LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050924\
Data File : BG061151.D
Acq On : 9 May 2024 14:48
Operator : MA/JU
Sample : P2414-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1011UMR-SS004-0212-01

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: BG061151.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.073	8	14	21	rBV	35080	80638	4.31%	0.857%
2	3.150	21	27	40	rVB	239290	414118	22.15%	4.400%
3	3.673	110	116	125	rBV	26078	42290	2.26%	0.449%
4	5.523	424	431	442	rBV	406134	642253	34.36%	6.824%
5	7.110	693	701	710	rBV	417544	720613	38.55%	7.656%
6	7.932	833	841	847	rBV	89943	150564	8.05%	1.600%
7	9.084	1029	1037	1046	rBV	273415	488023	26.11%	5.185%
8	10.723	1308	1316	1324	rBV	113680	200971	10.75%	2.135%
9	11.458	1437	1441	1450	rBV3	13777	27176	1.45%	0.289%
10	13.185	1726	1735	1742	rBV	701709	1096731	58.67%	11.652%
11	14.560	1962	1969	1977	rBV	190468	289156	15.47%	3.072%
12	14.760	1996	2003	2004	rBV3	28289	32760	1.75%	0.348%
13	14.777	2004	2006	2012	rVB3	33098	43667	2.34%	0.464%
14	16.052	2216	2223	2236	rBV	671740	1062229	56.82%	11.286%
15	17.310	2431	2437	2442	rBV	252601	380331	20.35%	4.041%
16	17.351	2442	2444	2451	rVB2	19124	21750	1.16%	0.231%
17	18.208	2583	2590	2598	rBV6	29661	54615	2.92%	0.580%
18	19.366	2782	2787	2792	rBV	53866	72987	3.90%	0.775%
19	19.472	2801	2805	2808	rBV4	13128	19480	1.04%	0.207%
20	19.513	2808	2812	2816	rVB3	34281	43659	2.34%	0.464%
21	19.671	2835	2839	2841	rBV3	39790	49973	2.67%	0.531%
22	19.701	2841	2844	2846	rVV3	47459	67383	3.60%	0.716%
23	19.724	2846	2848	2854	rVB	45748	63262	3.38%	0.672%
24	19.930	2877	2883	2892	rBV	1478237	1869305	100.00%	19.860%
25	21.240	3101	3106	3114	rBV6	33456	78439	4.20%	0.833%
26	21.569	3152	3162	3167	rBV	294287	519066	27.77%	5.515%
27	21.769	3190	3196	3201	rVB7	11770	22353	1.20%	0.237%
28	23.015	3401	3408	3419	rVB4	58320	129539	6.93%	1.376%
29	23.226	3438	3444	3451	rVB4	21218	42458	2.27%	0.451%
30	23.708	3520	3526	3533	rBV3	22765	67933	3.63%	0.722%
31	23.820	3543	3545	3552	rVB7	13958	21170	1.13%	0.225%
32	24.407	3637	3645	3650	rBV4	14456	44060	2.36%	0.468%
33	24.542	3663	3668	3676	rBV5	14692	30874	1.65%	0.328%
34	24.695	3684	3694	3718	rBV	149211	522407	27.95%	5.550%

