LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022223\
Data File : BG056697.D
Acq On : 22 Feb 2023 14:32
Operator : CG/JU
Sample : 01640-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

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-BG021523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056697.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.454	320	326	332	rBV	90115	140064	11.82%	2.568%
2	5.936	401	408	416	rVB	221217	350472	29.59%	6.426%
3	7.552	675	683	690	rBV	239123	407149	34.37%	7.465%
4	8.427	823	832	840	rBV2	50527	85359	7.21%	1.565%
5	9.602	1022	1032	1041	rBV	137598	243120	20.52%	4.458%
6	11.265	1308	1315	1322	rVB	67677	121598	10.27%	2.230%
7	13.662	1715	1723	1729	rVB	426569	632580	53.40%	11.599%
8	15.031	1950	1956	1963	rVB	138582	210465	17.77%	3.859%
9	16.365	2177	2183	2189	rBV	41421	59989	5.06%	1.100%
10	16.506	2200	2207	2217	rVB	437081	666175	56.24%	12.215%
11	17.769	2415	2422	2429	rBV	209148	321372	27.13%	5.892%
12	18.603	2559	2564	2573	rBV	80537	118245	9.98%	2.168%
13	19.021	2632	2635	2642	rVB4	9552	12605	1.06%	0.231%
14	19.855	2774	2777	2780	rBV3	24410	31764	2.68%	0.582%
15	20.331	2852	2858	2864	rBV	900391	1184508	100.00%	21.718%
16	21.653	3078	3083	3089	rBV2	65550	98701	8.33%	1.810%
17	22.076	3149	3155	3162	rBV	171192	307056	25.92%	5.630%
18	22.246	3181	3184	3191	rVB2	23557	38392	3.24%	0.704%
19	22.916	3292	3298	3302	rBV3	27105	48636	4.11%	0.892%
20	23.674	3423	3427	3433	rVB5	21095	38568	3.26%	0.707%
21	25.619	3747	3758	3770	rVB2	107814	337108	28.46%	6.181%

