LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055613.D
Acq On : 14 Nov 2022 20:48
Operator : CG/JU
Sample : N5531-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28B

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055613.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.320	3	5	23	rVB	260547	441463	13.52%	2.496%
2	5.318	339	345	355	rBV	147899	236762	7.25%	1.338%
3	5.793	418	426	437	rBV	1025738	1679253	51.44%	9.493%
4	7.403	690	700	713	rBV	1026716	1790105	54.83%	10.120%
5	8.261	839	846	854	rBV	193802	338077	10.36%	1.911%
6	9.436	1036	1046	1054	rBV	630907	1126307	34.50%	6.367%
7	10.841	1278	1285	1299	rBV	82327	150735	4.62%	0.852%
8	11.093	1320	1328	1336	rVB	276616	481580	14.75%	2.722%
9	13.514	1730	1740	1748	rBV	1605306	2527717	77.43%	14.289%
10	14.883	1966	1973	1980	rBV	428774	672227	20.59%	3.800%
11	16.369	2218	2226	2237	rBV	1368077	2178103	66.72%	12.313%
12	17.627	2433	2440	2448	rBV	544762	804267	24.64%	4.547%
13	18.267	2545	2549	2554	rBV2	26533	33281	1.02%	0.188%
14	18.485	2581	2586	2595	rBV2	124777	202311	6.20%	1.144%
15	19.742	2797	2800	2806	rBV	65131	105872	3.24%	0.598%
16	20.218	2875	2881	2886	rBV	2353179	3264678	100.00%	18.455%
17	21.534	3101	3105	3117	rVB	60564	117215	3.59%	0.663%
18	21.928	3166	3172	3183	rVB	483340	820693	25.14%	4.639%
19	25.359	3748	3756	3769	rVB	232503	718964	22.02%	4.064%

