LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061108.D
Acq On : 3 May 2024 16:09
Operator : MA/JU
Sample : P2354-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : V359

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: BG061108.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.071	10	14	22	rBV4	11561	26571	4.12%	0.457%
2	3.153	22	28	39	rVB	215032	352988	54.69%	6.070%
3	5.057	344	352	359	rBV	91980	135967	21.07%	2.338%
4	5.527	423	432	443	rVB	223721	365395	56.62%	6.283%
5	7.107	693	701	712	rBV	315045	572684	88.74%	9.847%
6	7.225	715	721	727	rVB4	4847	9383	1.45%	0.161%
7	7.936	834	842	848	rBV2	100538	171320	26.55%	2.946%
8	9.087	1031	1038	1048	rVB	194619	340869	52.82%	5.861%
9	9.634	1124	1131	1137	rVB4	6854	13205	2.05%	0.227%
10	10.498	1271	1278	1284	rBV2	17154	30579	4.74%	0.526%
11	10.727	1309	1317	1323	rBV	133615	234124	36.28%	4.026%
12	10.774	1323	1325	1331	rVB3	5343	6807	1.05%	0.117%
13	11.467	1438	1443	1450	rVB4	6560	11576	1.79%	0.199%
14	12.219	1565	1571	1578	rVB2	14396	24497	3.80%	0.421%
15	13.183	1729	1735	1743	rBV	335316	488212	75.65%	8.395%
16	14.563	1959	1970	1976	rBV	217532	348383	53.98%	5.990%
17	14.775	1999	2006	2012	rBV5	9979	24661	3.82%	0.424%
18	16.050	2216	2223	2232	rBV	315253	499167	77.34%	8.583%
19	16.308	2263	2267	2274	rVB5	8764	14828	2.30%	0.255%
20	17.125	2401	2406	2415	rVB5	6632	13108	2.03%	0.225%
21	17.313	2432	2438	2443	rBV	279399	421805	65.36%	7.253%
22	17.348	2443	2444	2449	rVB	13058	14598	2.26%	0.251%
23	18.212	2583	2591	2600	rBV4	35053	69896	10.83%	1.202%
24	19.364	2783	2787	2793	rVB2	11111	17864	2.77%	0.307%
25	19.487	2804	2808	2812	rBV7	8108	11103	1.72%	0.191%
26	19.722	2845	2848	2857	rVB	14375	33035	5.12%	0.568%
27	19.810	2857	2863	2864	rBV5	4570	8072	1.25%	0.139%
28	19.928	2878	2883	2889	rVB	497143	645381	100.00%	11.097%
29	20.245	2935	2937	2941	rVB5	7183	9650	1.50%	0.166%
30	21.244	3104	3107	3111	rVB5	12310	16423	2.54%	0.282%
31	21.567	3155	3162	3169	rBV	283348	497626	77.11%	8.557%
32	22.372	3297	3299	3303	rVB5	11376	10597	1.64%	0.182%
33	23.964	3567	3570	3571	rBV3	6229	7019	1.09%	0.121%
34	24.693	3686	3694	3707	rBV	113355	352517	54.62%	6.061%
35	28.559	4350	4352	4355	rVB4	7884	7275	1.13%	0.125%
36	30.310	4648	4650	4653	rBV4	6534	8531	1.32%	0.147%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061108.D
Acq On : 3 May 2024 16:09
Operator : MA/JU
Sample : P2354-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
V359