Sum of corrected areas: 5453926

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022223\
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Acq On : 22 Feb 2023 14:32
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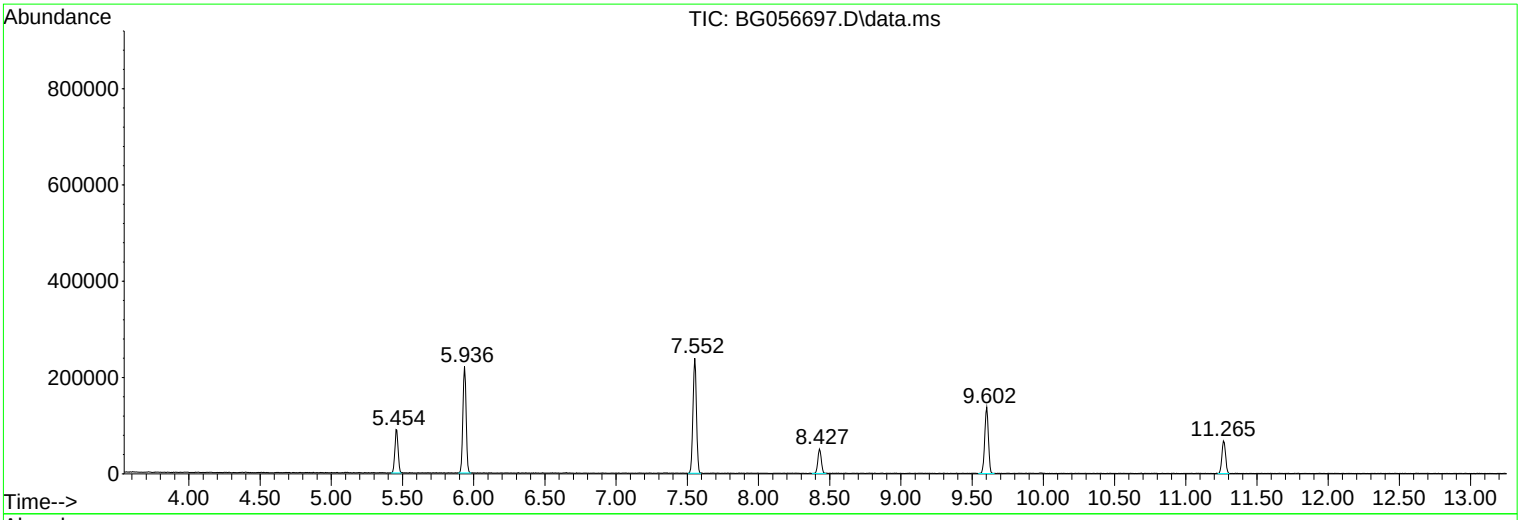
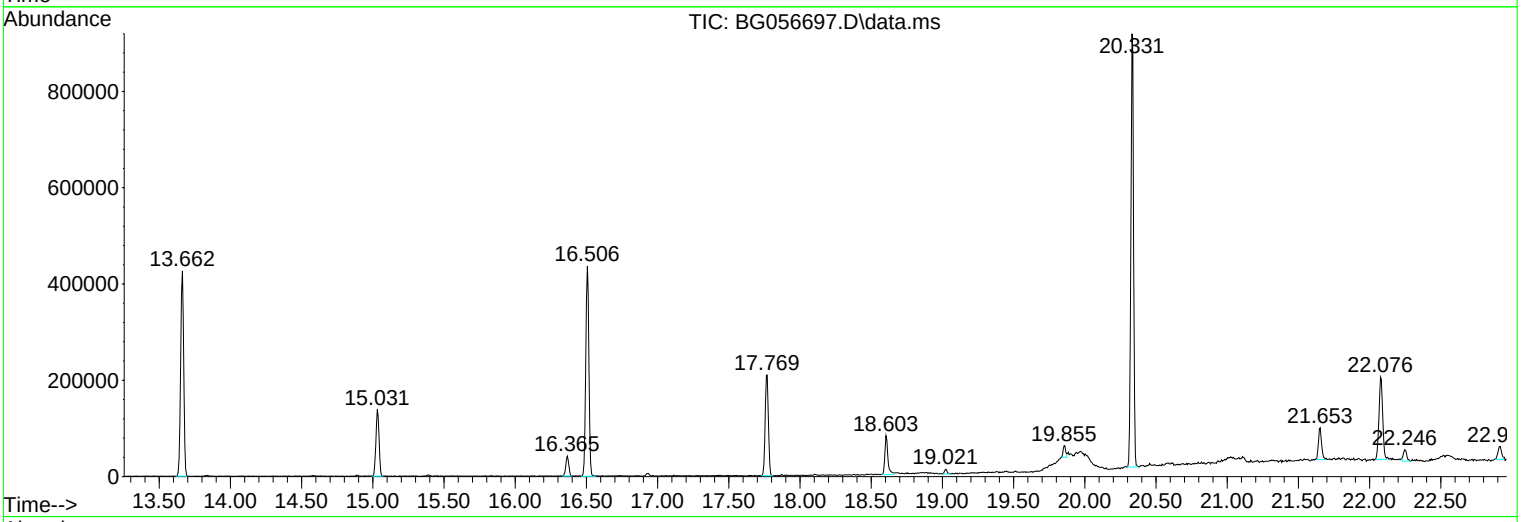
Misc :
ALS Vial : 6 Sample Multiplier: 1