Sum of corrected areas: 17689610

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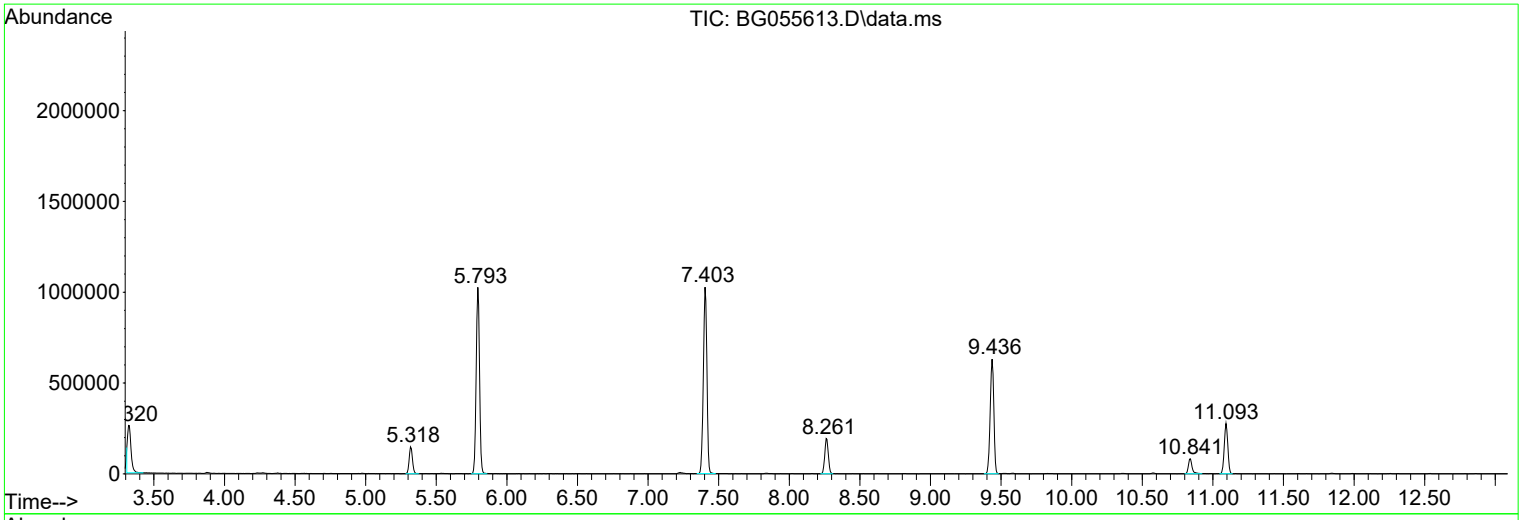
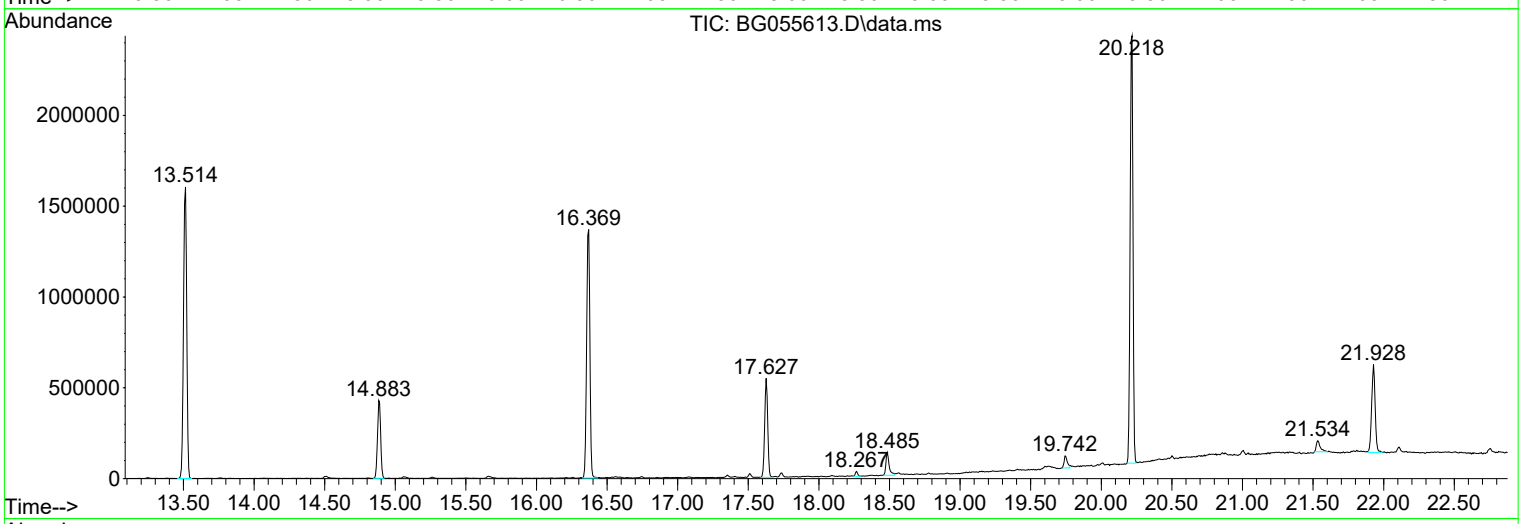
Misc :
ALS Vial : 13 Sample Multiplier: 1

