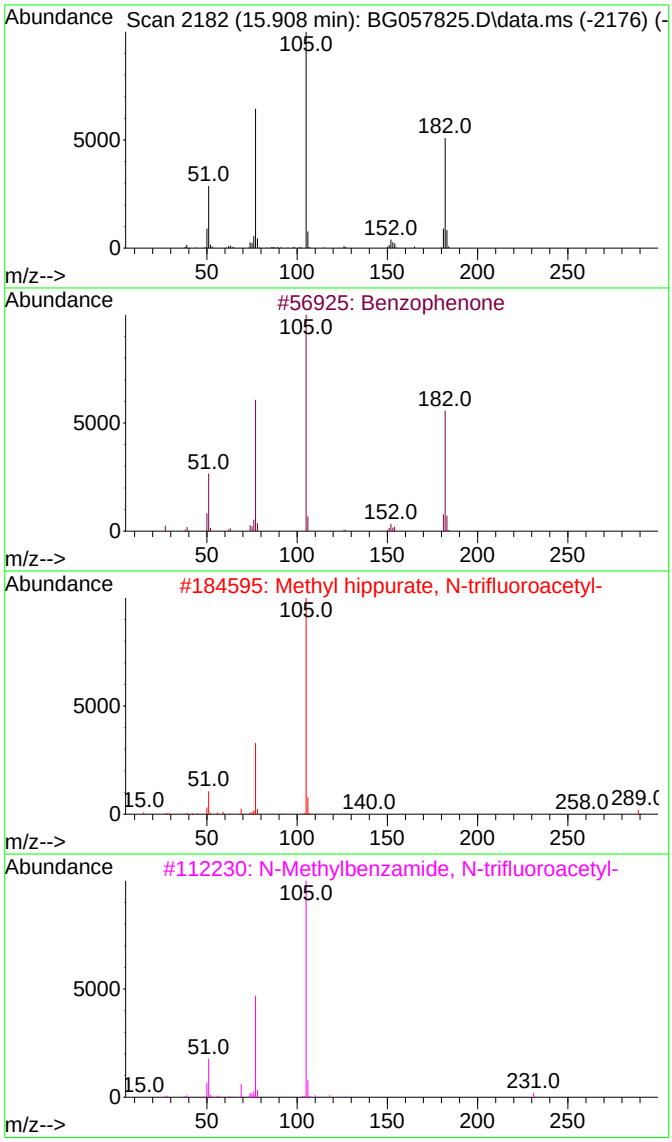
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

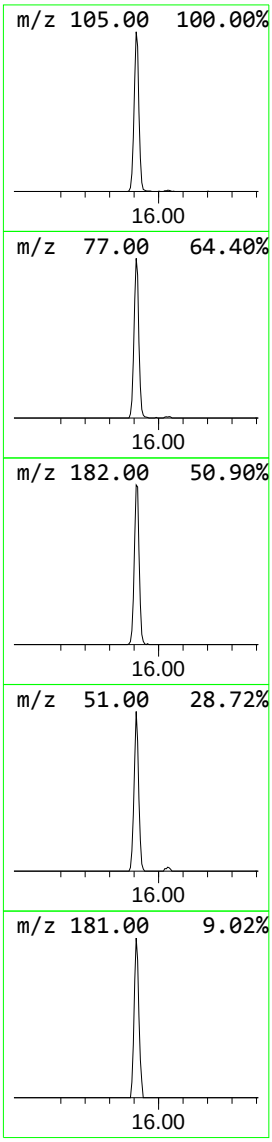
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.908	10.63 ng	295214	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Methyl hippurate, N-trifluoroace...	289	C12H10F3NO4	073749-76-5	47
3	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057825.D
Acq On : 23 Jun 2023 2:32
Operator : CG/JU
Sample : 03320-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-12