Sum of corrected areas: 9412233

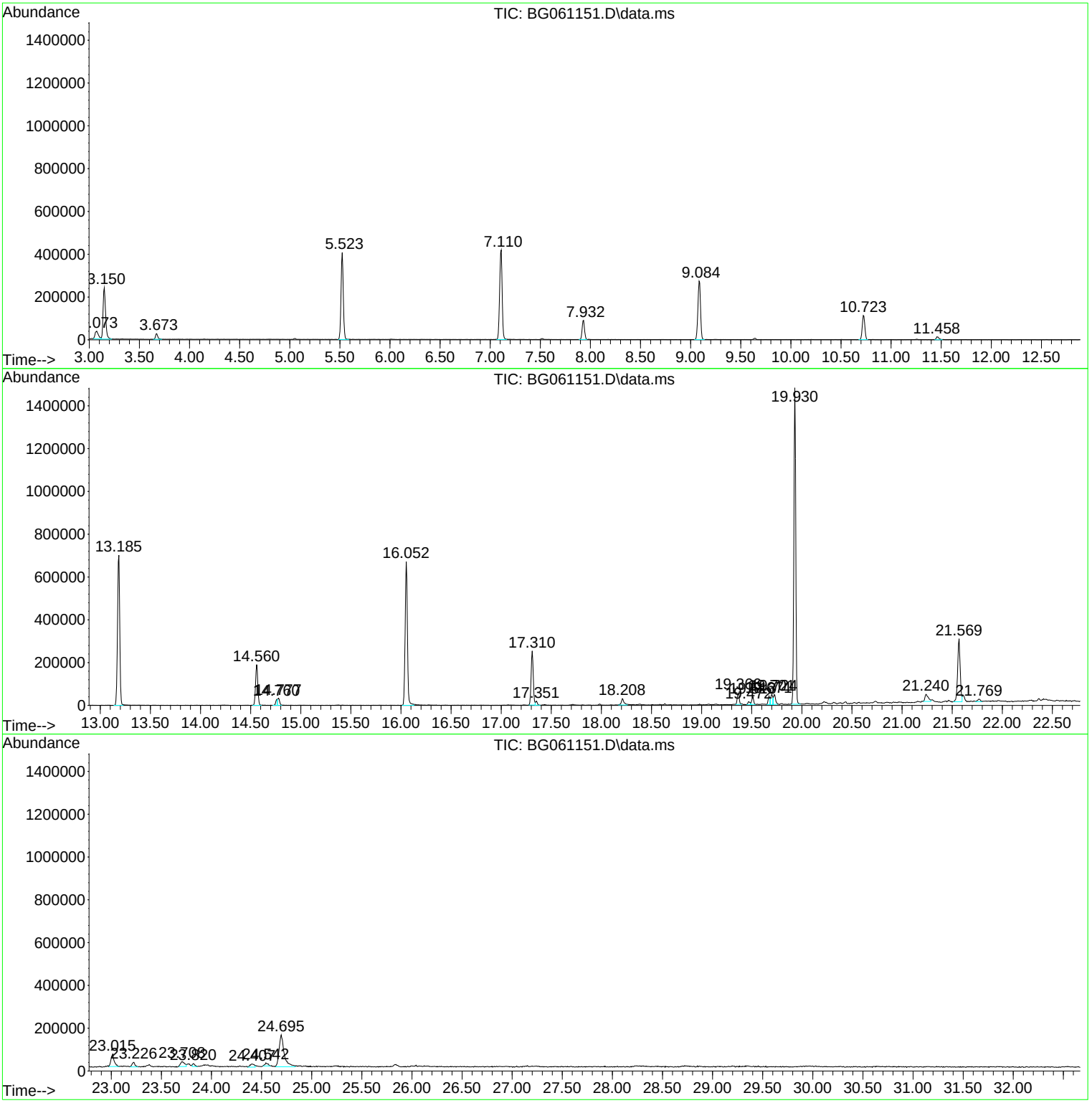
Instrument :
BNA_G
ClientSampleId :
1011UMR-SS004-0212-01

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050924\
Data File : BG061151.D
Acq On : 9 May 2024 14:48
Operator : MA/JU
Sample : P2414-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS004-0212-01

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\BG050924\
Data File : BG061151.D
Acq On : 9 May 2024 14:48
Operator : MA/JU
Sample : P2414-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
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1011UMR-SS004-0212-01

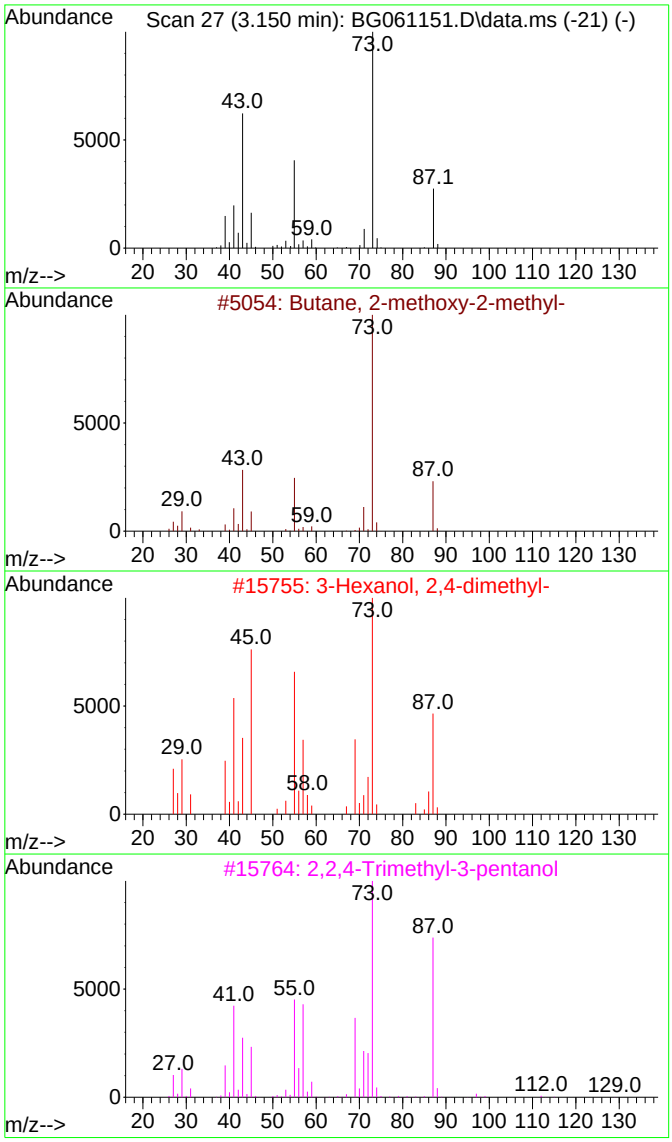
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