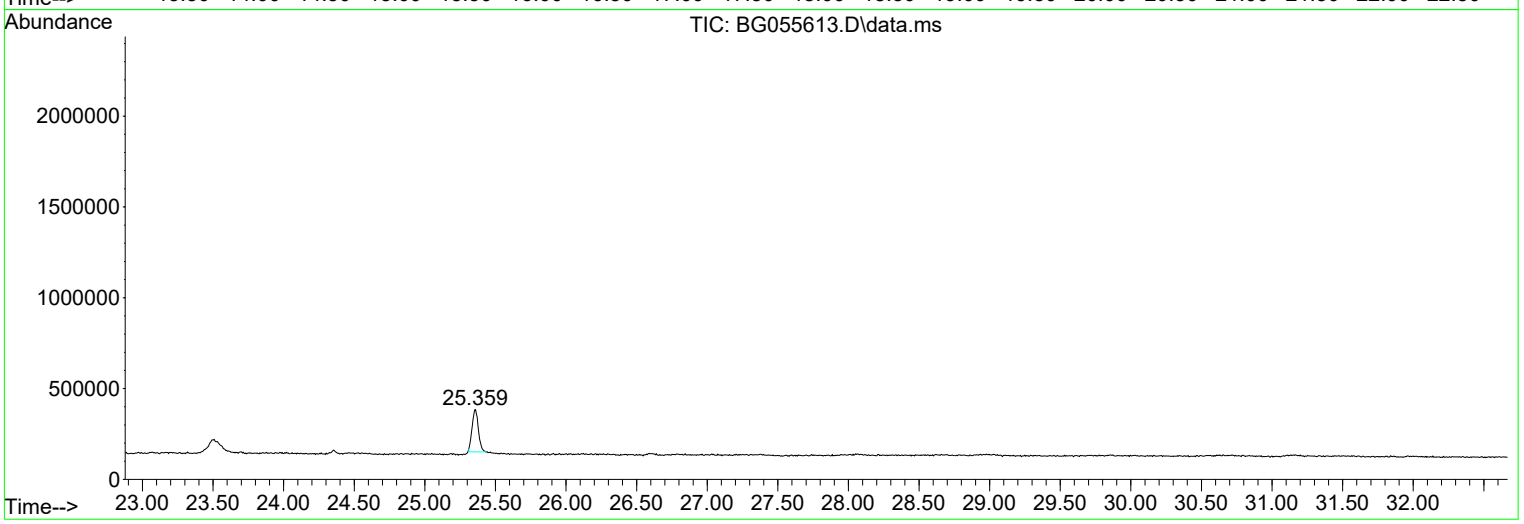
Instrument :
BNA_G
ClientSampleId :
SB-28B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

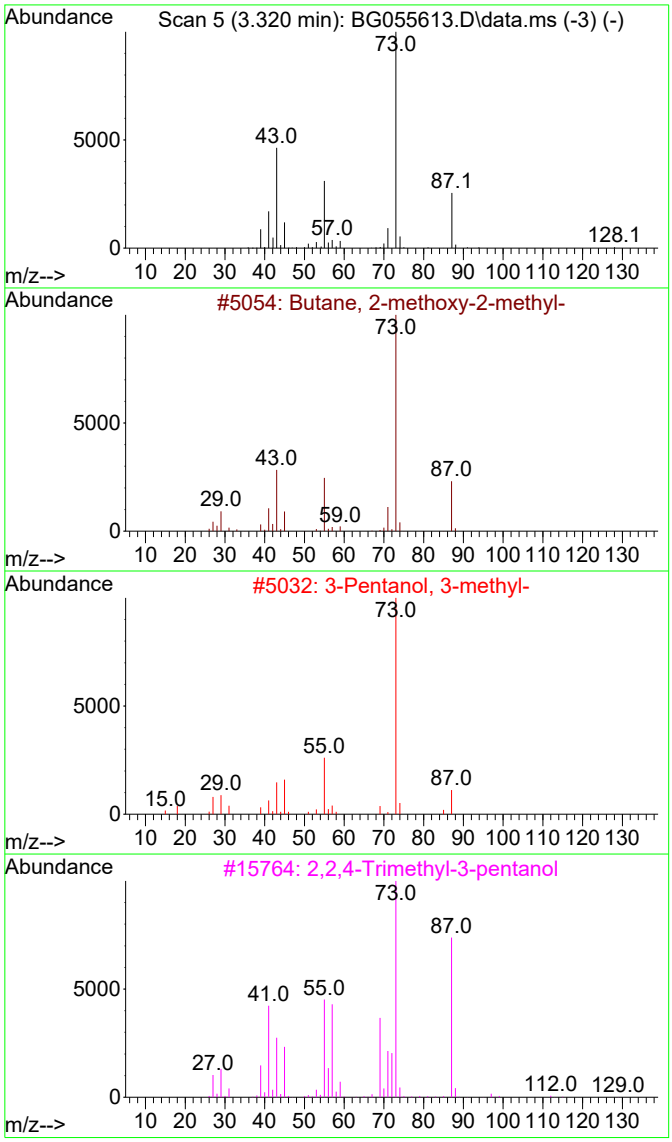
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