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

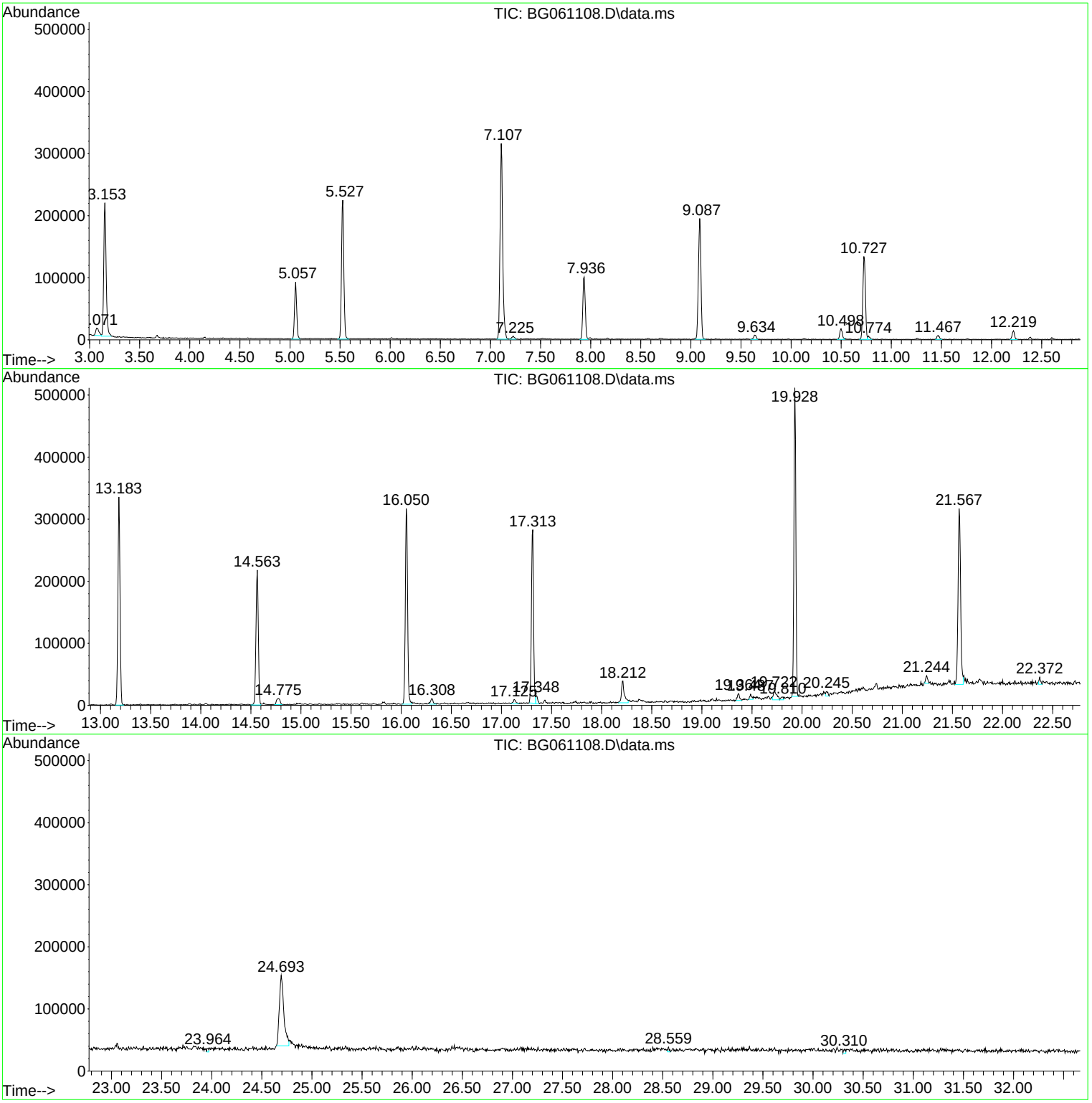
Sum of corrected areas: 5815716

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061108.D
Acq On : 3 May 2024 16:09
Operator : MA/JU
Sample : P2354-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
V359

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 : BG061108.D
Acq On : 3 May 2024 16:09
Operator : MA/JU
Sample : P2354-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
V359

