LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061104.D
Acq On : 3 May 2024 13:25
Operator : MA/JU
Sample : P2331-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	22	28	42	rVB	253009	420876	17.96%	3.881%
2	3.669	112	116	126	rBV	29714	46546	1.99%	0.429%
3	5.526	425	432	443	rVB	518937	816239	34.84%	7.527%
4	7.112	693	702	710	rBV	550433	956120	40.81%	8.817%
5	7.935	835	842	848	rBV	96293	161694	6.90%	1.491%
6	9.086	1029	1038	1049	rBV	356173	635945	27.14%	5.864%
7	10.726	1310	1317	1324	rBV	129327	227569	9.71%	2.098%
8	11.460	1436	1442	1450	rBV4	11630	23472	1.00%	0.216%
9	13.182	1728	1735	1743	rBV	962173	1503800	64.18%	13.867%
10	14.562	1963	1970	1976	rBV	221615	333630	14.24%	3.077%
11	16.055	2216	2224	2236	rBV	957114	1454583	62.08%	13.413%
12	17.306	2431	2437	2442	rBV	266437	412614	17.61%	3.805%
13	17.347	2442	2444	2451	rVB	30744	38607	1.65%	0.356%
14	18.211	2582	2591	2601	rBV2	126073	209595	8.95%	1.933%
15	19.363	2779	2787	2793	rBV	69964	103999	4.44%	0.959%
16	19.480	2802	2807	2817	rBV6	31323	60708	2.59%	0.560%
17	19.721	2844	2848	2856	rVB	49602	83139	3.55%	0.767%
18	19.927	2874	2883	2890	rBV	1836476	2343038	100.00%	21.606%
19	21.237	3101	3106	3112	rBV4	51285	99075	4.23%	0.914%
20	21.566	3153	3162	3167	rBV	295735	551618	23.54%	5.087%
21	24.686	3683	3693	3701	rBV	119339	361510	15.43%	3.334%

Sum of corrected areas: 10844377

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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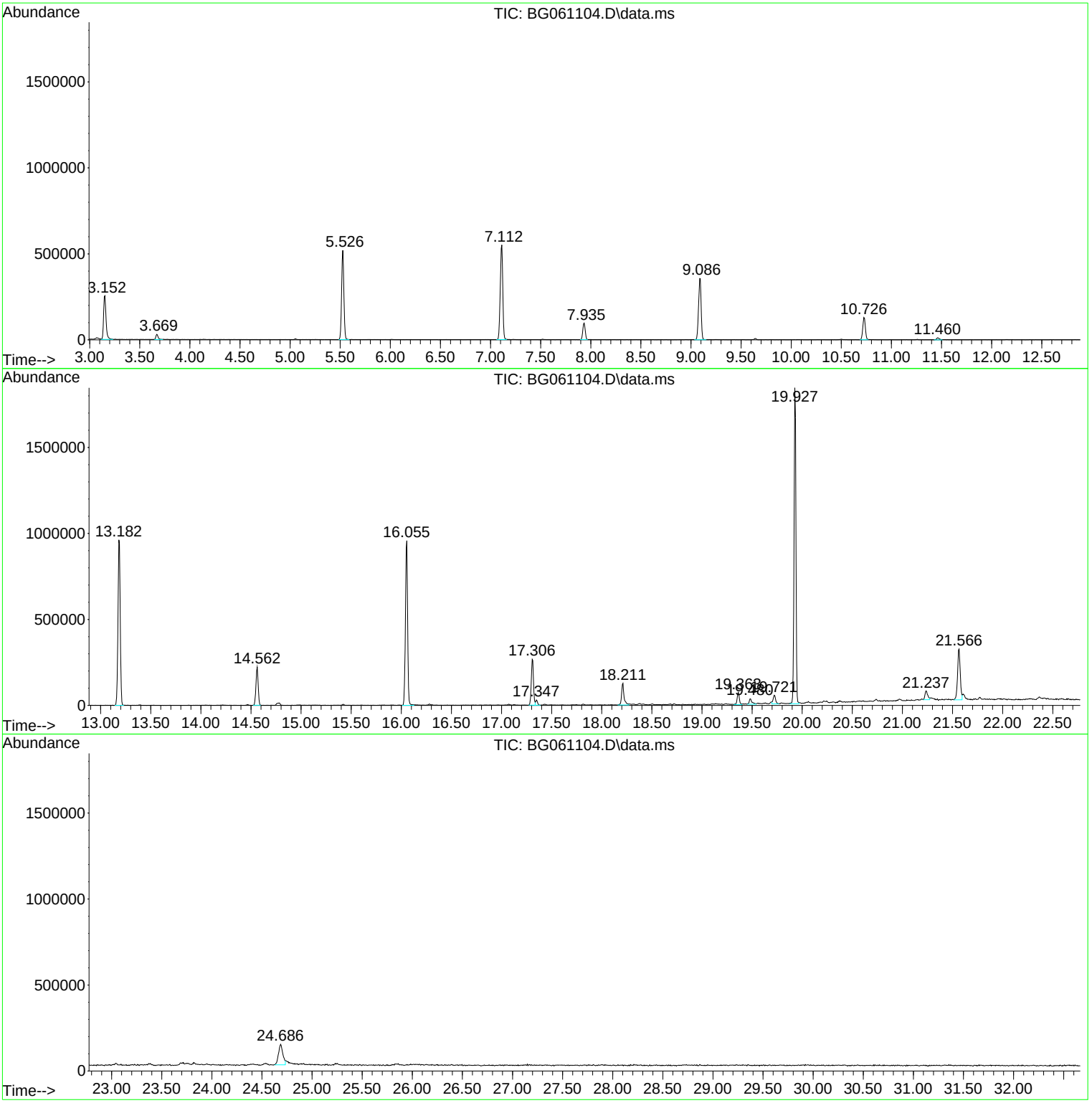