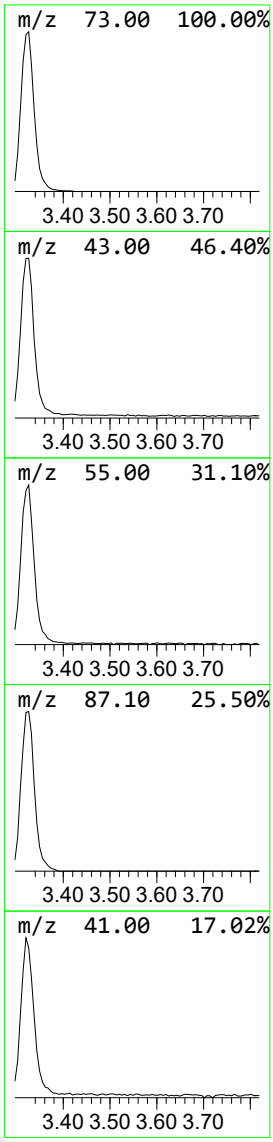
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.320	26.12 ng	441463	1,4-Dichlorobenzene-d4	8.267

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	40
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	33
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Operator : CG/JU
Sample : N5531-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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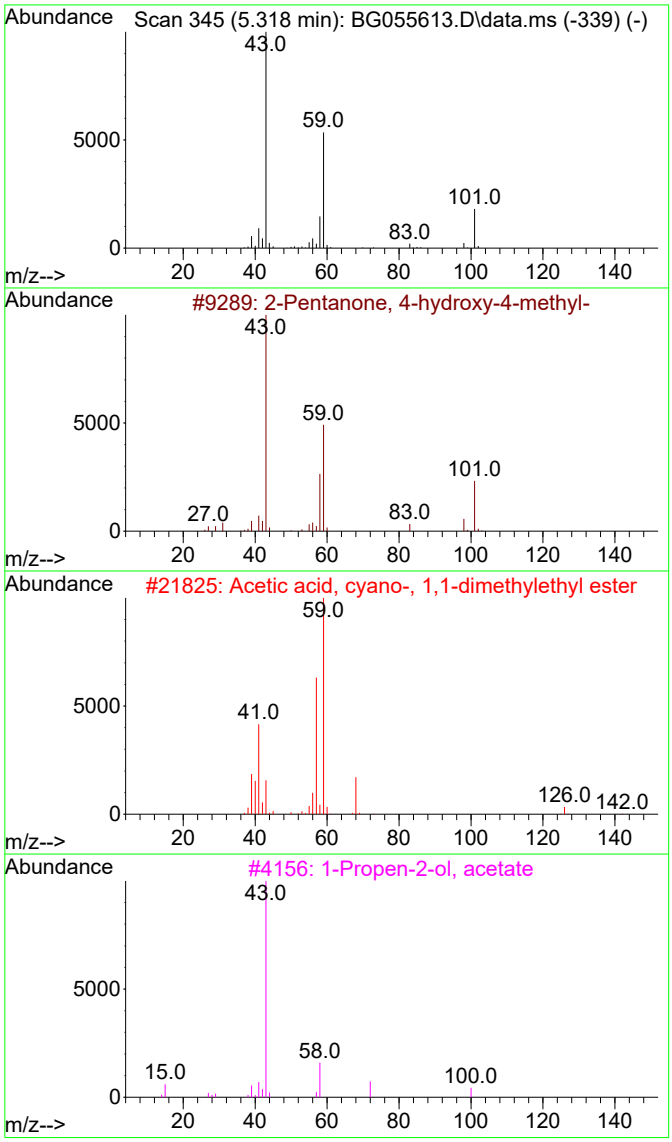
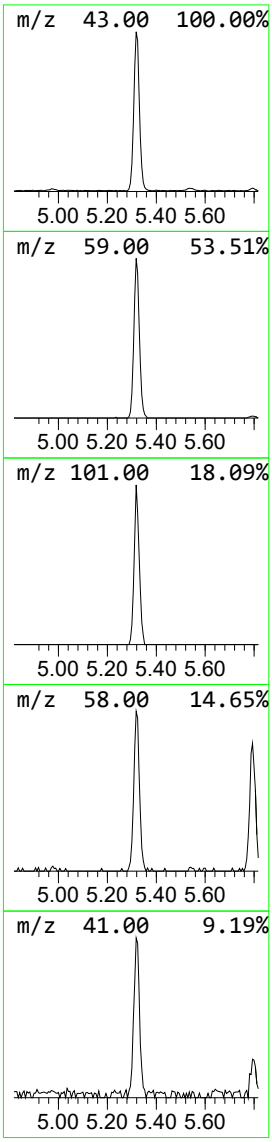
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.318	14.01 ng	236762	1,4-Dichlorobenzene-d4	8.267

