LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051024\
Data File : BG061166.D
Acq On : 10 May 2024 16:57
Operator : MA/JU
Sample : P2423-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-HH

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: BG061166.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.070	9	14	22	rBV7	10585	25541	1.54%	0.304%
2	3.152	22	28	40	rVB	211277	355497	21.38%	4.236%
3	3.669	110	116	124	rBV	21537	35159	2.11%	0.419%
4	5.526	425	432	442	rVB	371165	594918	35.78%	7.088%
5	7.106	694	701	716	rBV	416290	709727	42.69%	8.456%
6	7.929	834	841	848	rBV	101147	169374	10.19%	2.018%
7	9.086	1030	1038	1046	rBV	256806	457291	27.51%	5.448%
8	10.726	1309	1317	1326	rBV	133535	239517	14.41%	2.854%
9	13.182	1727	1735	1745	rBV	697371	1075286	64.68%	12.811%
10	14.556	1963	1969	1977	rBV	211016	332793	20.02%	3.965%
11	16.049	2217	2223	2234	rBV	600644	931115	56.01%	11.094%
12	17.306	2431	2437	2443	rBV	275915	416912	25.08%	4.967%
13	18.211	2587	2591	2598	rBV2	32882	56441	3.39%	0.672%
14	19.927	2877	2883	2891	rBV	1328467	1662520	100.00%	19.808%
15	20.244	2933	2937	2941	rVB2	18069	22203	1.34%	0.265%
16	20.731	3016	3020	3024	rBV2	22951	31867	1.92%	0.380%
17	21.231	3100	3105	3113	rBV2	64927	122950	7.40%	1.465%
18	21.566	3155	3162	3174	rVB	292415	496370	29.86%	5.914%
19	21.766	3192	3196	3200	rBV	28335	41824	2.52%	0.498%
20	22.365	3293	3298	3305	rBV2	26927	45991	2.77%	0.548%
21	23.005	3402	3407	3410	rBV3	29643	55814	3.36%	0.665%
22	23.223	3439	3444	3450	rVB7	15453	29788	1.79%	0.355%
23	24.692	3685	3694	3709	rBV	142429	484317	29.13%	5.770%