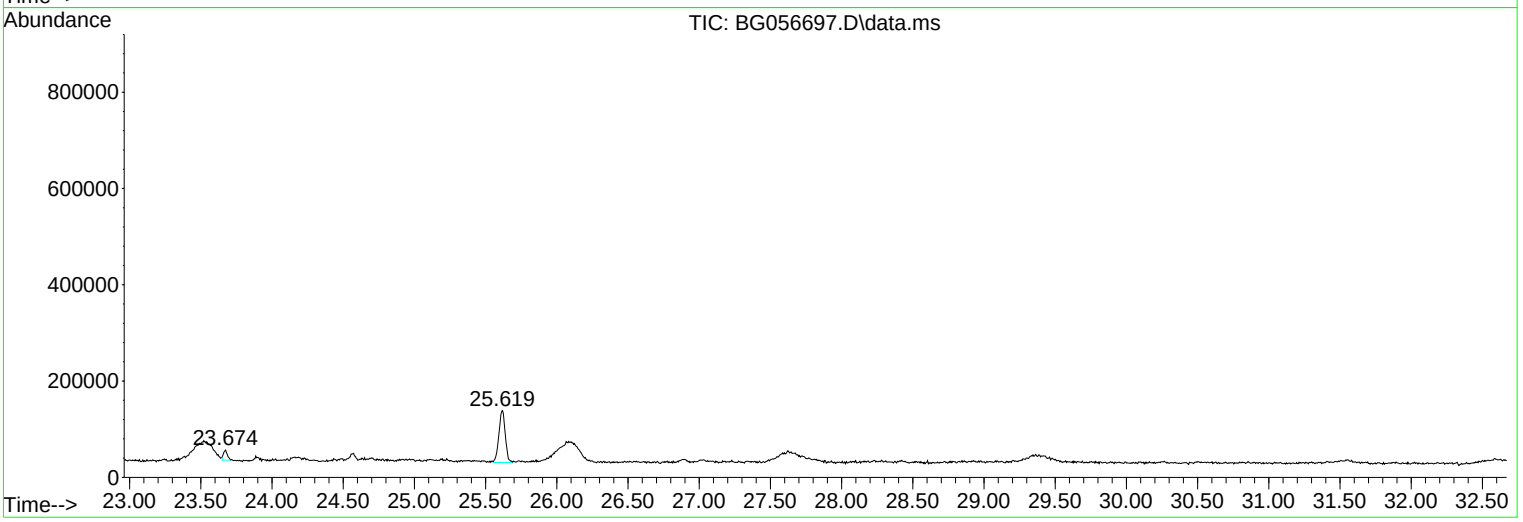
Instrument :
BNA_G
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.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 : BG056697.D
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Instrument :
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ClientSampleId :
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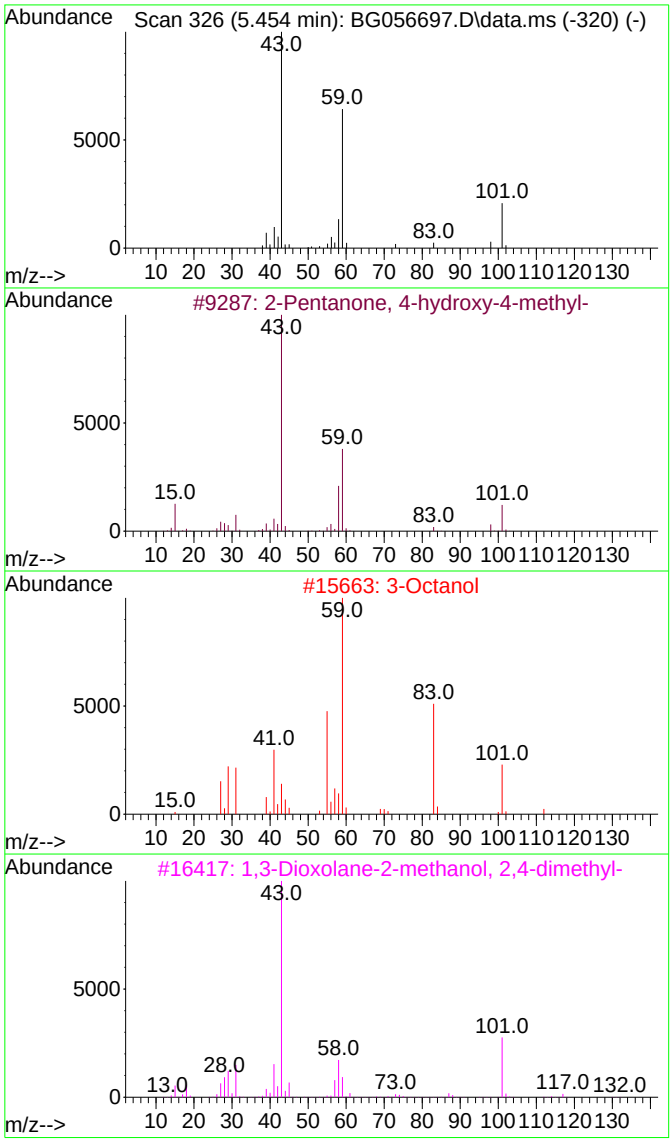
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

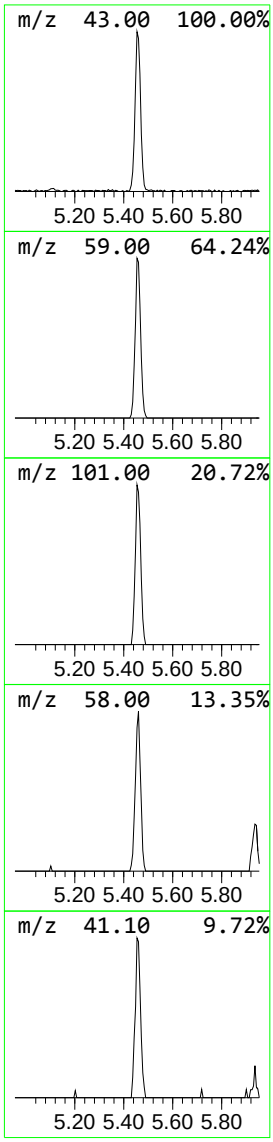
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.454	32.82 ng	140064	1,4-Dichlorobenzene-d4	8.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Octanol	130	C8H18O	000589-98-0	45
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17