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2-Pentanone	86	C5H10O	000107-87-9	10
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Data File : BG055613.D
Acq On : 14 Nov 2022 20:48
Operator : CG/JU
Sample : N5531-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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TIC Library : C:\Database\NIST20.L
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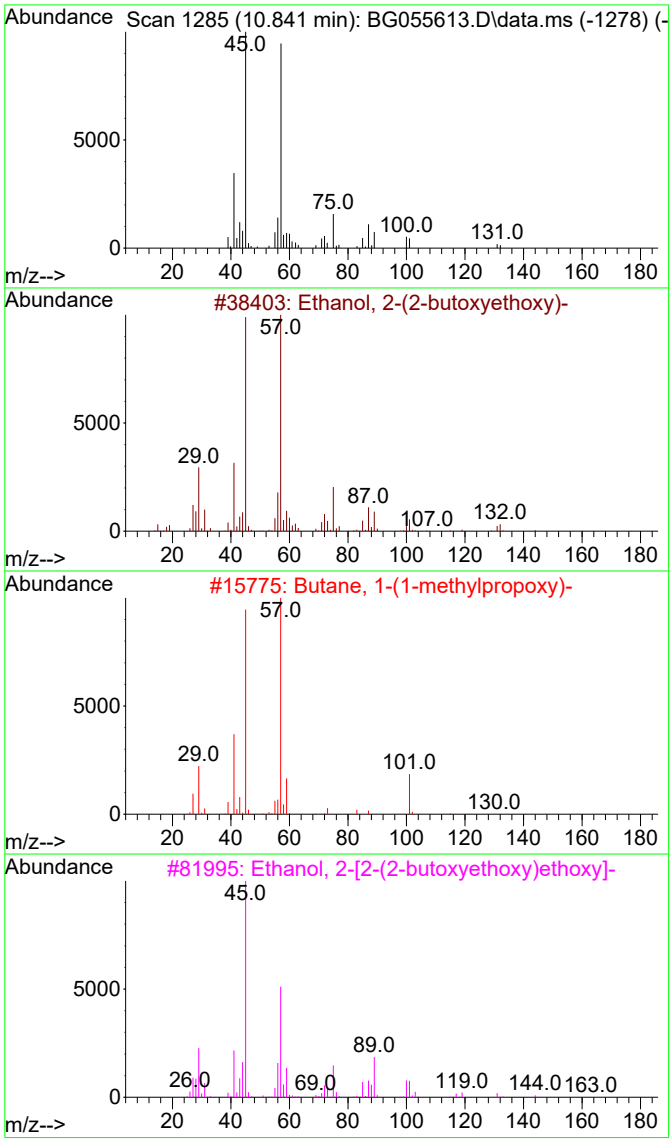
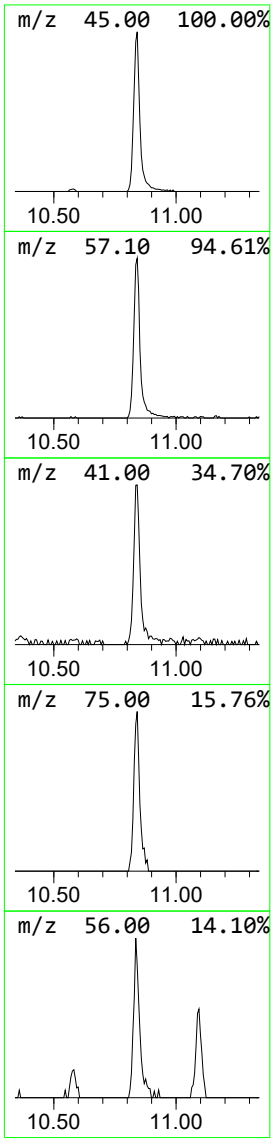
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.841	6.26 ng	150735	Naphthalene-d8	11.093