Sum of corrected areas: 8393215

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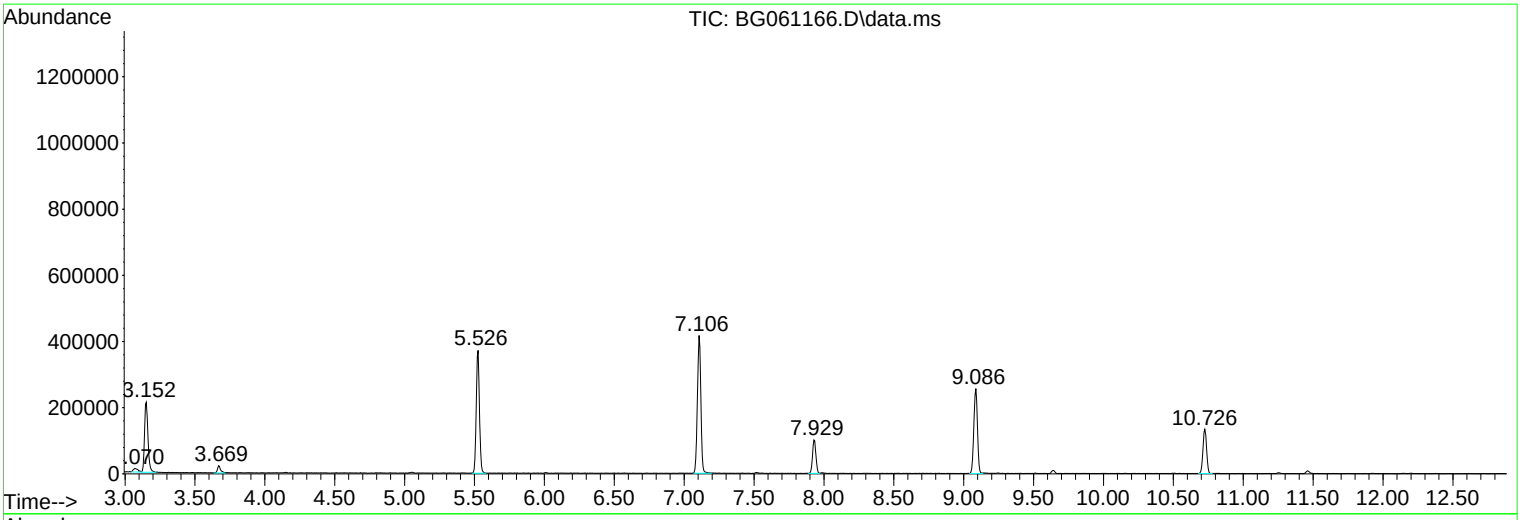
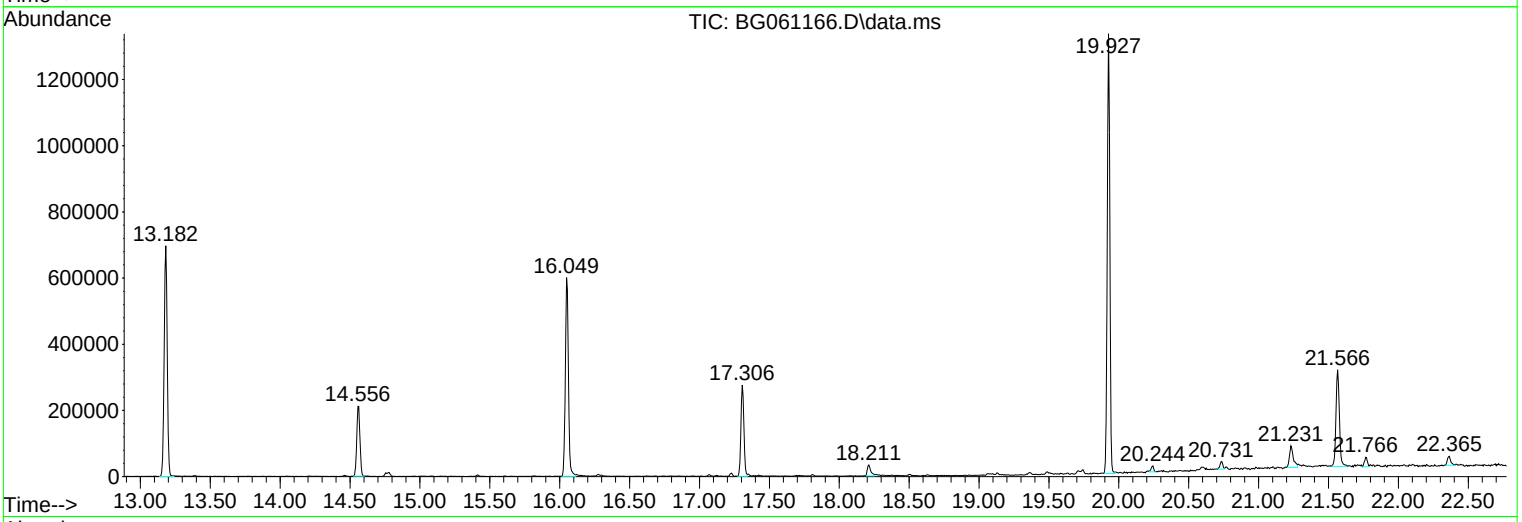
Misc :
ALS Vial : 8 Sample Multiplier: 1