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061104.D
Acq On : 3 May 2024 13:25
Operator : MA/JU
Sample : P2331-05
Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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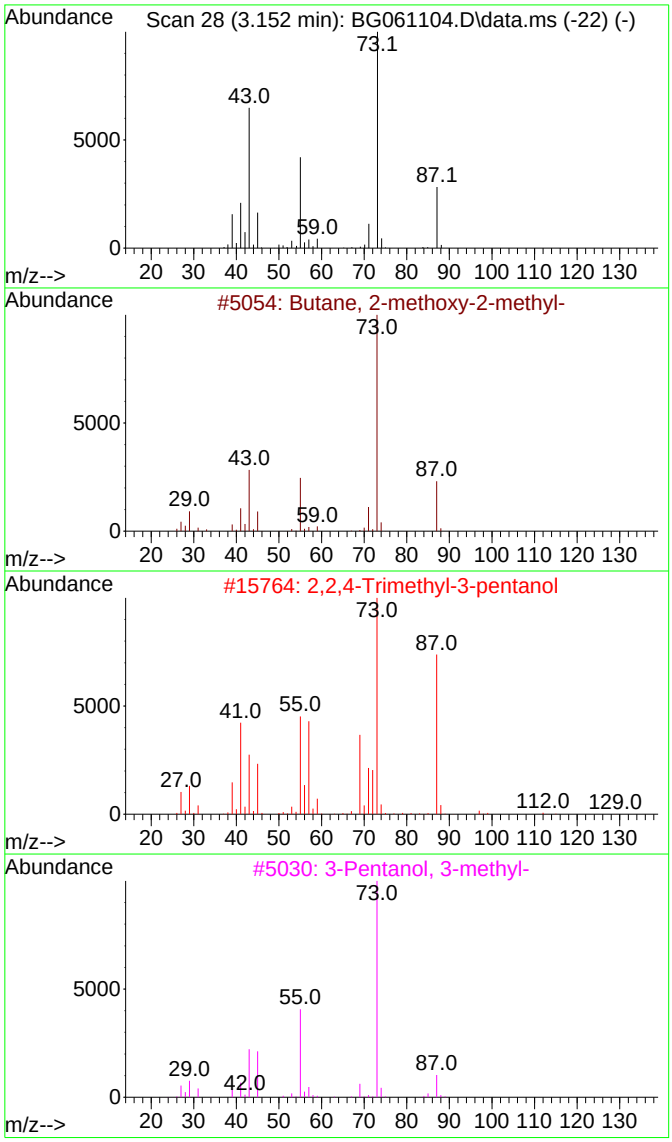
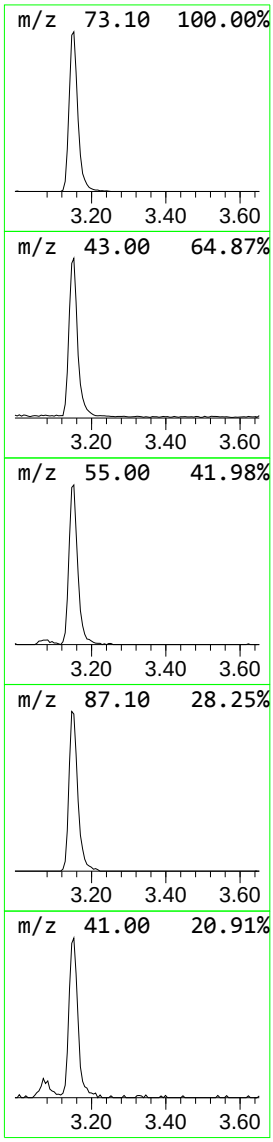
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	52.06 ng	420876	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	25





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Operator : MA/JU
Sample : P2331-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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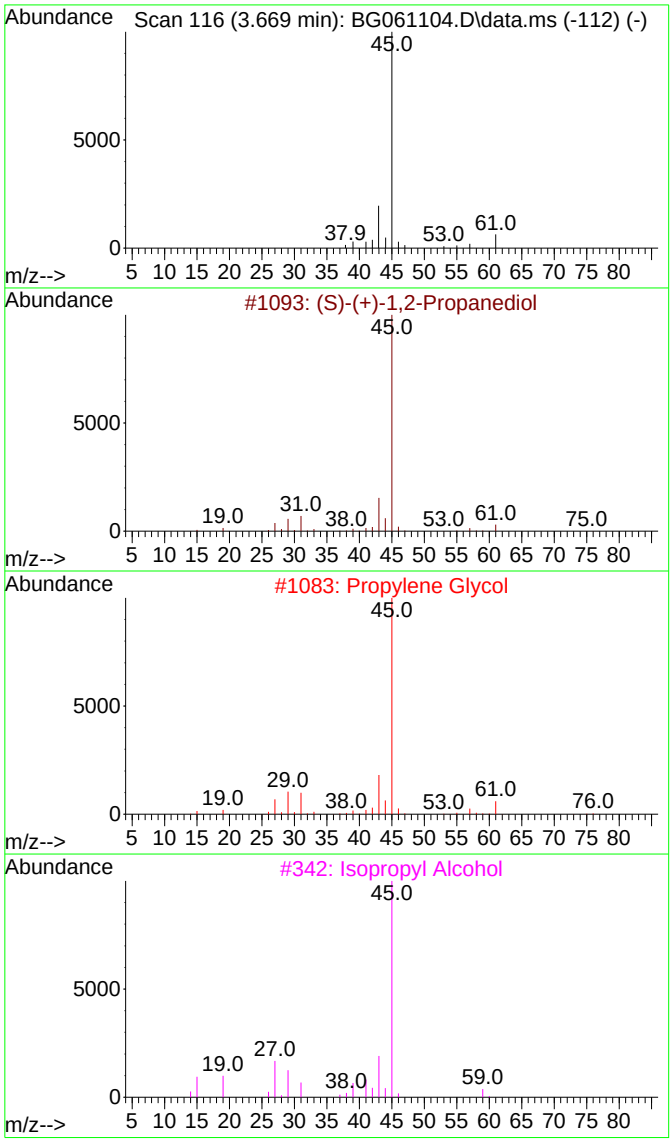
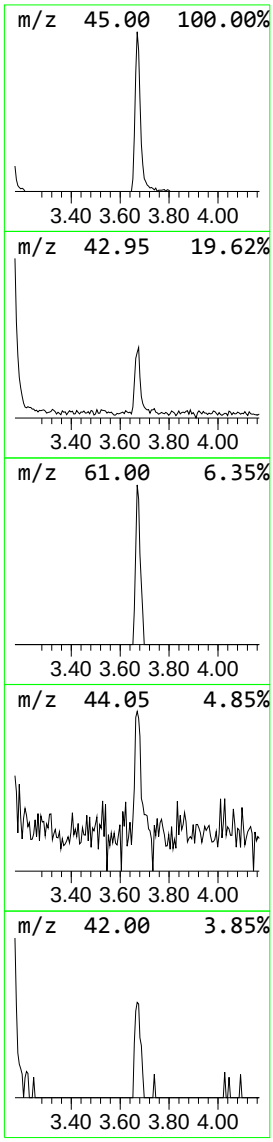