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	43
5	Propanoic acid, 3-methoxy-2-meth...	132	C6H12O3	003852-11-7	43





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Instrument :
BNA_G
ClientSampleId :
SB-28B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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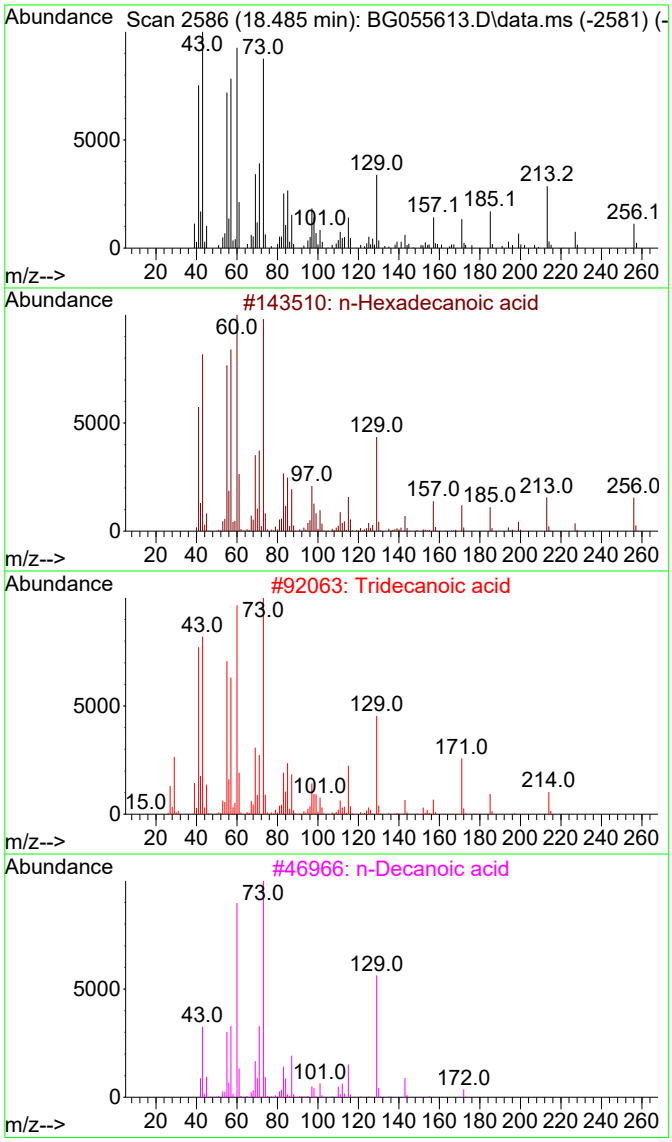
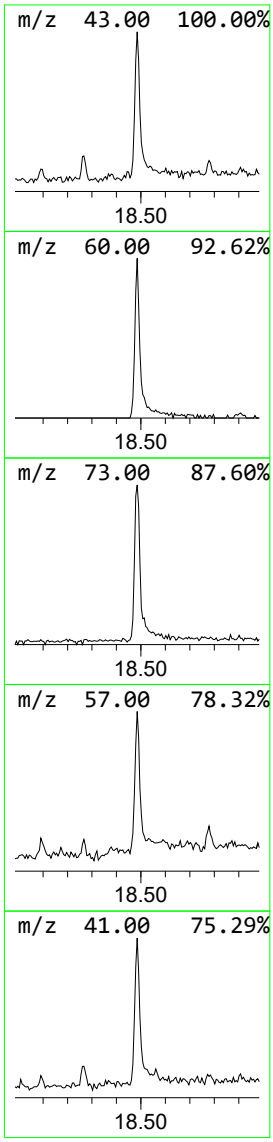
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.485	5.03 ng	202311	Phenanthrene-d10	17.627