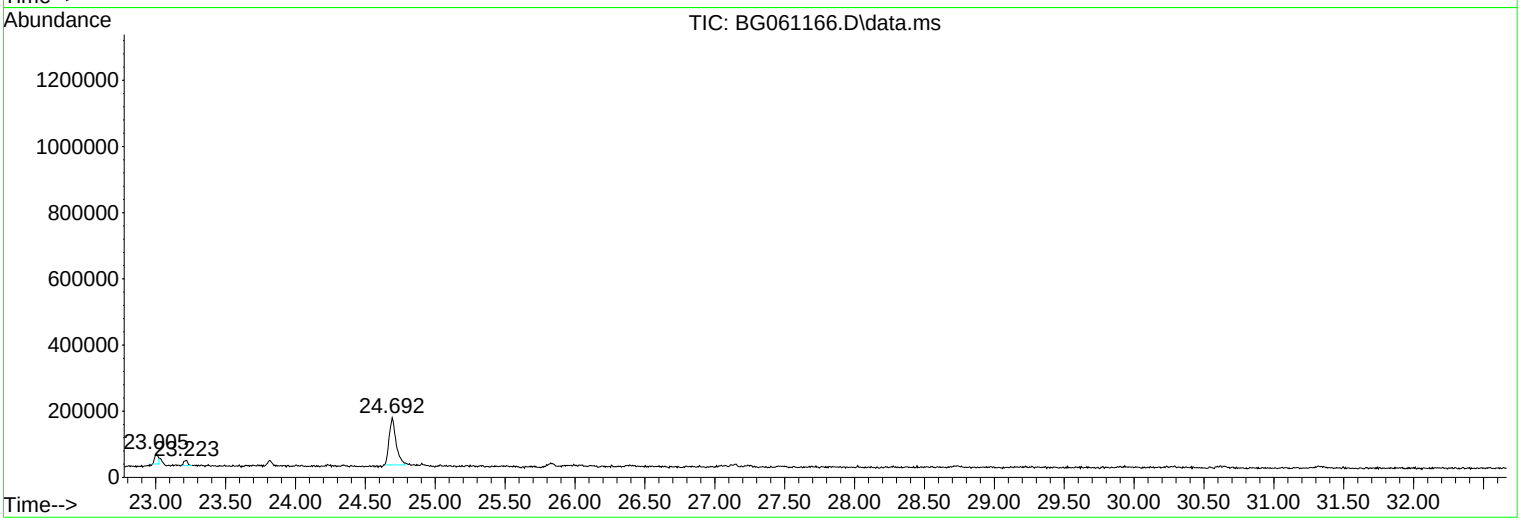
Instrument :
BNA_G
ClientSampleId :
WC-HH

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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Data File : BG061166.D
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Operator : MA/JU
Sample : P2423-05
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

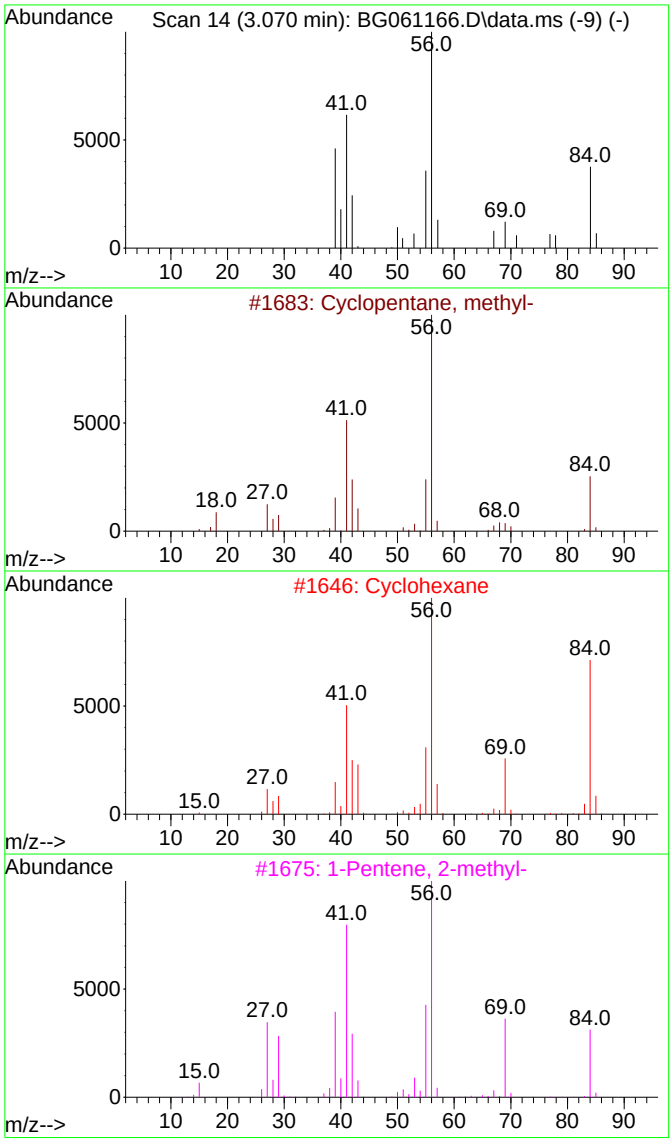
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