Peak Number 2 unknown3.669 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.669	5.76 ng	46546	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5	L-Lactic acid	90	C3H6O3	000079-33-4	9





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Data File : BG061104.D
Acq On : 3 May 2024 13:25
Operator : MA/JU
Sample : P2331-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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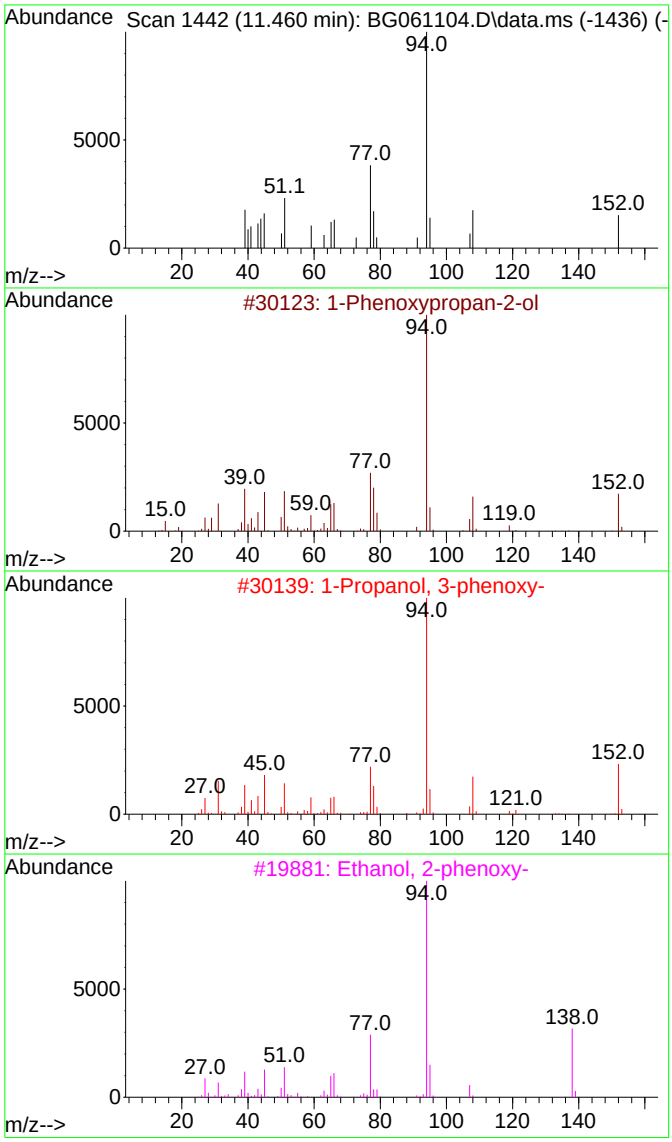
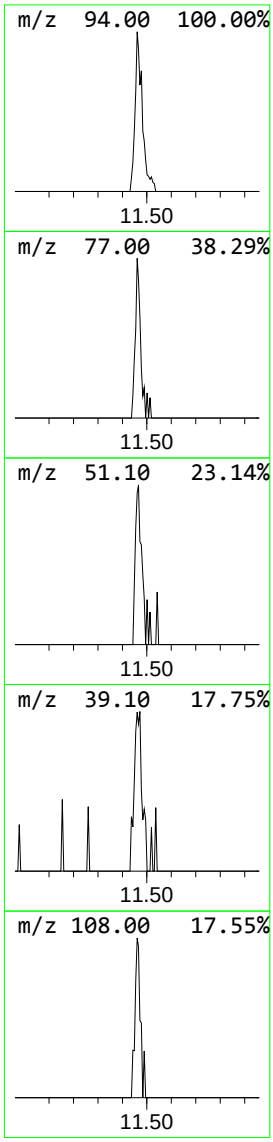
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.460	2.06 ng	23472	Naphthalene-d8	10.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	90
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	80
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	72