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

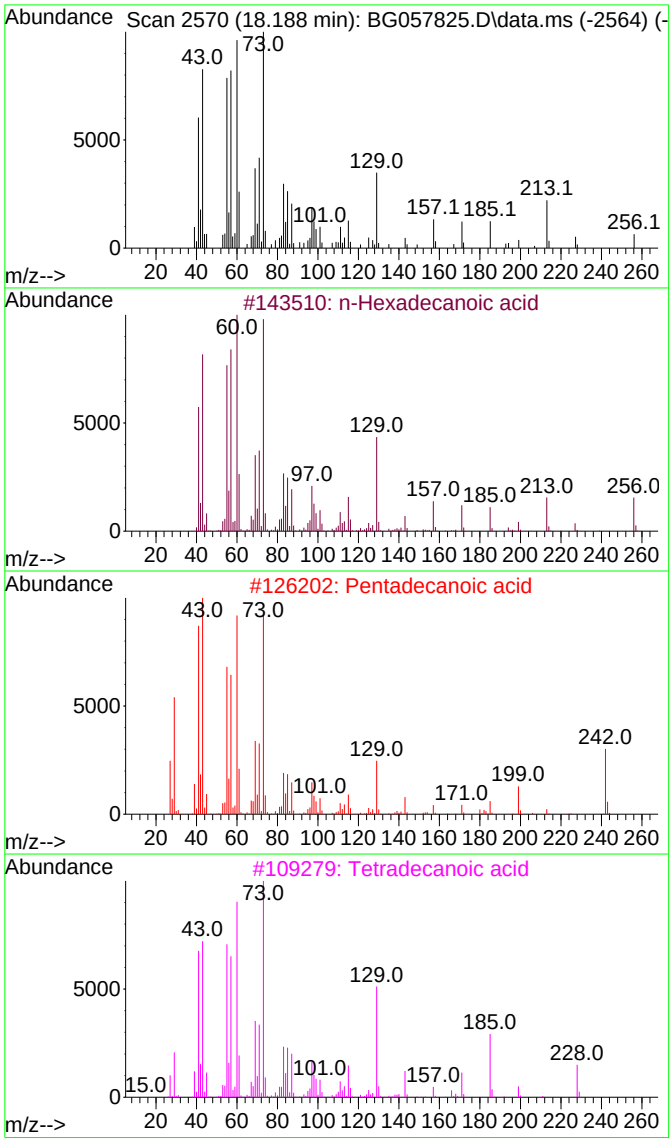
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

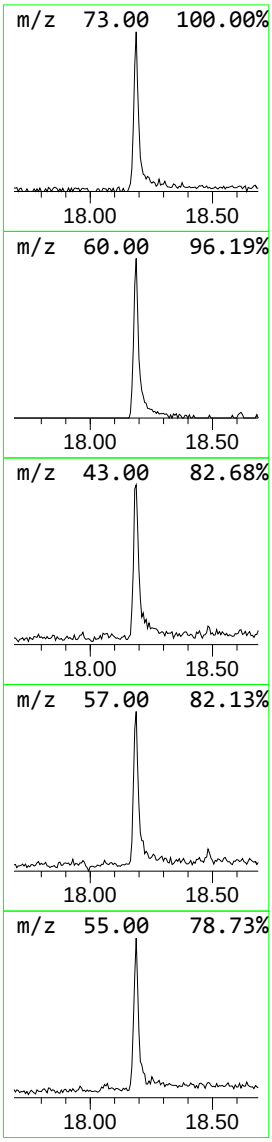
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.188	5.00 ng	169385	Phenanthrene-d10	17.295

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	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Nonanoic acid	158	C9H18O2	000112-05-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057825.D
Acq On : 23 Jun 2023 2:32
Operator : CG/JU
Sample : 03320-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-12