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	92
3	n-Decanoic acid	172	C10H20O2	000334-48-5	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	62





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Operator : CG/JU
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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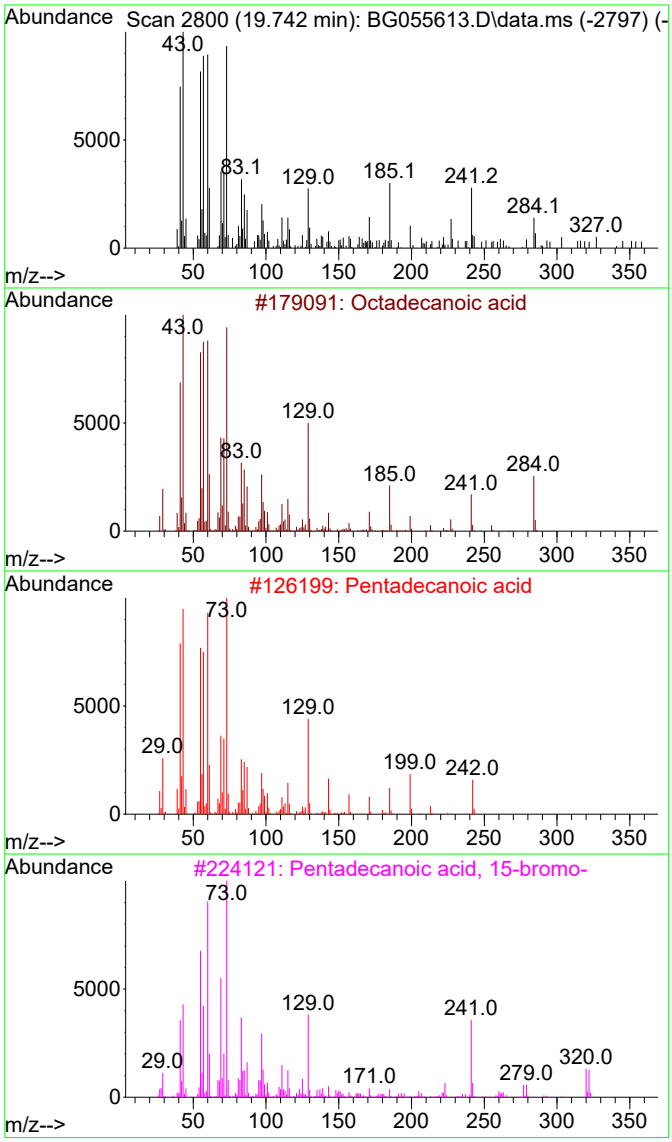
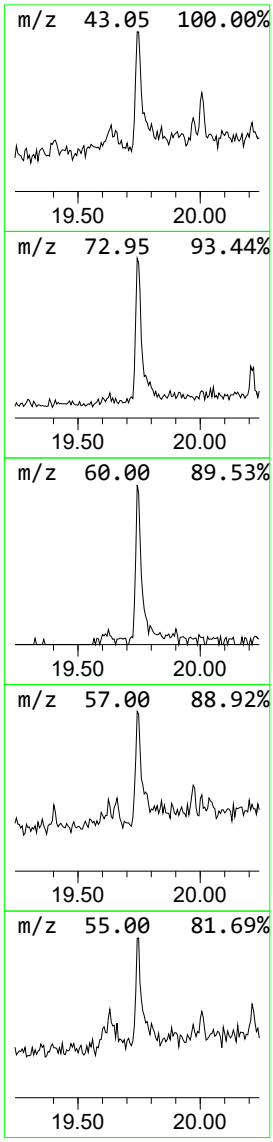
Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.742	2.63 ng	105872	Phenanthrene-d10	17.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	97
3	Pentadecanoic acid, 15-bromo-	320	C15H29BrO2	056523-59-2	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Tricosanoic acid	354	C23H46O2	002433-96-7	55