4	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	40
5	2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	38





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Data File : BG061104.D
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Operator : MA/JU
Sample : P2331-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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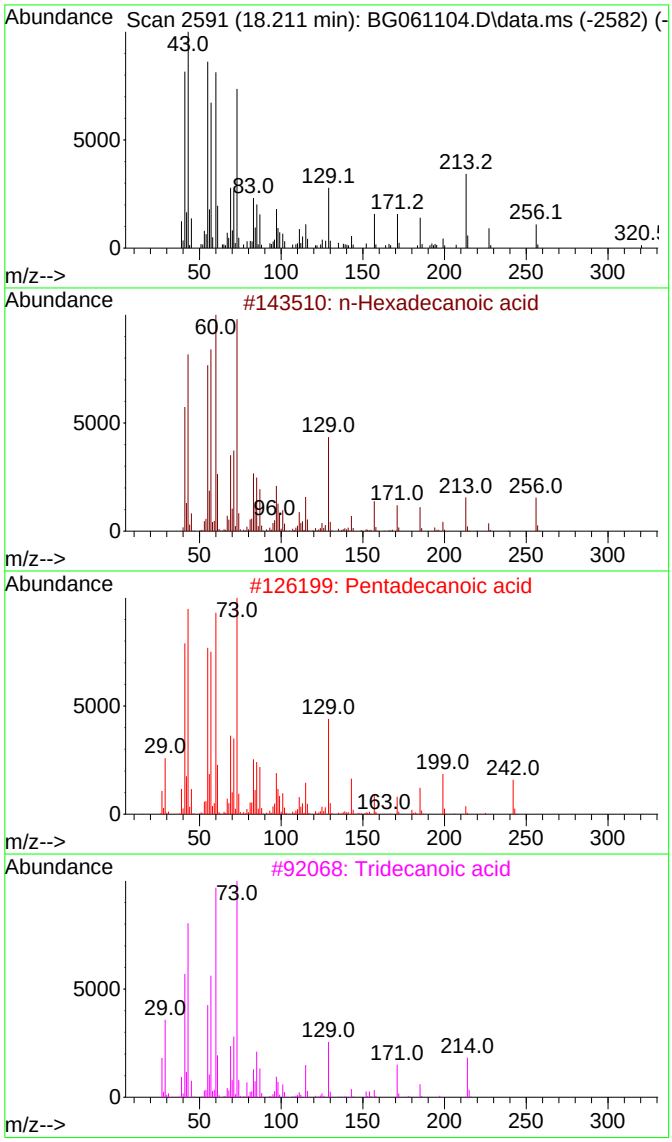
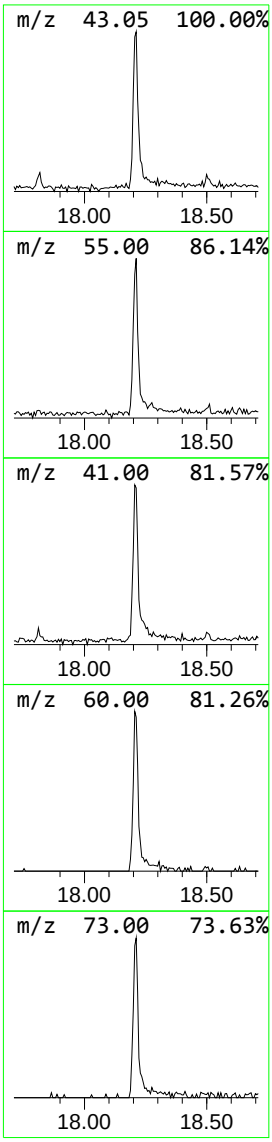
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	10.16 ng	209595	Phenanthrene-d10	17.306

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Octadecanoic acid	284	C18H36O2	000057-11-4	60
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061104.D