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Sample : 01640-04
Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.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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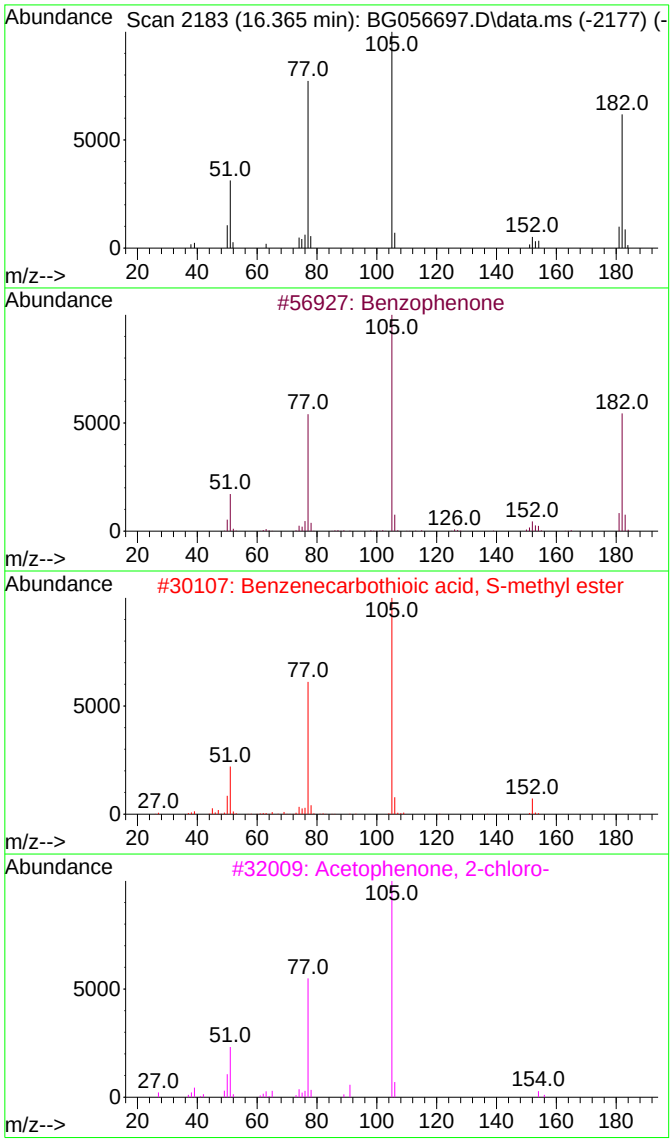
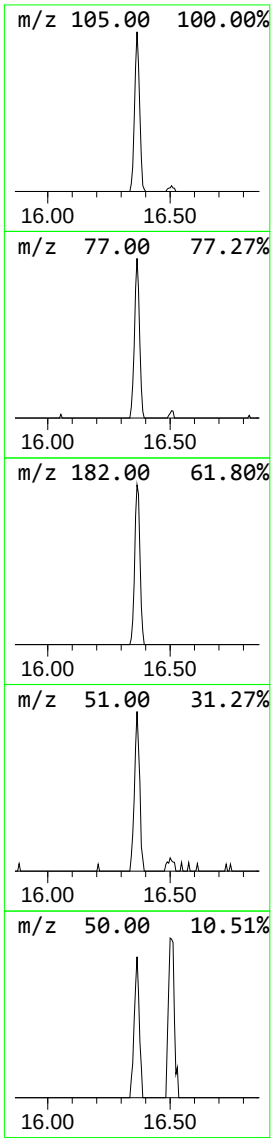
Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.365	5.70 ng	59989	Acenaphthene-d10	15.031