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BNA_G
ClientSampleId :
SB-28B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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TIC Library : C:\Database\NIST20.L
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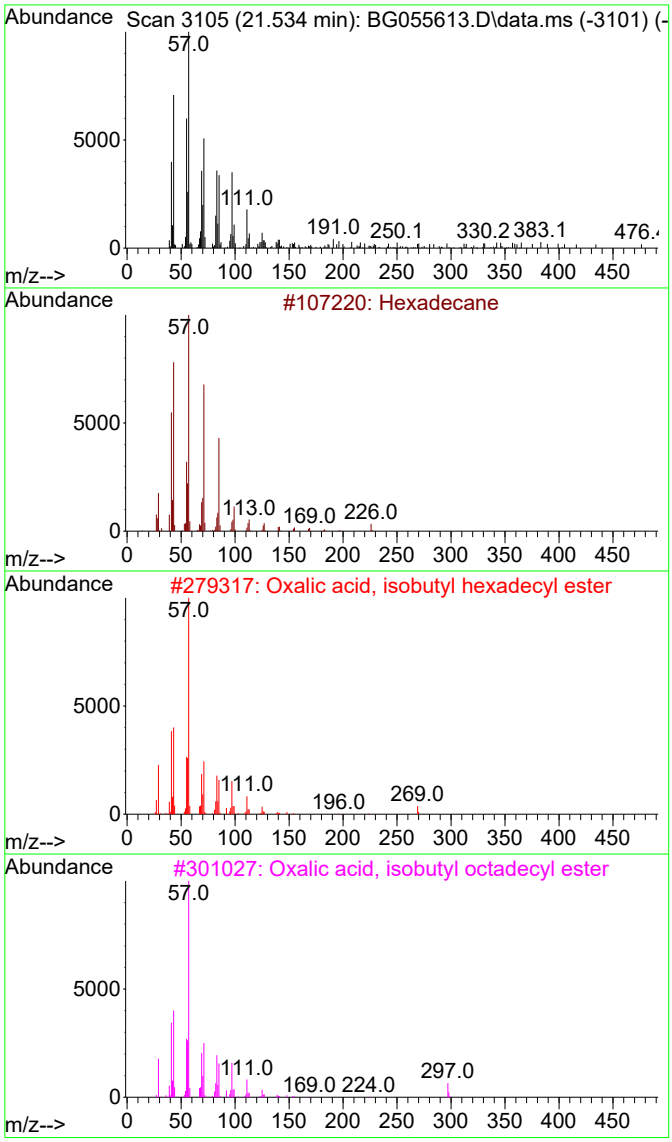
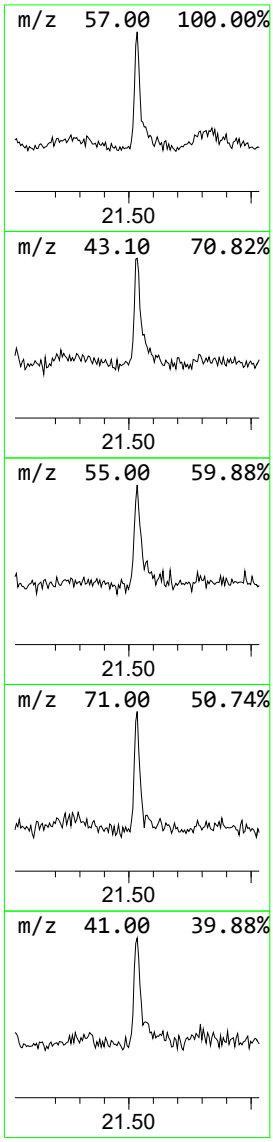
****

Peak Number 6 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.534	2.86 ng	117215	Chrysene-d12	21.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	92
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
3	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
5	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	86





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-metho...	3.320	26.1	ng	441463	1	8.267	338077	20.0
2-Pentanone, 4-...	5.318	14.0	ng	236762	1	8.267	338077	20.0
Ethanol, 2-(2-b...	10.841	6.3	ng	150735	2	11.093	481580	20.0
n-Hexadecanoic ...	18.485	5.0	ng	202311	4	17.627	804267	20.0
Octadecanoic acid	19.742	2.6	ng	105872	4	17.627	804267	20.0
Hexadecane	21.534	2.9	ng	117215	5	21.927	820693	20.0