Acq On : 3 May 2024 13:25
Operator : MA/JU
Sample : P2331-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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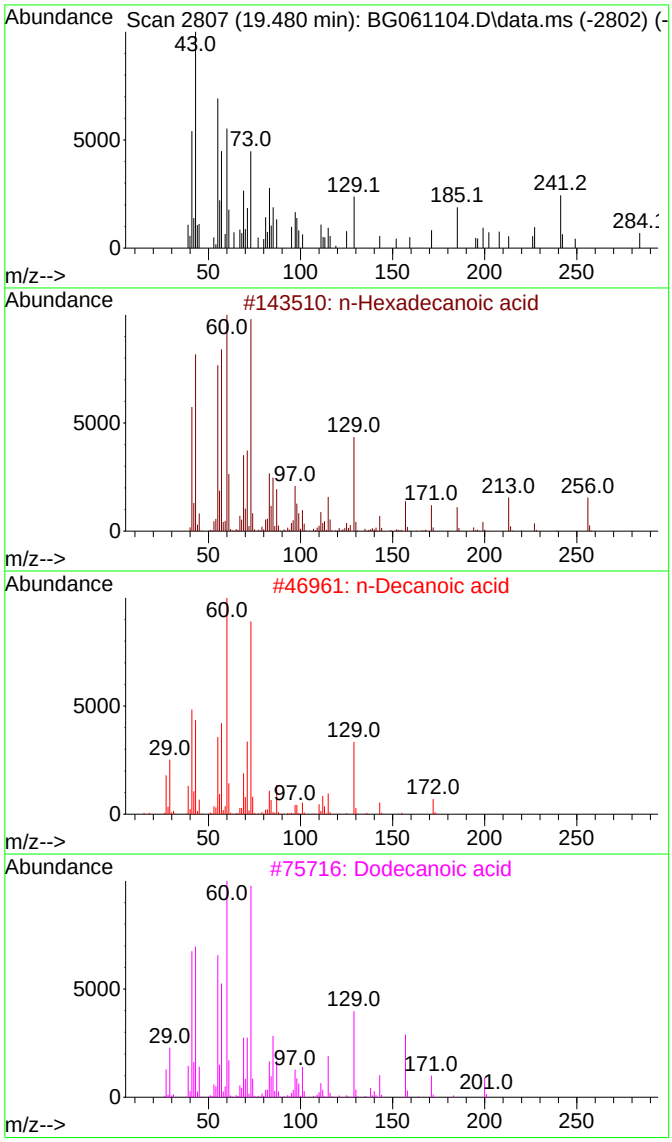
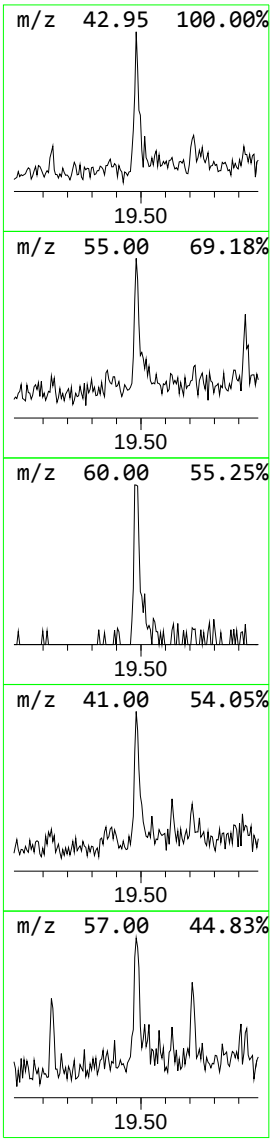
Peak Number 5 unknown19.480 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.480	2.20 ng	60708	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	38
2	n-Decanoic acid	172	C10H20O2	000334-48-5	35
3	Dodecanoic acid	200	C12H24O2	000143-07-7	35
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	22
5	Octanoic acid	144	C8H16O2	000124-07-2	14





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Operator : MA/JU