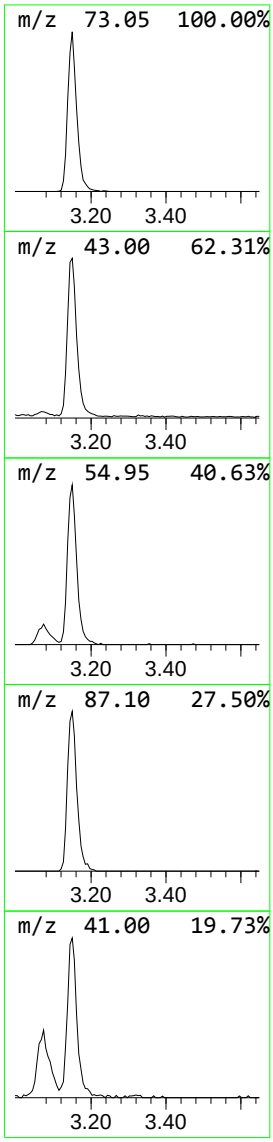
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.150	55.01 ng	414118	1,4-Dichlorobenzene-d4	7.926

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	50
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	25





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Data File : BG061151.D
Acq On : 9 May 2024 14:48
Operator : MA/JU
Sample : P2414-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS004-0212-01

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

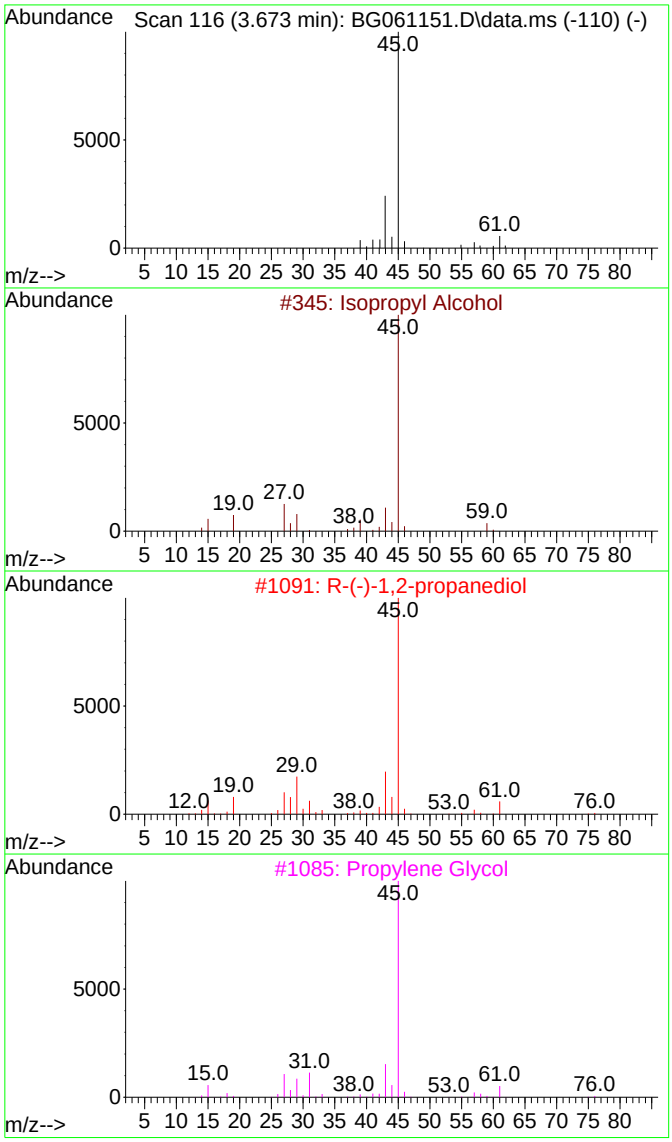
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

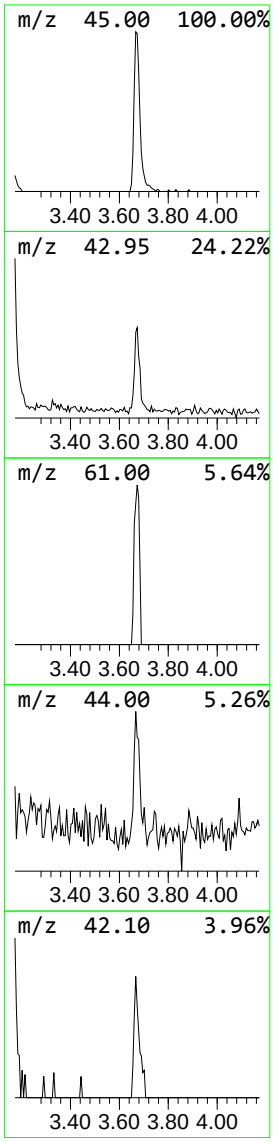
****

Peak Number 3 unknown3.673 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.673	5.62 ng	42290	1,4-Dichlorobenzene-d4	7.926