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

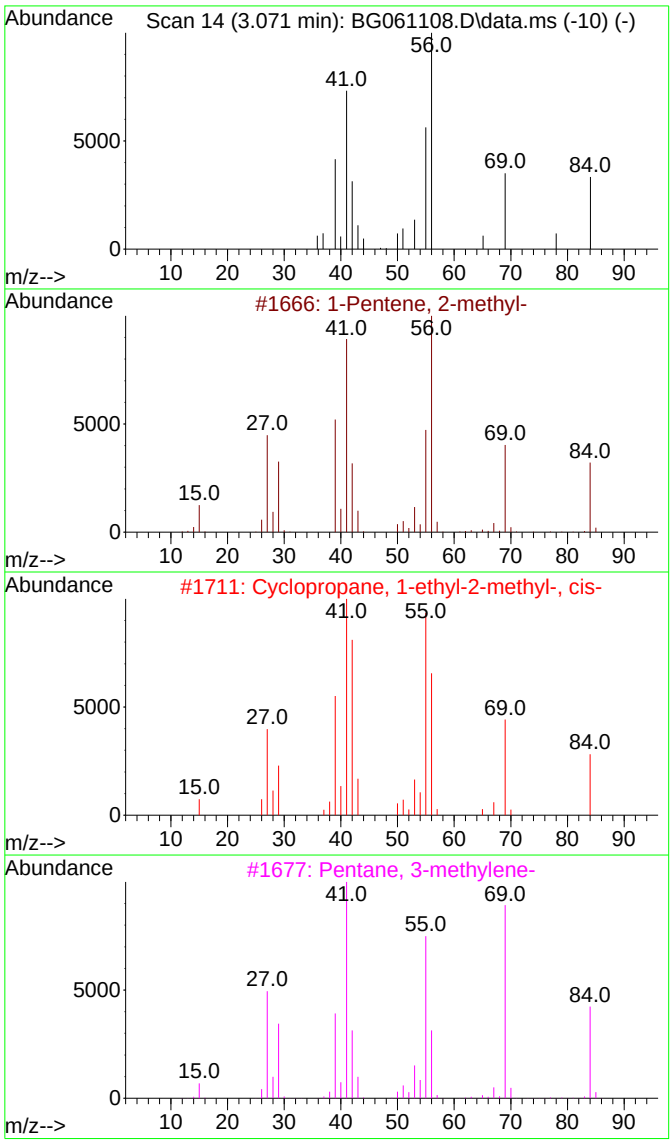
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

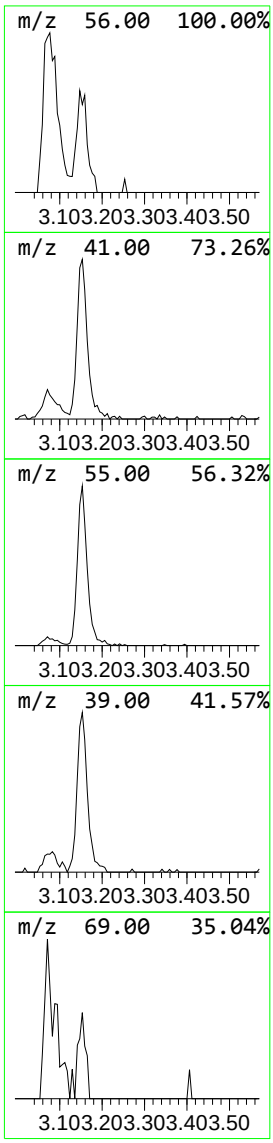
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.071	3.10 ng	26571	1,4-Dichlorobenzene-d4	7.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	91
2	Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	64
3	Pentane, 3-methylene-	84	C6H12	000760-21-4	50
4	3-Hexene, (Z)-	84	C6H12	007642-09-3	49
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061108.D
Acq On : 3 May 2024 16:09
Operator : MA/JU
Sample : P2354-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
V359