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	62
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
4	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	50
5	2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022223\
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Acq On : 22 Feb 2023 14:32
Operator : CG/JU
Sample : 01640-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.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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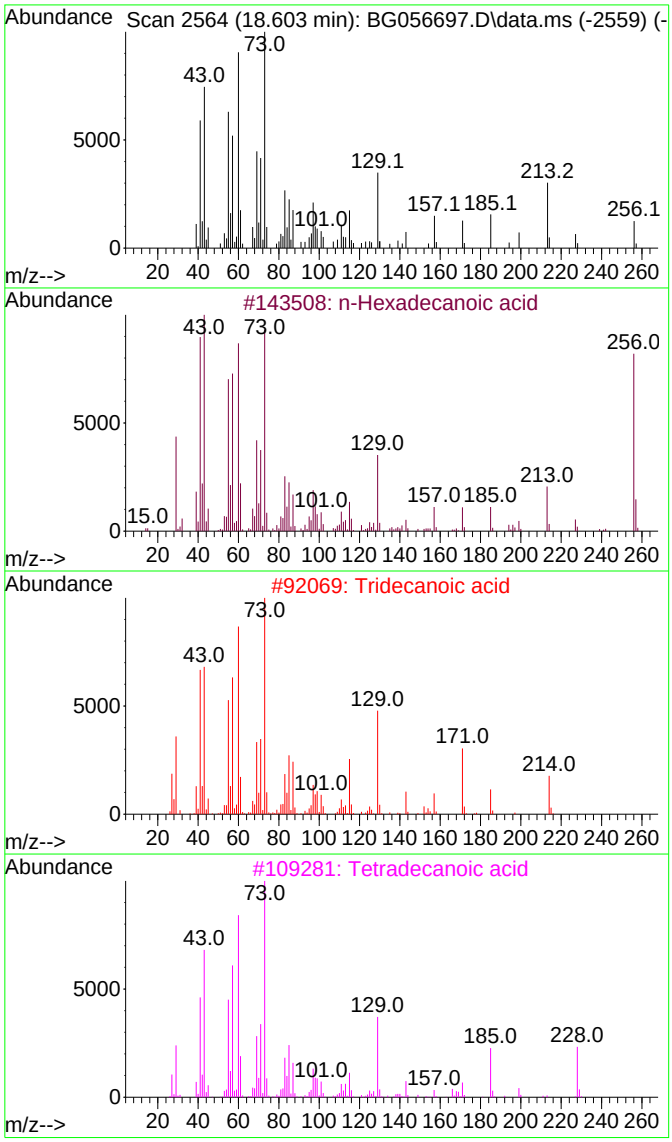
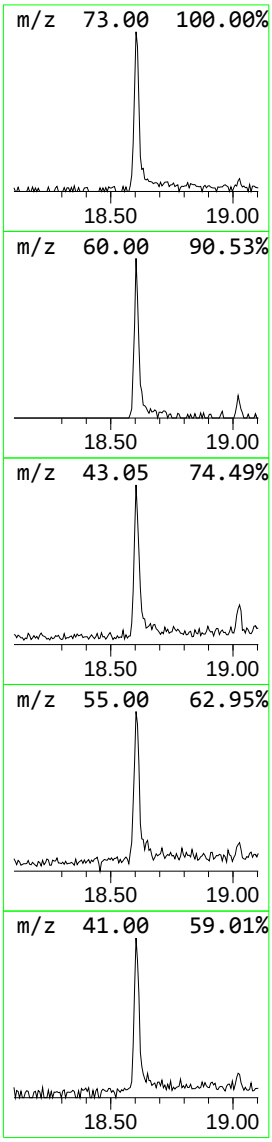
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.604	7.36 ng	118245	Phenanthrene-d10	17.763

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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022223\
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Operator : CG/JU
Sample : 01640-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.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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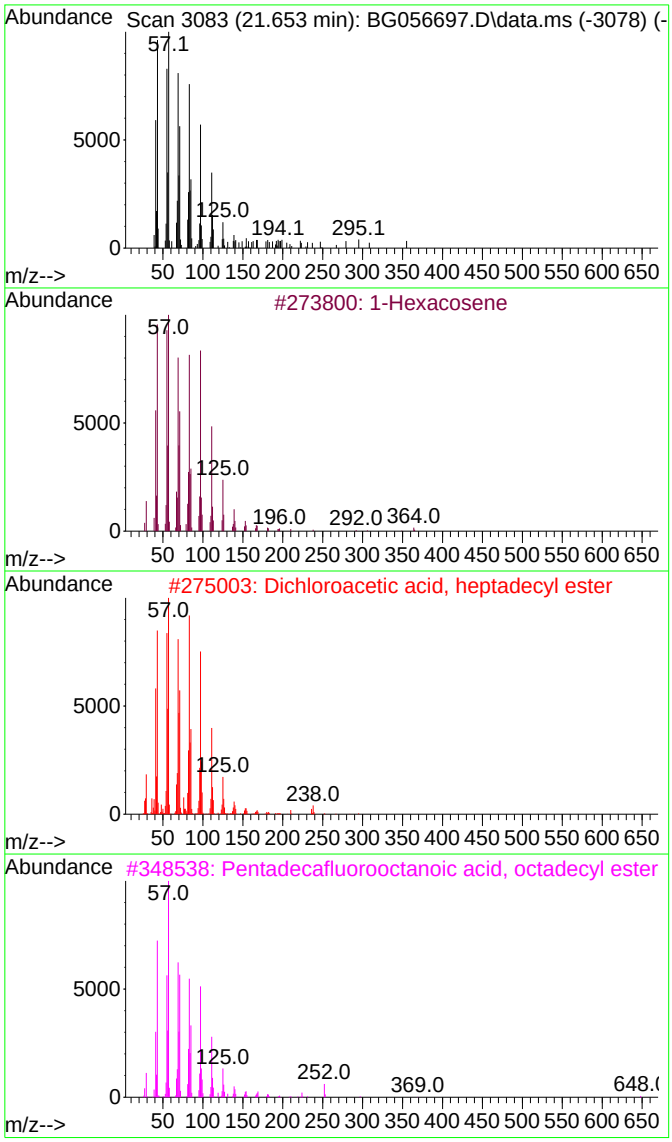
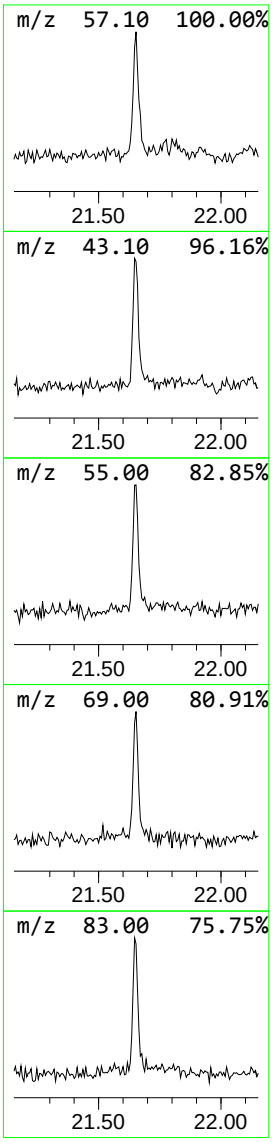
Peak Number 4 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.653	6.43 ng	98701	Chrysene-d12	22.076