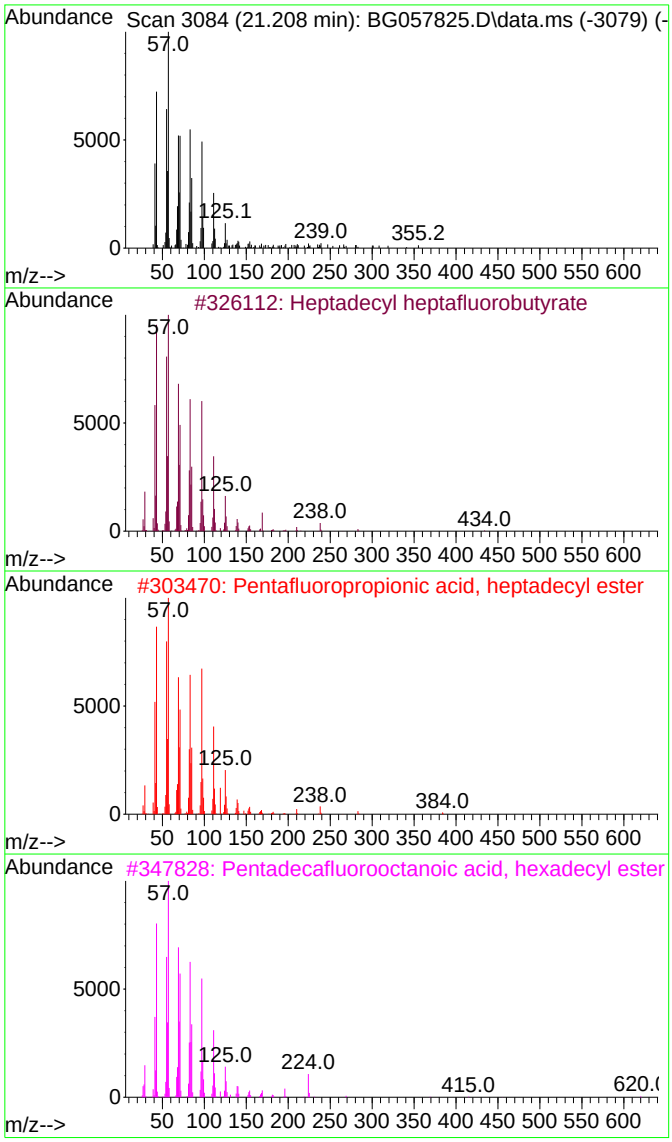
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

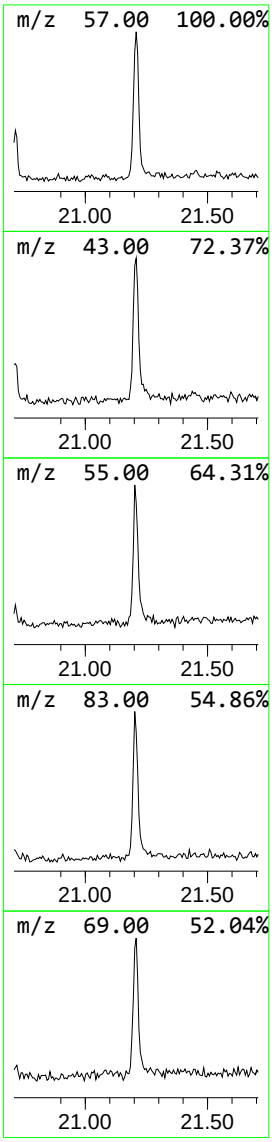
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.208	5.52 ng	191046	Chrysene-d12	21.549

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	91
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057825.D
Acq On : 23 Jun 2023 2:32
Operator : CG/JU
Sample : 03320-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-12