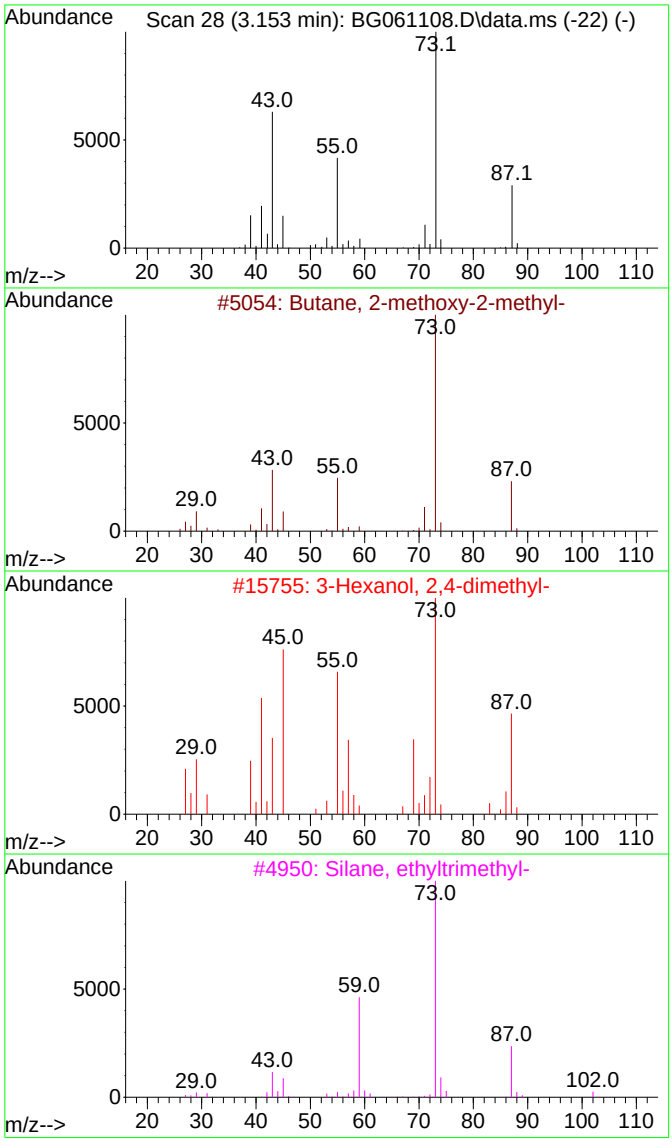
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

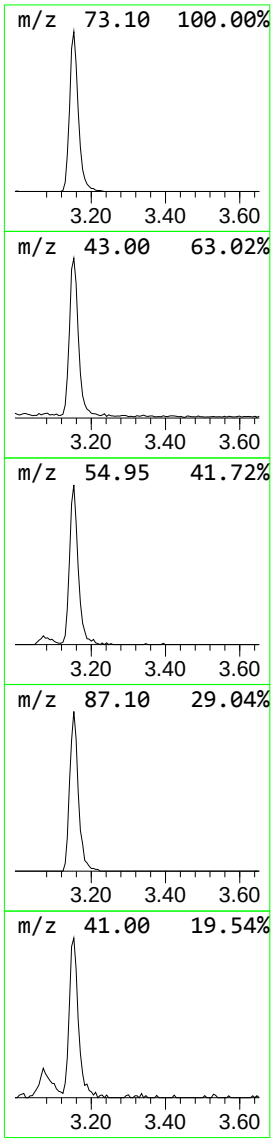
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.153	41.21 ng	352988	1,4-Dichlorobenzene-d4	7.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	36
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061108.D
Acq On : 3 May 2024 16:09
Operator : MA/JU
Sample : P2354-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
V359

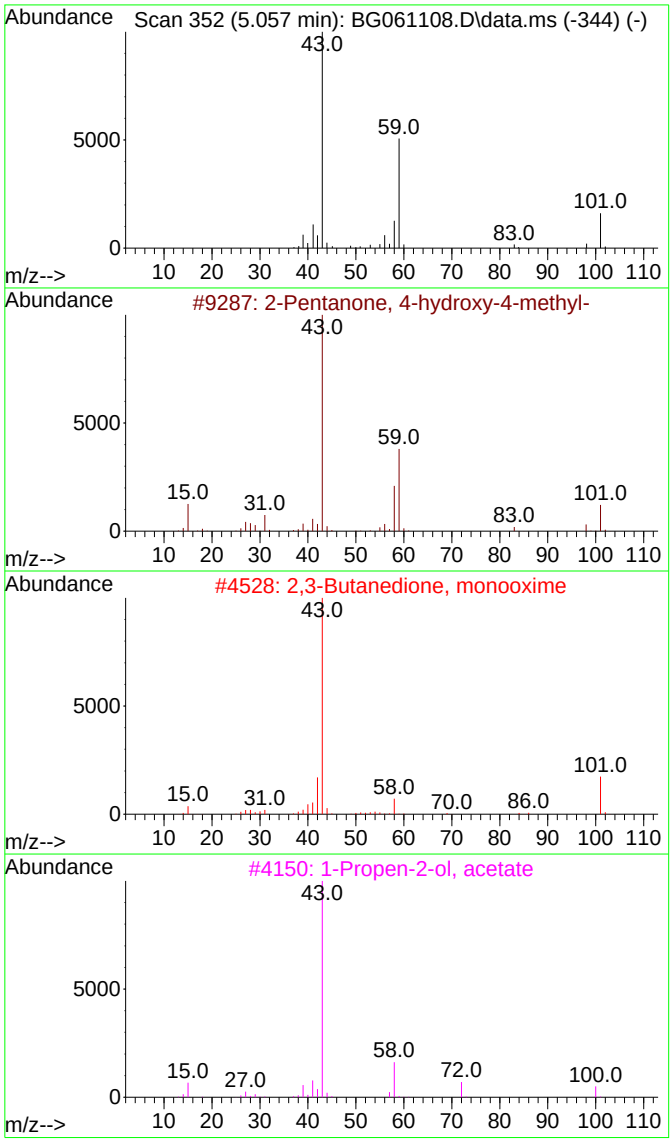
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