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	91
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	62





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Operator : CG/JU
Sample : 01640-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.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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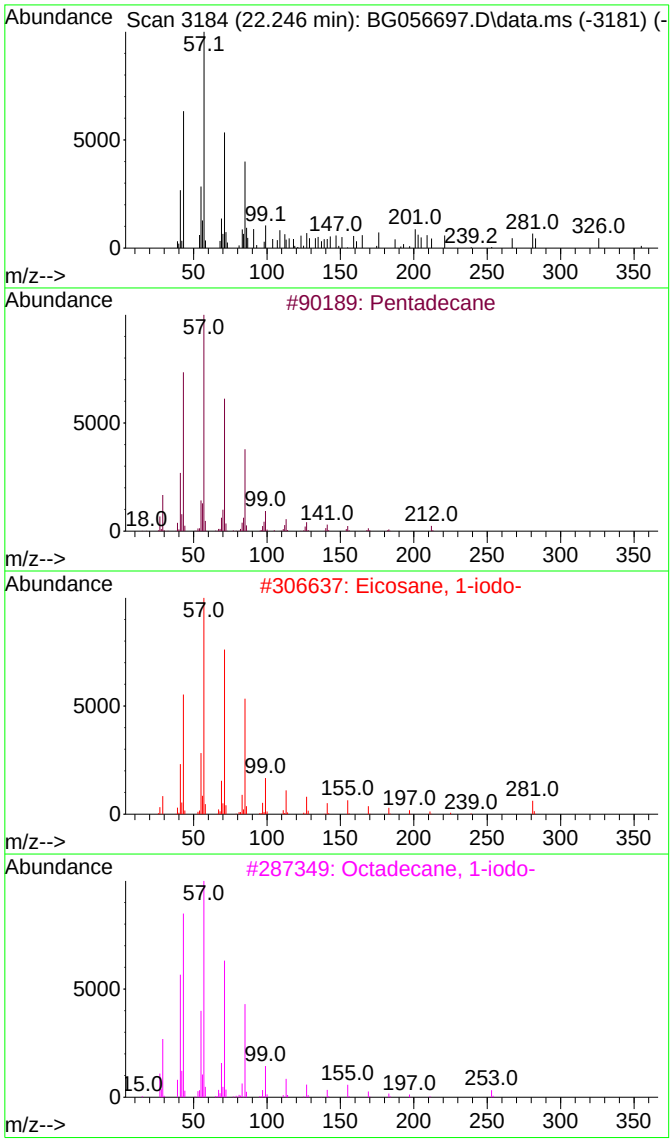
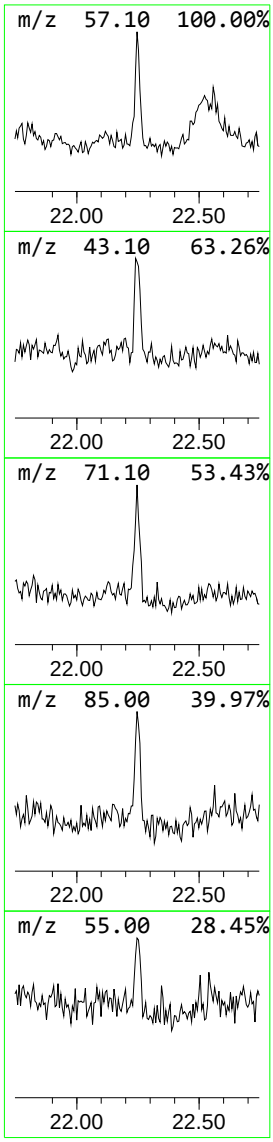
Peak Number 5 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.246	2.50 ng	38392	Chrysene-d12	22.076