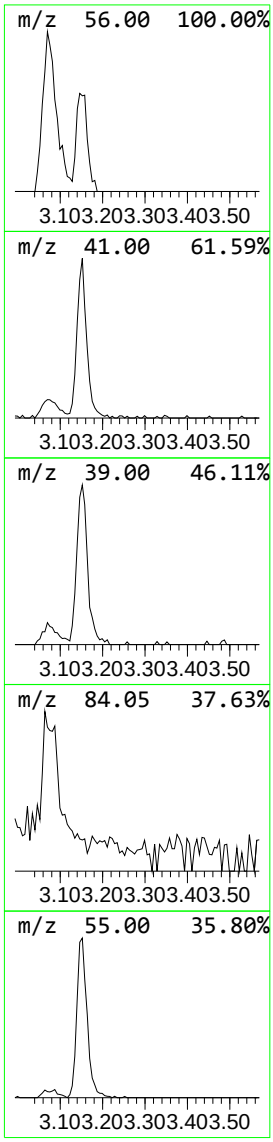
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.070	3.02 ng	25541	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	50
2	Cyclohexane	84	C6H12	000110-82-7	50
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
4	2-Amino-oxazole	84	C3H4N2O	004570-45-0	40
5	Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	37





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Acq On : 10 May 2024 16:57
Operator : MA/JU
Sample : P2423-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-HH

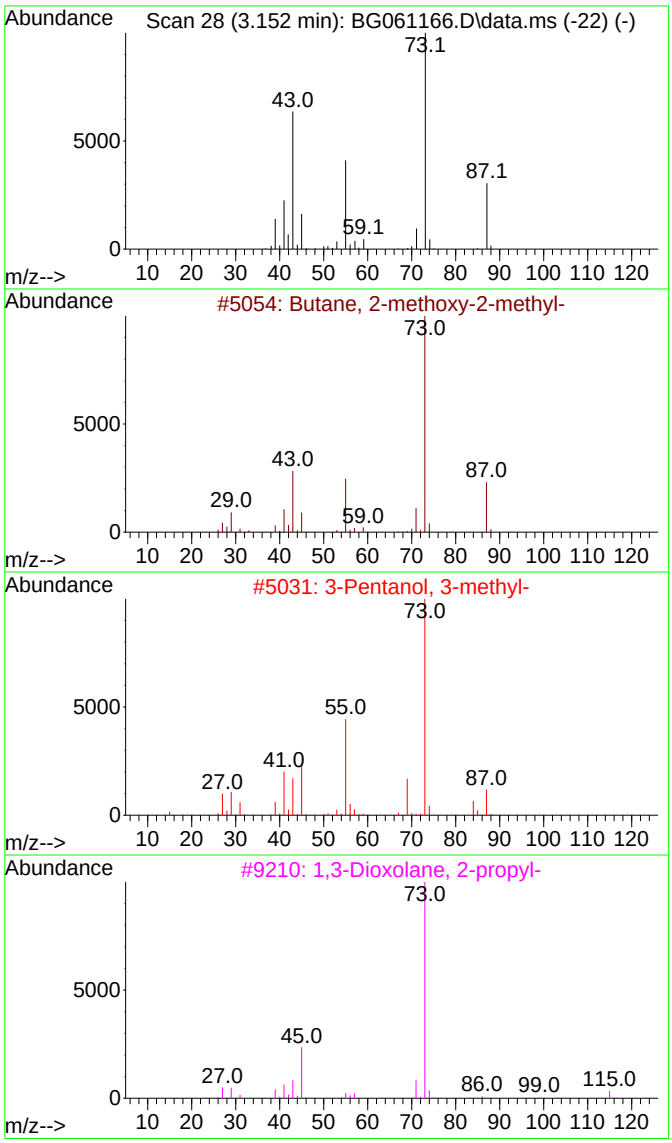
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