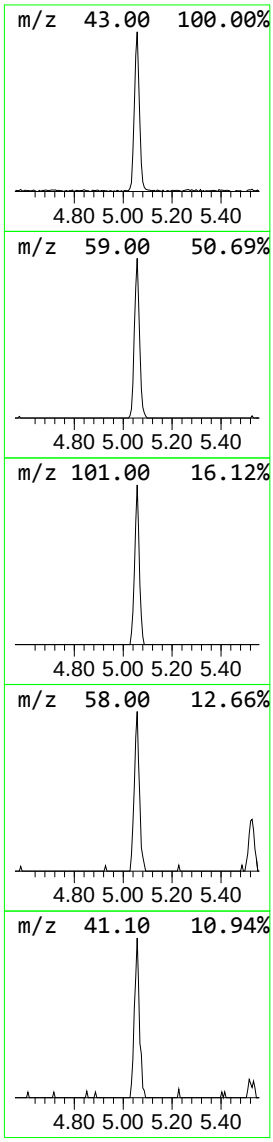
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	15.87 ng	135967	1,4-Dichlorobenzene-d4	7.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
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Operator : MA/JU
Sample : P2354-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
V359

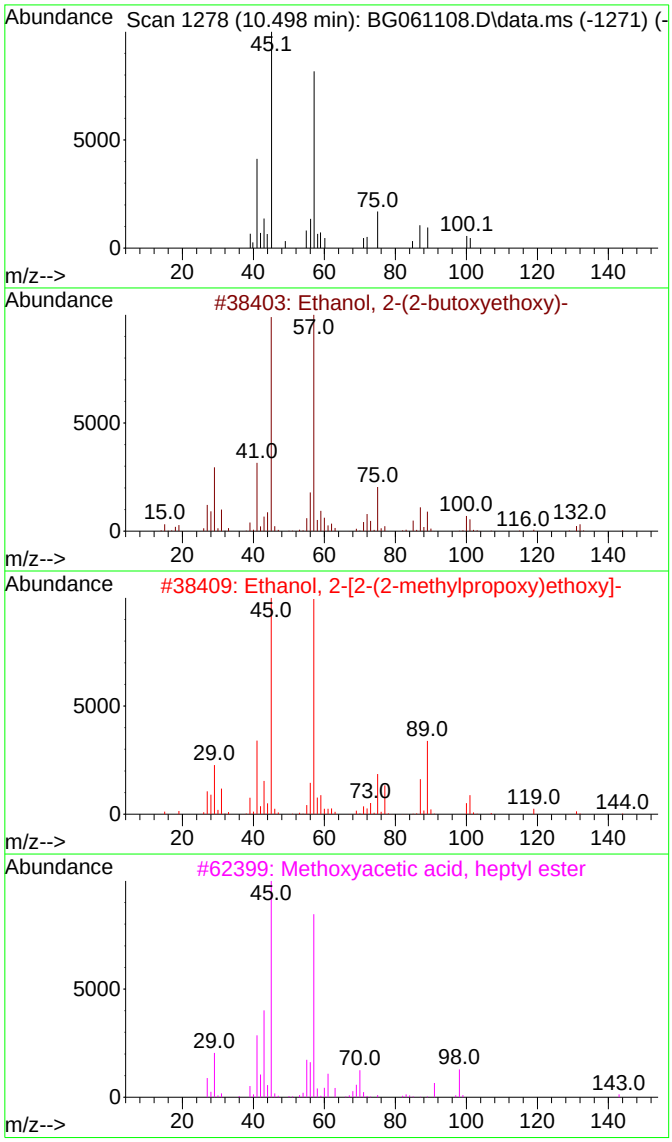
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