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	72
2	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	64
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	64
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	59
5	Heneicosane	296	C21H44	000629-94-7	59





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Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.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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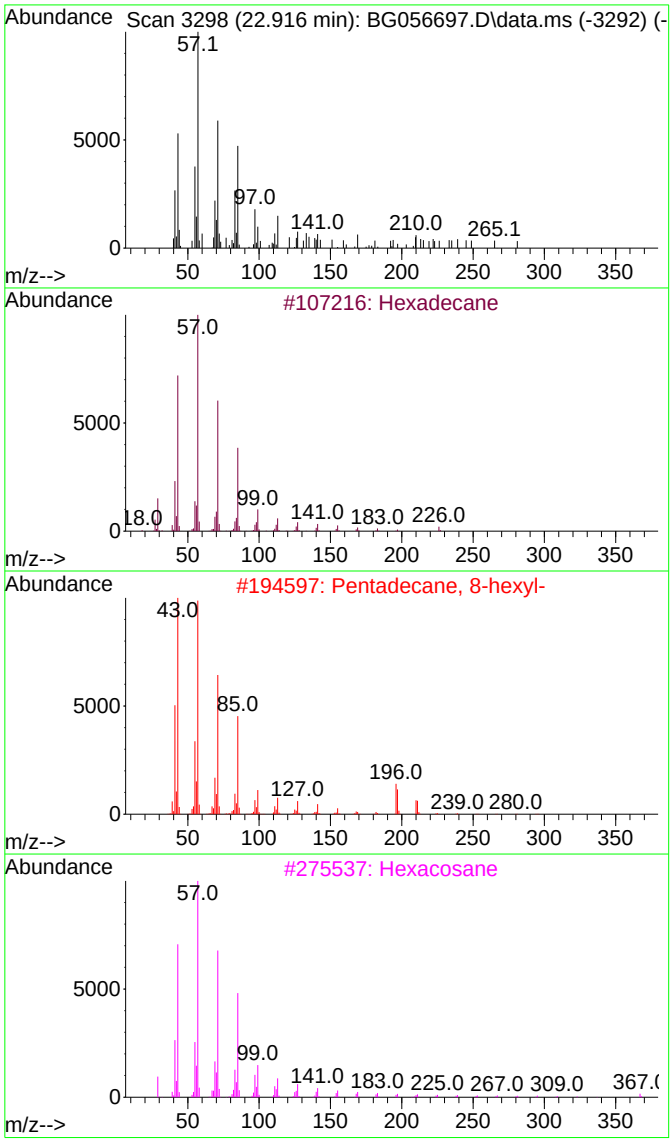
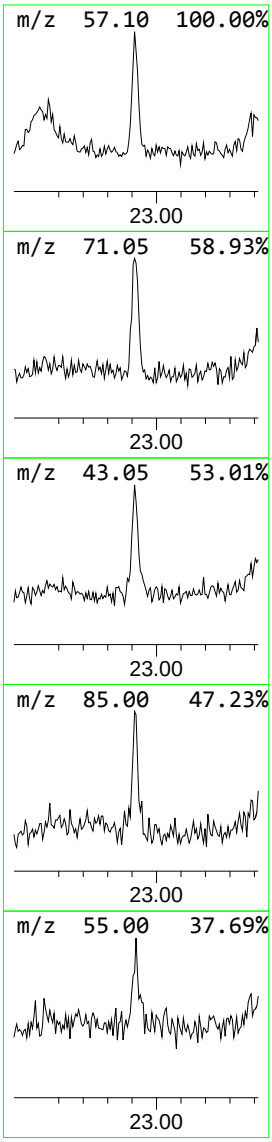
Peak Number 6 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.916	3.17 ng	48636	Chrysene-d12	22.076