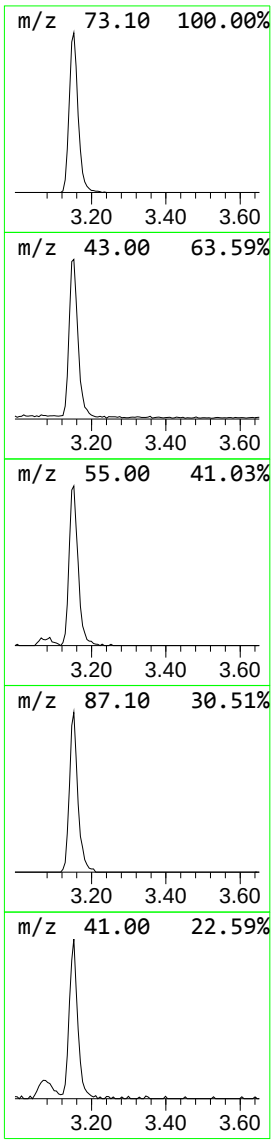
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	41.98 ng	355497	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	72
2	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
3	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	9





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Acq On : 10 May 2024 16:57
Operator : MA/JU
Sample : P2423-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-HH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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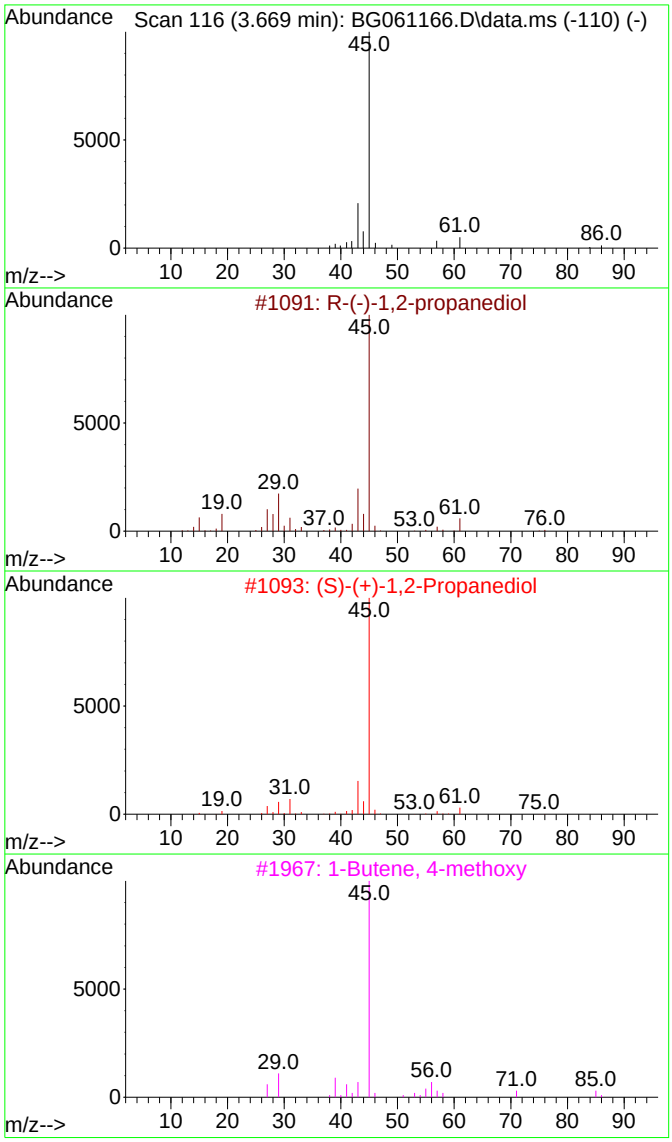
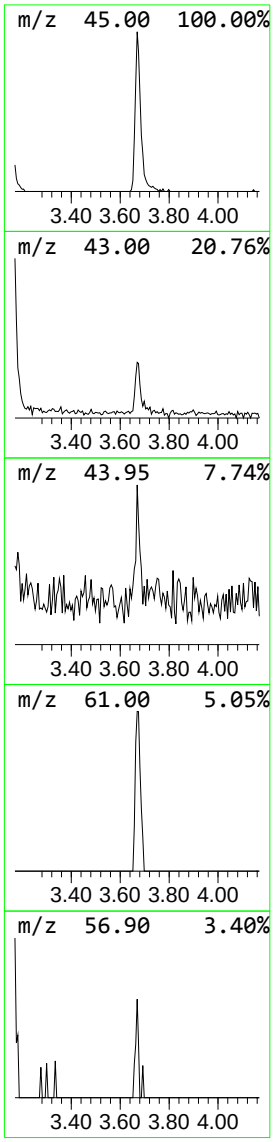
Peak Number 3 unknown3.669 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.669	4.15 ng	35159	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	2-Pentanol	88	C5H12O	006032-29-7	9