Sample : P2331-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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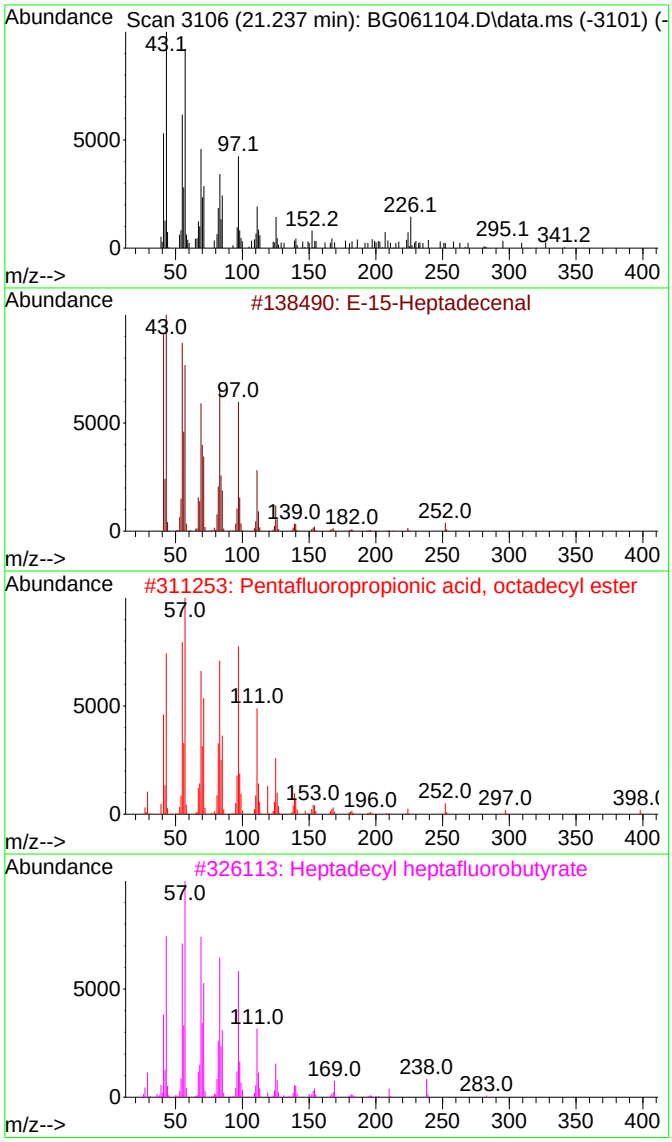
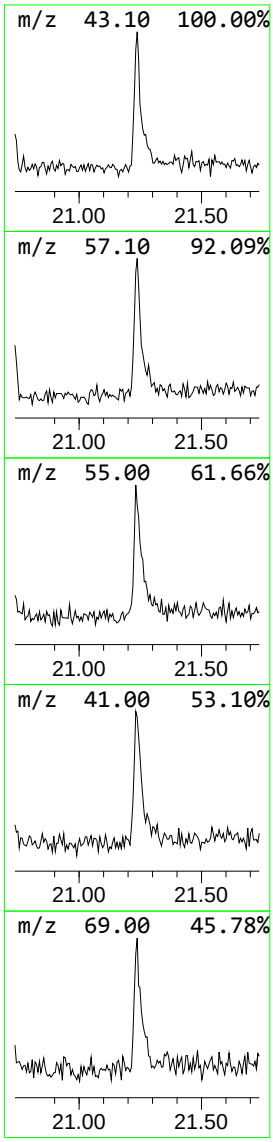
Peak Number 6 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	3.59 ng	99075	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	81
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76
5	1-Docosene	308	C22H44	001599-67-3	76





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...	3.152	52.1	ng	420876	1	7.935	161694	20.0
unknown3.669	3.669	5.8	ng	46546	1	7.935	161694	20.0
1-Phenoxypropan...	11.460	2.1	ng	23472	2	10.726	227569	20.0
n-Hexadecanoic ...	18.211	10.2	ng	209595	4	17.306	412614	20.0
unknown19.480	19.480	2.2	ng	60708	5	21.566	551618	20.0
E-15-Heptadecenal	21.237	3.6	ng	99075	5	21.566	551618	20.0