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5	Formamide	45	CH3NO	000075-12-7	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050924\
Data File : BG061151.D
Acq On : 9 May 2024 14:48
Operator : MA/JU
Sample : P2414-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS004-0212-01

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

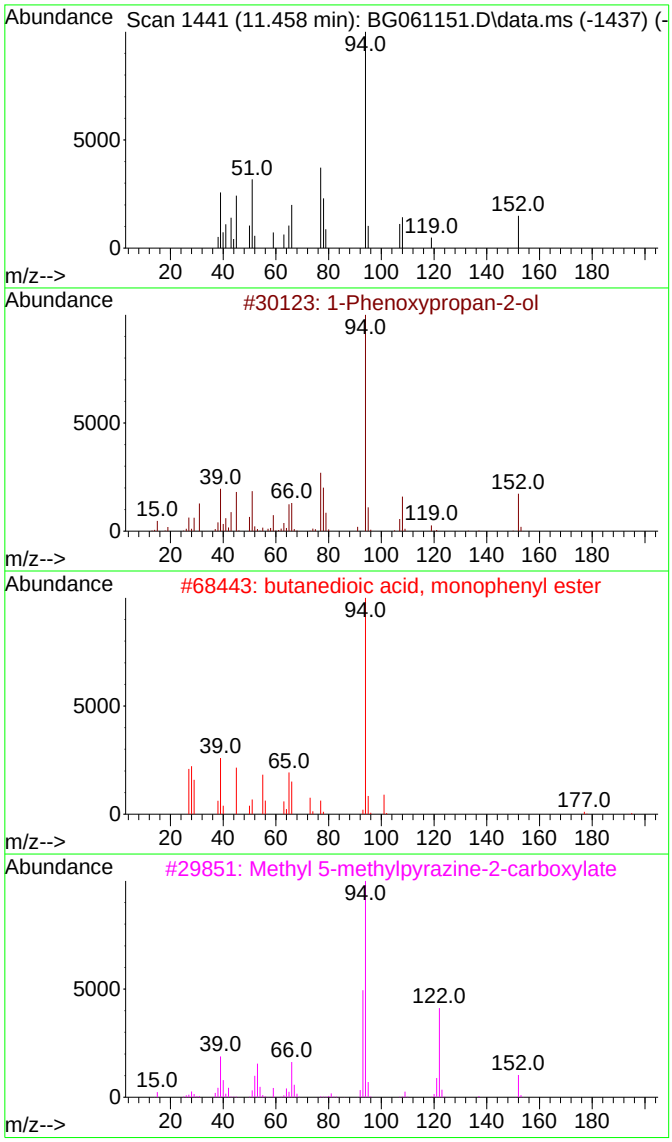
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

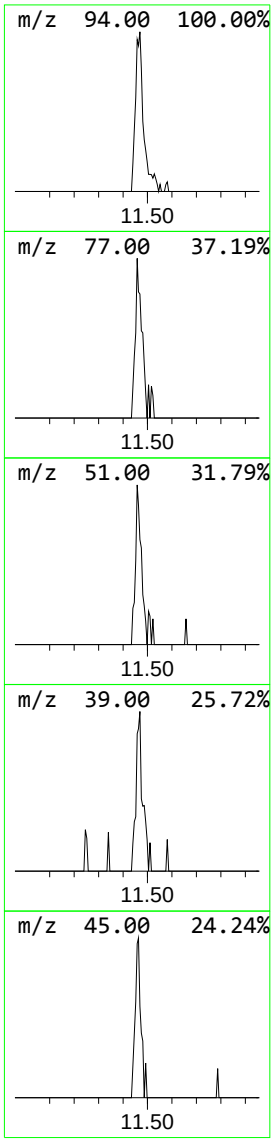
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.458	2.70 ng	27176	Naphthalene-d8	10.723

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	58
2	butanedioic acid, monophenyl ester	194	C10H10O4	1000400-29-4	53
3	Methyl 5-methylpyrazine-2-carbox...	152	C7H8N2O2	041110-33-2	50
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	45
5	2-Vinylfuran	94	C6H6O	001487-18-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050924\
Data File : BG061151.D
Acq On : 9 May 2024 14:48
Operator : MA/JU
Sample : P2414-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS004-0212-01