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Data File : BG061166.D
Acq On : 10 May 2024 16:57
Operator : MA/JU
Sample : P2423-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-HH

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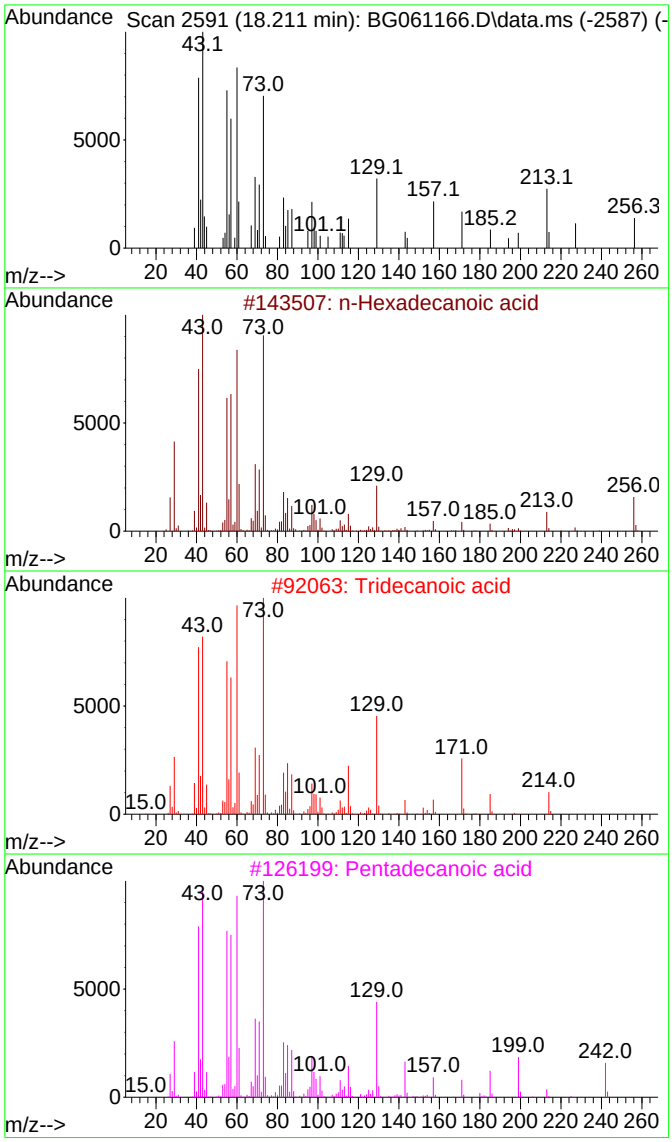
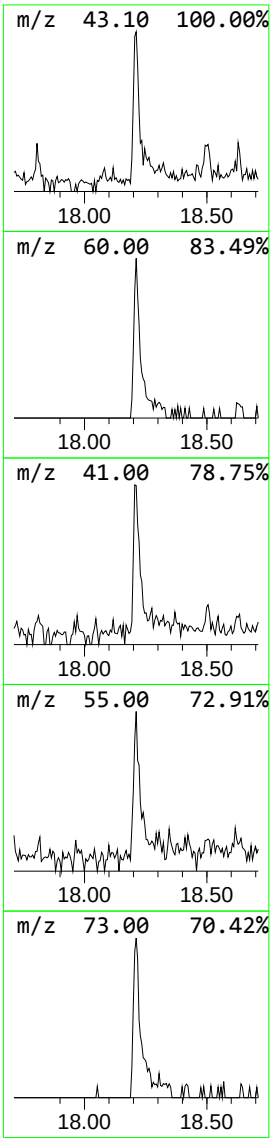
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	2.71 ng	56441	Phenanthrene-d10	17.306