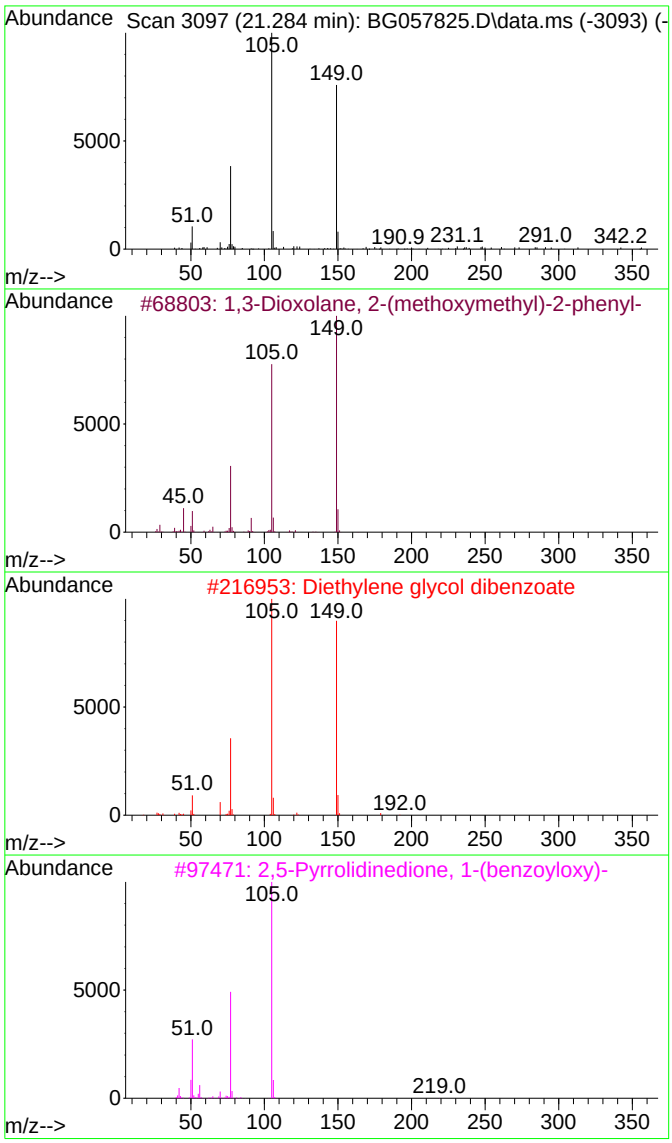
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

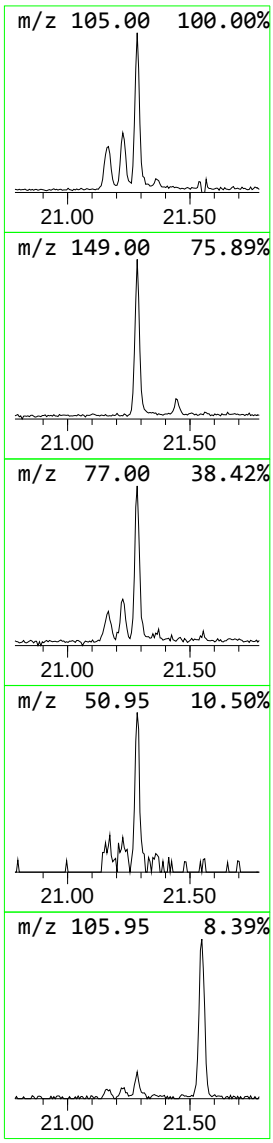
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.284	2.03 ng	70167	Chrysene-d12	21.549

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
3	2,5-Pyrrolidinedione, 1-(benzoyl...	219	C11H9NO4	023405-15-4	35
4	3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	35
5	N-(2,4-Dihydroxy-6-methyl-5-pyri...	245	C12H11N3O3	1000472-87-2	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057825.D
Acq On : 23 Jun 2023 2:32
Operator : CG/JU
Sample : 03320-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-12

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.027	51.4	ng	667180	1	7.923	259383	20.0
2-Pentanone, 4-...	6.108	2.1	ng	27177	1	7.923	259383	20.0
Benzophenone	15.908	10.6	ng	295214	3	14.557	555698	20.0
n-Hexadecanoic ...	18.188	5.0	ng	169385	4	17.295	676999	20.0
Heptadecyl hept...	21.208	5.5	ng	191046	5	21.549	692603	20.0
1,3-Dioxolane, ...	21.284	2.0	ng	70167	5	21.549	692603	20.0