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

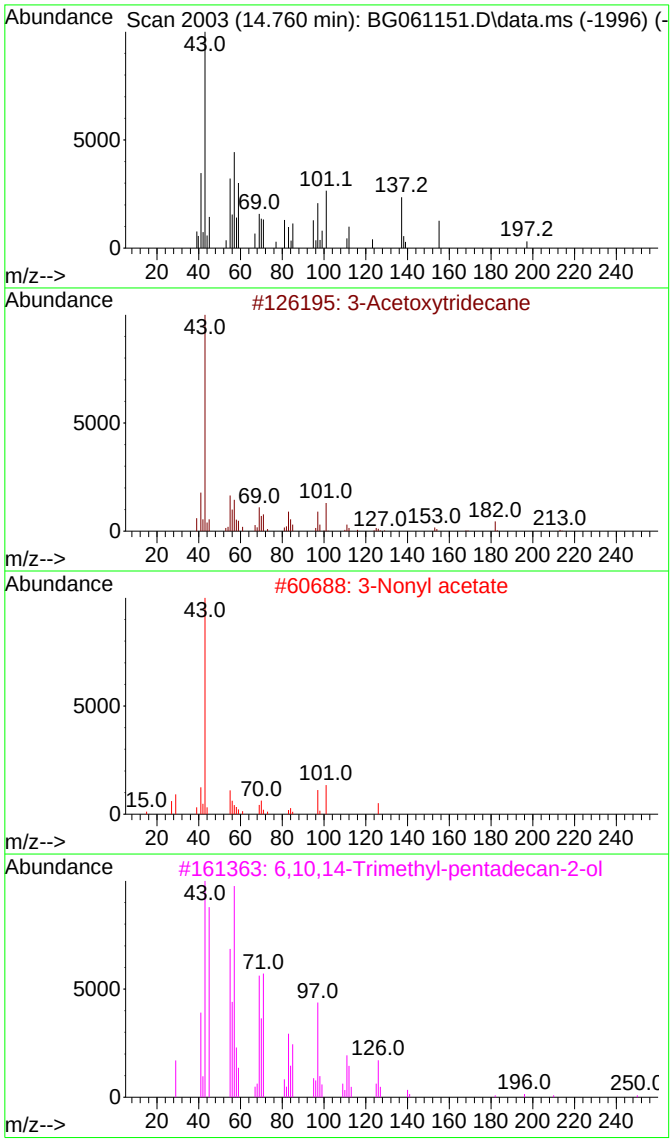
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

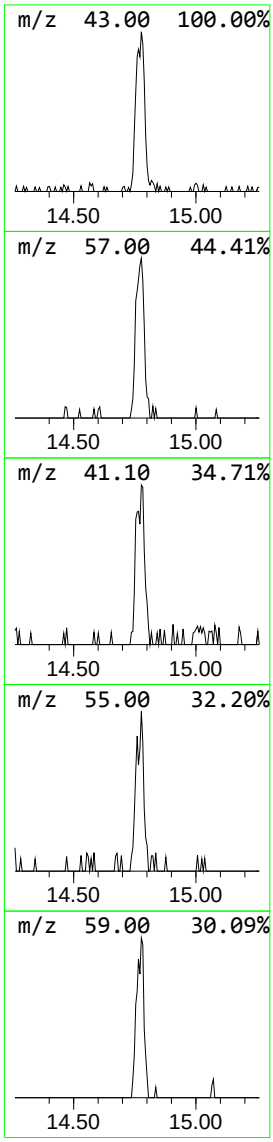
****

Peak Number 5 unknown14.760 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.760	2.27 ng	32760	Acenaphthene-d10	14.560

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Acetoxytridecane	242	C15H30O2	1010245-61-3	25
2	3-Nonyl acetate	186	C11H22O2	1010429-16-2	22
3	6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	10
4	Undecane, 1-bromo-	234	C11H23Br	000693-67-4	10
5	2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	10





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Operator : MA/JU
Sample : P2414-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS004-0212-01

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

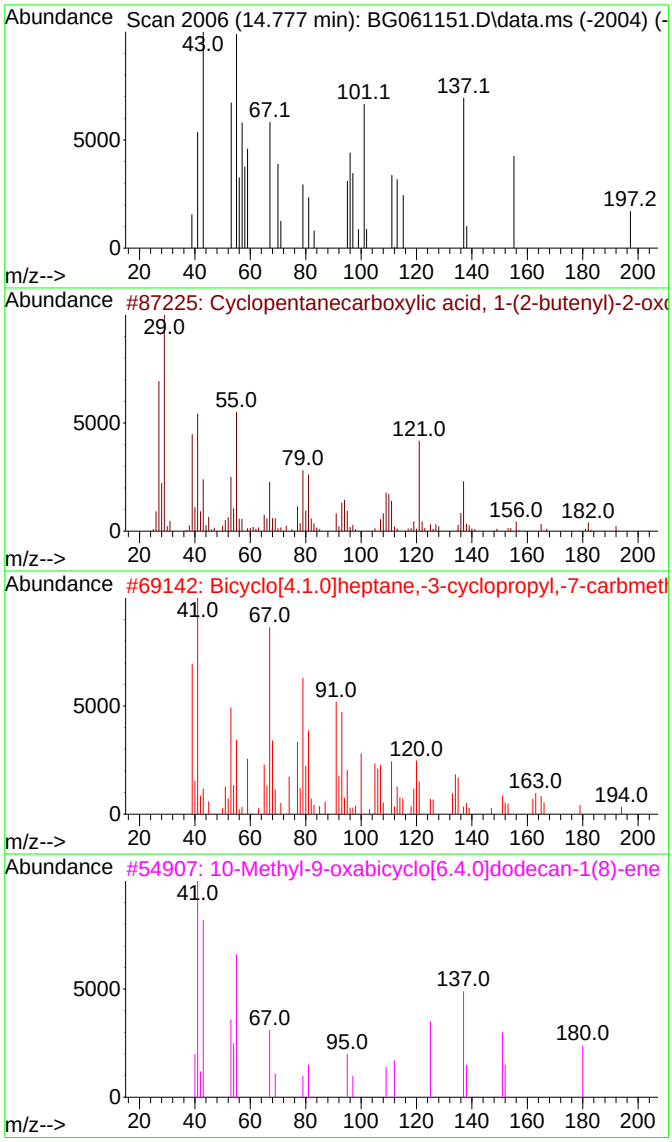
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