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43





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Operator : MA/JU
Sample : P2423-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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TIC Library : C:\Database\NIST20.L
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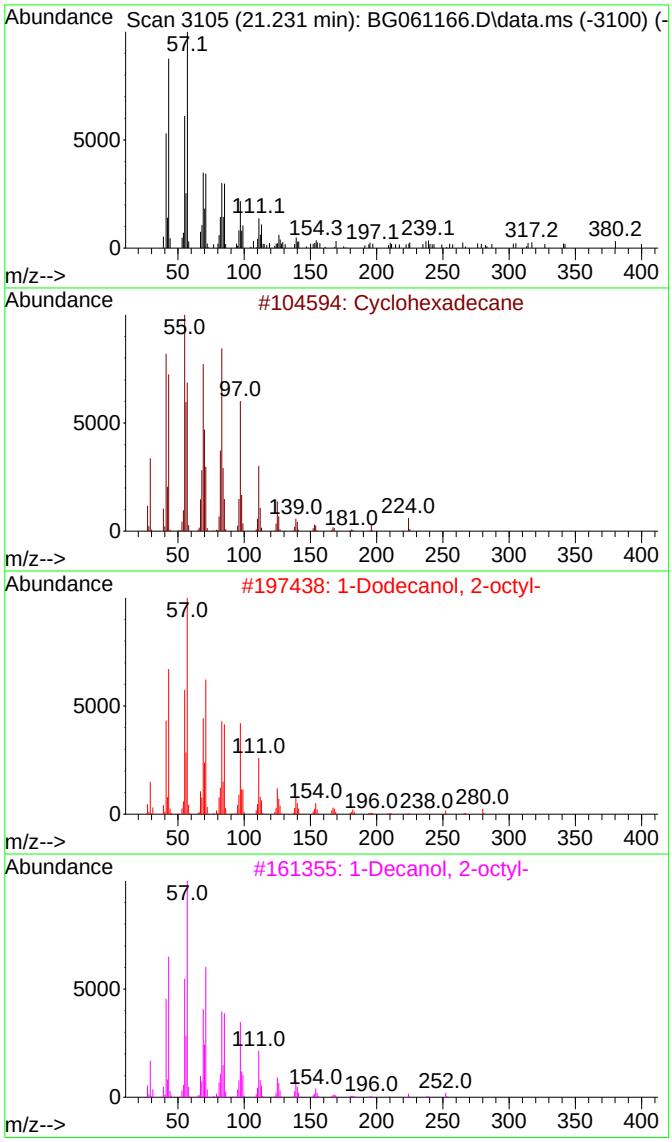
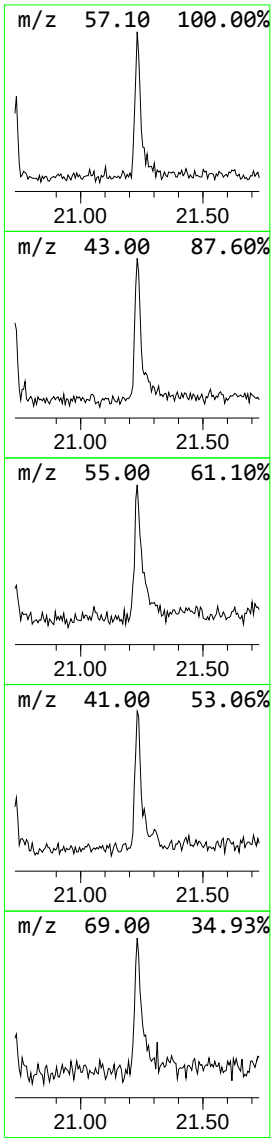
Peak Number 5 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.231	4.95 ng	122950	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	87
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87
3	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	83
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	83
5	Cetene	224	C16H32	000629-73-2	64