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	58
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	53
3	Hexacosane	366	C26H54	000630-01-3	52
4	Tritetracontane	605	C43H88	007098-21-7	52
5	Hentriacontane	437	C31H64	000630-04-6	52





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Operator : CG/JU
Sample : 01640-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.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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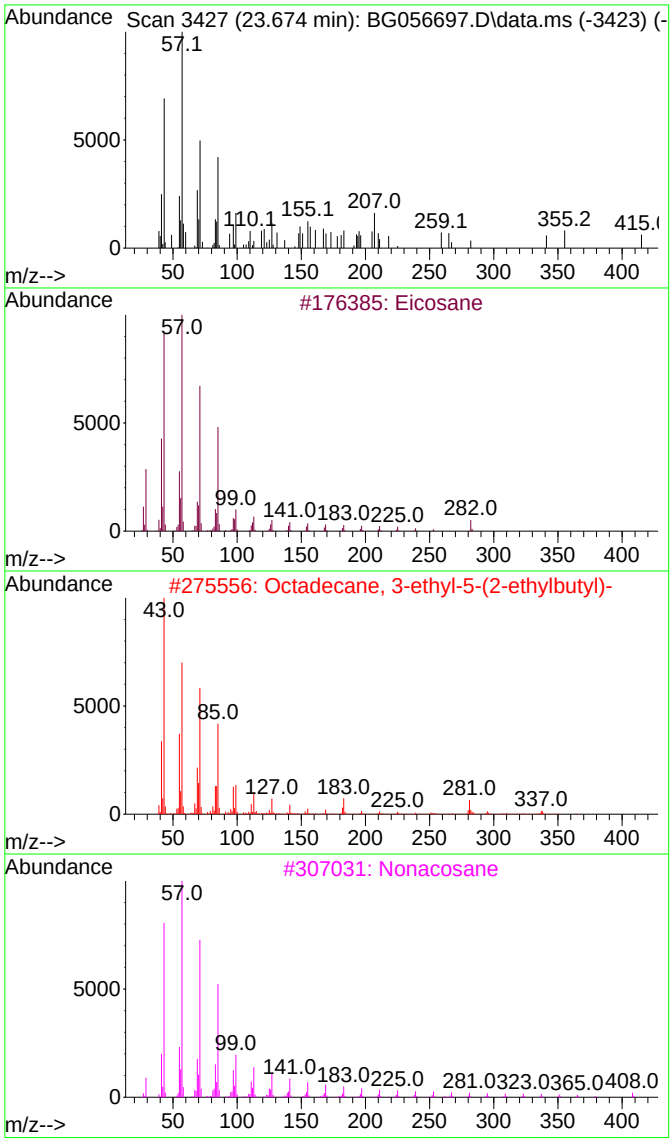
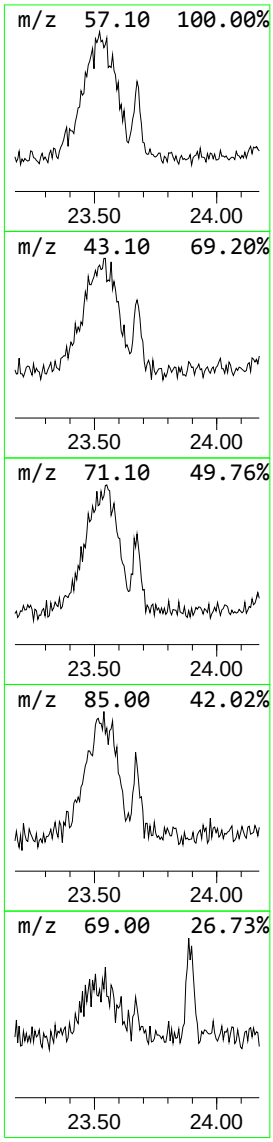
Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.674	2.51 ng	38568	Chrysene-d12	22.076

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	58
2	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	52
3	Nonacosane	408	C29H60	000630-03-5	50
4	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	47
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022223\
Data File : BG056697.D
Acq On : 22 Feb 2023 14:32
Operator : CG/JU
Sample : 01640-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.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-...	5.454	32.8	ng	140064	1	8.427	85359	20.0
Benzophenone	16.365	5.7	ng	59989	3	15.031	210465	20.0
n-Hexadecanoic ...	18.604	7.4	ng	118245	4	17.763	321372	20.0
1-Hexacosene	21.653	6.4	ng	98701	5	22.076	307056	20.0
Pentadecane	22.246	2.5	ng	38392	5	22.076	307056	20.0
Hexadecane	22.916	3.2	ng	48636	5	22.076	307056	20.0
Eicosane	23.674	2.5	ng	38568	5	22.076	307056	20.0