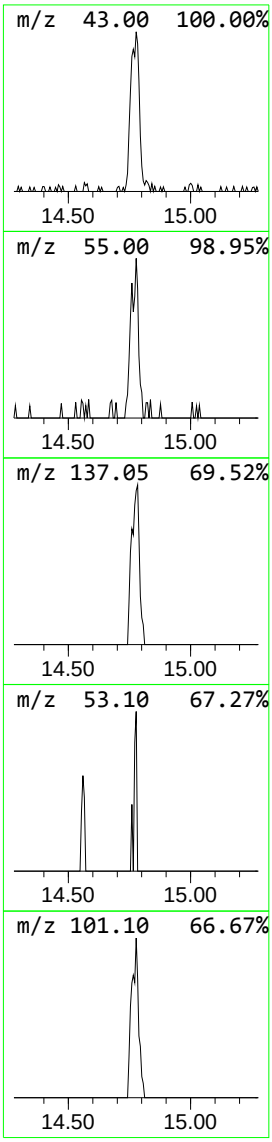
****

Peak Number 6 unknown14.777 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.777	3.02 ng	43667	Acenaphthene-d10	14.560

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxylic acid, 1-(...	210	C12H18O3	131534-41-3	25
2	Bicyclo[4.1.0]heptane,-3-cyclopr...	194	C12H18O2	1000222-97-0	23
3	10-Methyl-9-oxabicyclo[6.4.0]dod...	180	C12H20O	110288-22-7	23
4	Formaldehyde, methyl(2-propynyl)...	96	C5H8N2	110213-10-0	17
5	Carbonic acid, but-3-yn-1-yl und...	268	C16H28O3	1000383-17-7	16





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Data File : BG061151.D
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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
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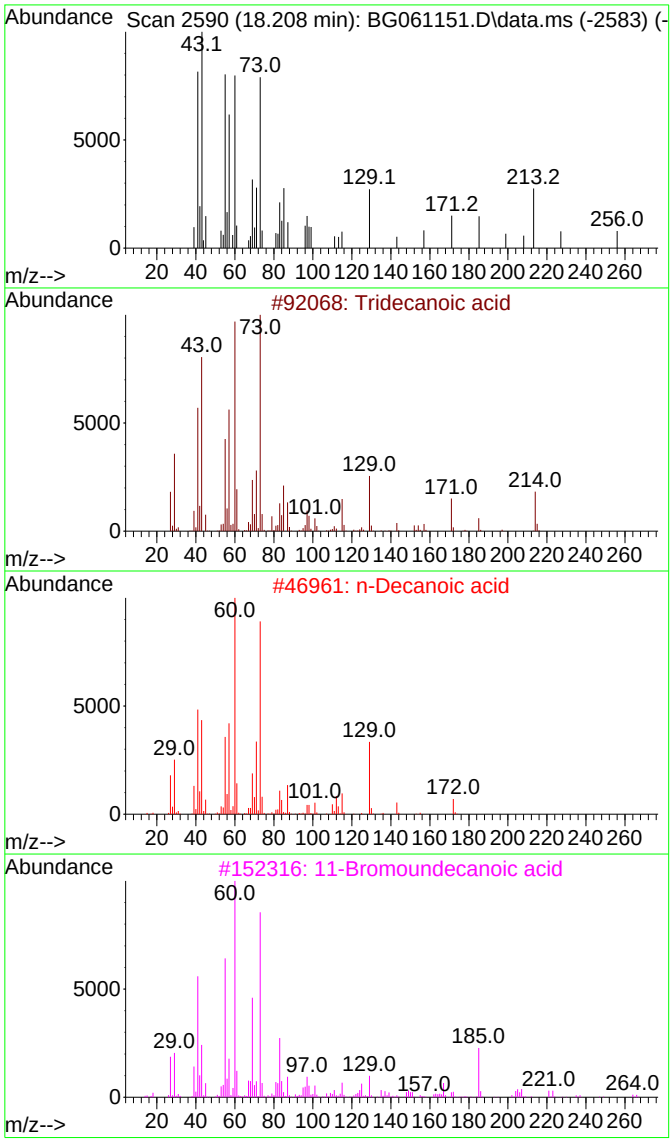
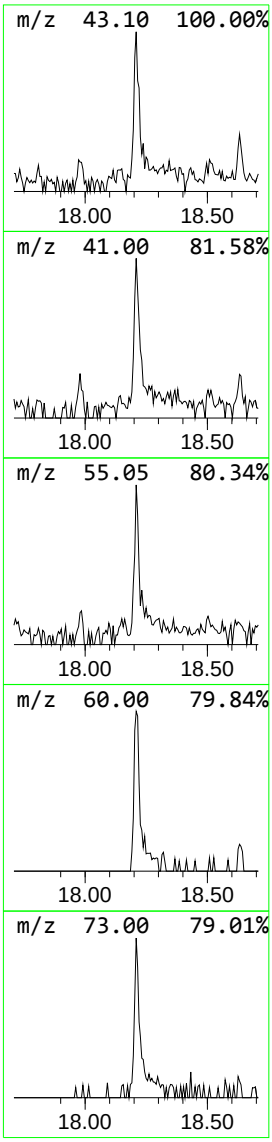
****