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

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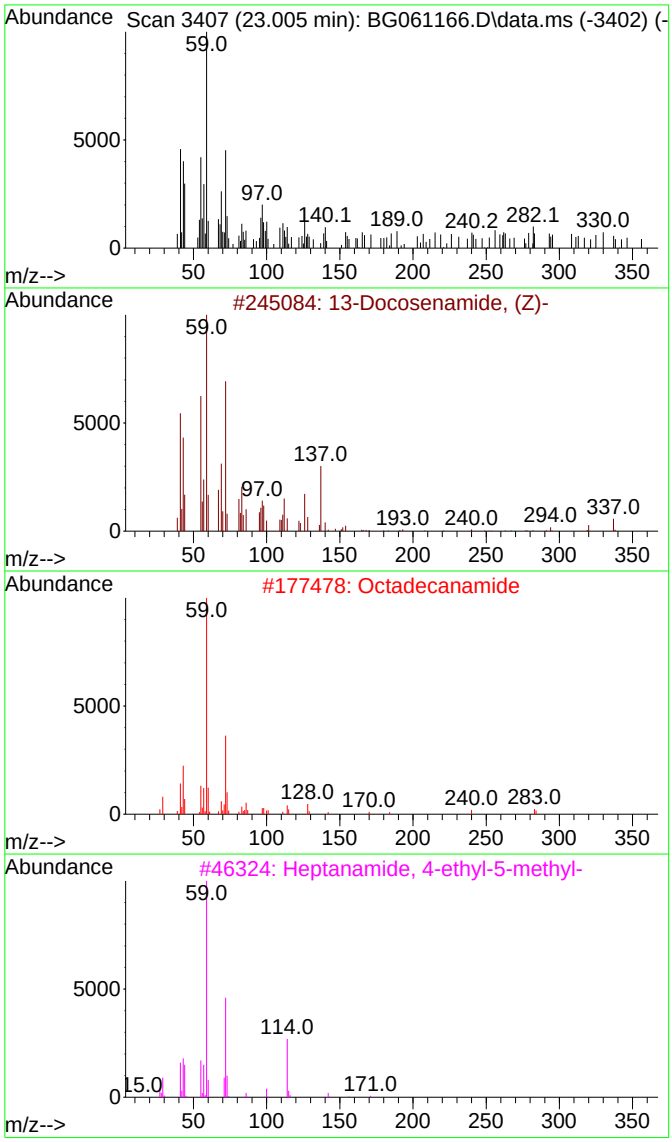
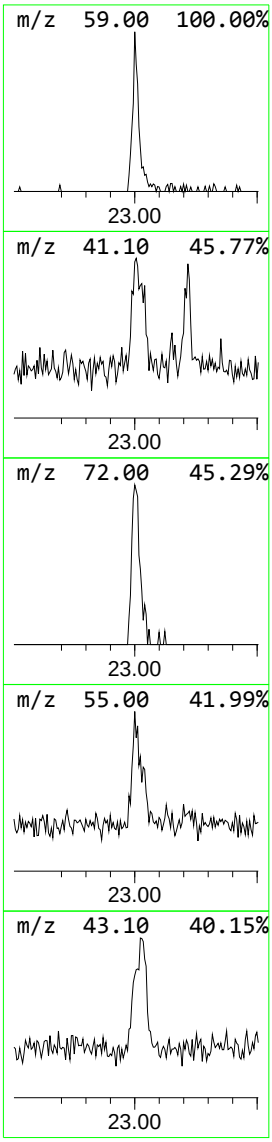
Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.005	2.25 ng	55814	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	86
2	Octadecanamide	283	C18H37NO	000124-26-5	70
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53
4	Dodecanamide	199	C12H25NO	001120-16-7	53
5	Hexadecanamide	255	C16H33NO	000629-54-9	53





Tentatively Identified Compound (LSC) summary

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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, m...	3.070	3.0	ng	25541	1	7.935	169374	20.0
Butane, 2-metho...	3.152	42.0	ng	355497	1	7.935	169374	20.0
unknown3.669	3.669	4.2	ng	35159	1	7.935	169374	20.0
n-Hexadecanoic ...	18.211	2.7	ng	56441	4	17.306	416912	20.0
Cyclohexadecane	21.231	5.0	ng	122950	5	21.566	496370	20.0
13-Docosenamide...	23.005	2.3	ng	55814	5	21.566	496370	20.0