Peak Number 7 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.209	2.87 ng	54615	Phenanthrene-d10	17.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	59
2	n-Decanoic acid	172	C10H20O2	000334-48-5	47
3	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	43
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
5	Octanoic acid	144	C8H16O2	000124-07-2	35





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Data File : BG061151.D
Acq On : 9 May 2024 14:48
Operator : MA/JU
Sample : P2414-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-SS004-0212-01

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

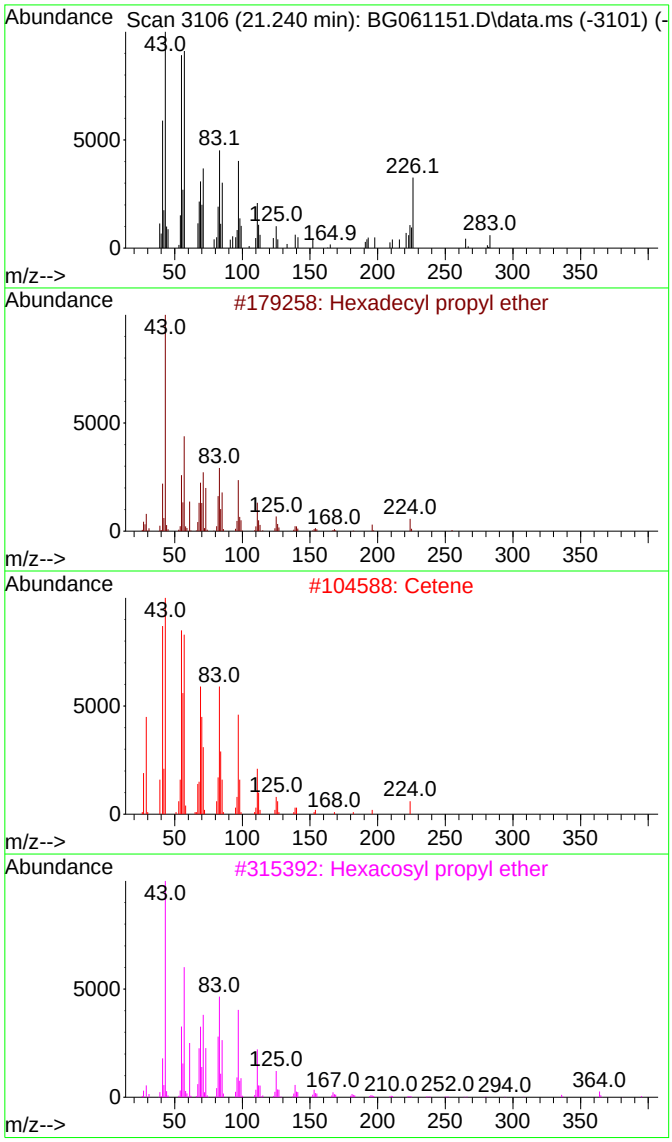
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

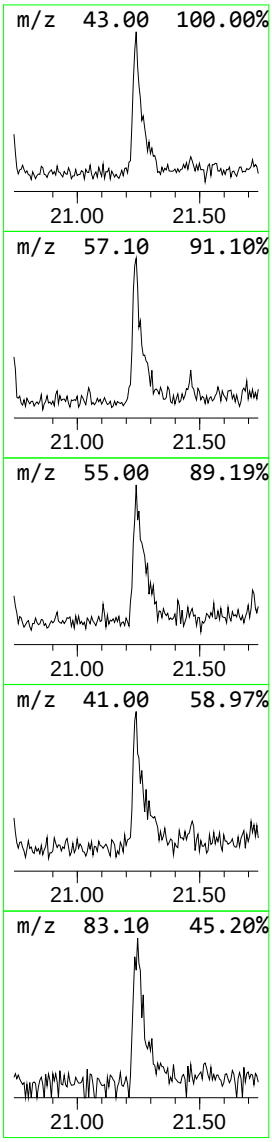
****

Peak Number 8 Hexadecyl propyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.240	3.02 ng	78439	Chrysene-d12	21.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecyl propyl ether	284	C19H40O	1000406-27-9	68
2	Cetene	224	C16H32	000629-73-2	66
3	Hexacosyl propyl ether	424	C29H60O	1000406-28-4	64
4	Octacosyl propyl ether	452	C31H64O	1000406-28-5	64
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	58





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BNA_G
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1011UMR-SS004-0212-01

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

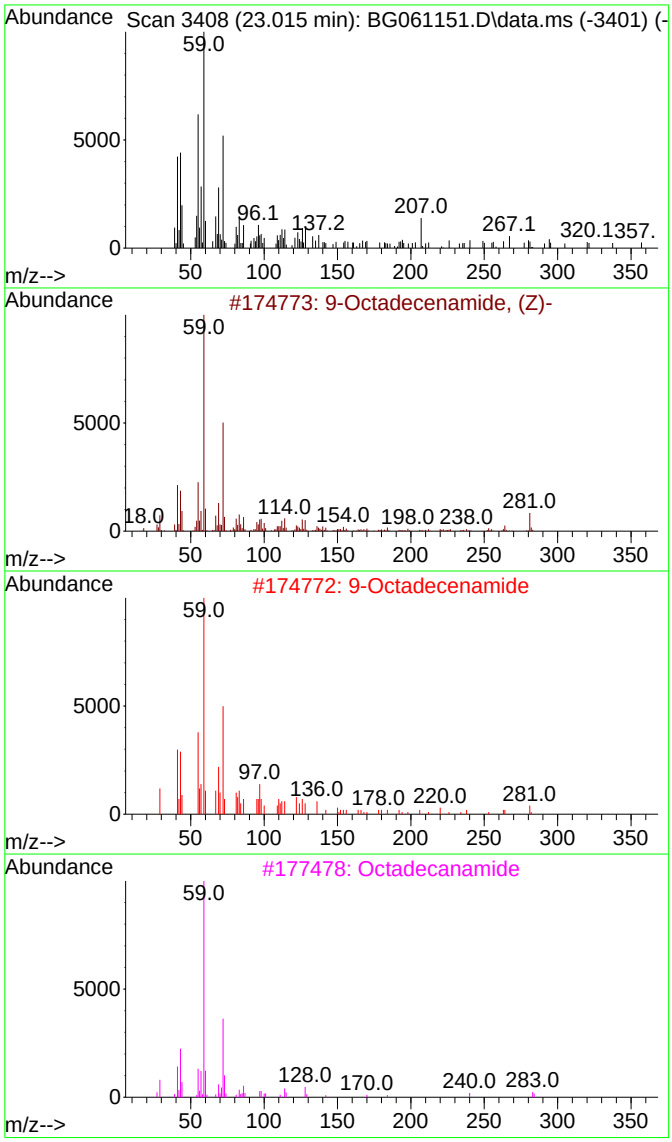
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

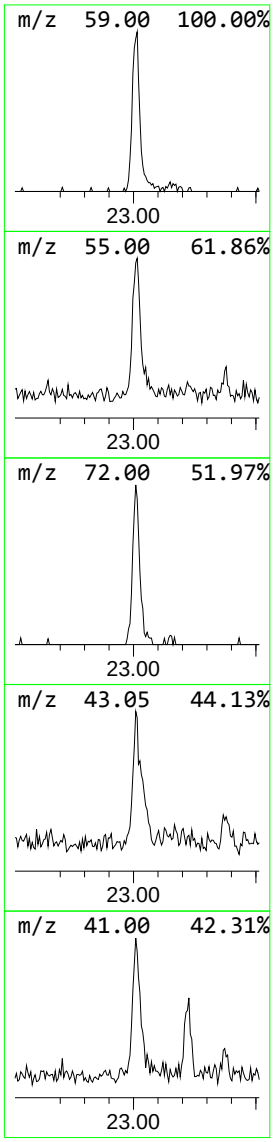
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.015	4.99 ng	129539	Chrysene-d12	21.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	9-Octadecenamide	281	C18H35NO	003322-62-1	90
3	Octadecanamide	283	C18H37NO	000124-26-5	90
4	Hexadecanamide	255	C16H33NO	000629-54-9	76
5	Palmitoleamide	253	C16H31NO	106010-22-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050924\
Data File : BG061151.D
Acq On : 9 May 2024 14:48
Operator : MA/JU
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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.150	55.0	ng	414118	1	7.926	150564	20.0
unknown3.673	3.673	5.6	ng	42290	1	7.926	150564	20.0
1-Phenoxypropan...	11.458	2.7	ng	27176	2	10.723	200971	20.0
unknown14.760	14.760	2.3	ng	32760	3	14.560	289156	20.0
unknown14.777	14.777	3.0	ng	43667	3	14.560	289156	20.0
Tridecanoic acid	18.209	2.9	ng	54615	4	17.310	380331	20.0
Hexadecyl propy...	21.240	3.0	ng	78439	5	21.569	519066	20.0
9-Octadecenamid...	23.015	5.0	ng	129539	5	21.569	519066	20.0