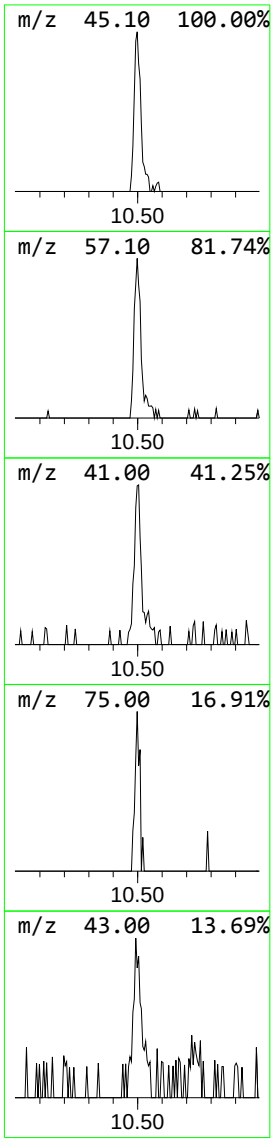
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.498	2.61 ng	30579	Naphthalene-d8	10.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
3	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50
4	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	38
5	2-Hexanol, 5-methyl-	116	C7H16O	000627-59-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061108.D
Acq On : 3 May 2024 16:09
Operator : MA/JU
Sample : P2354-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
V359

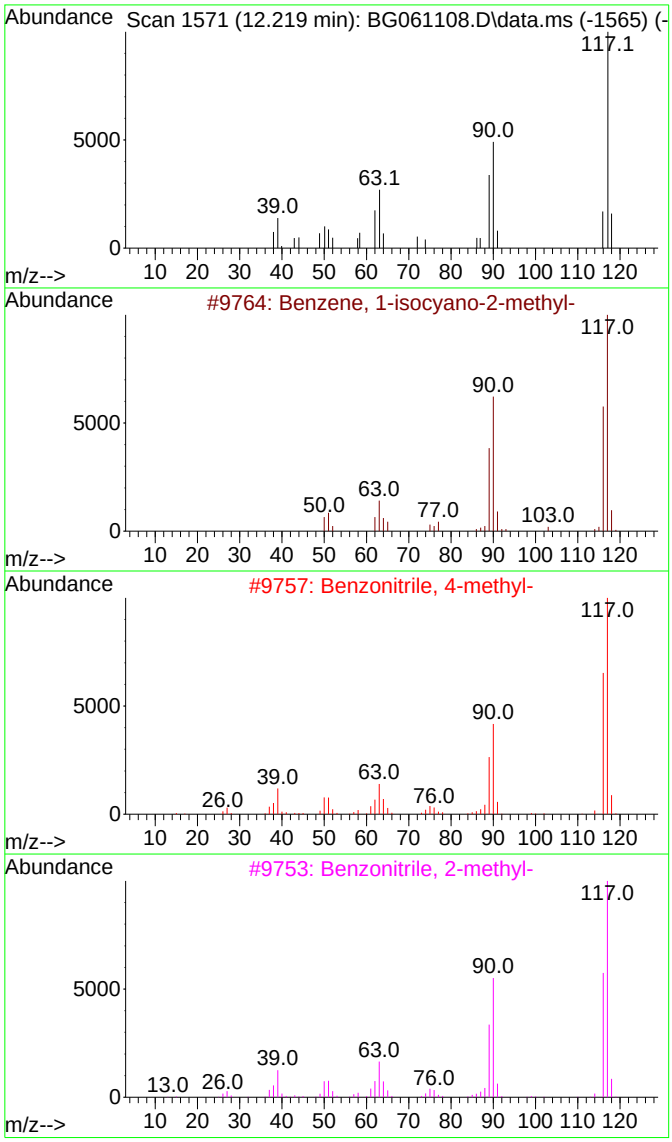
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

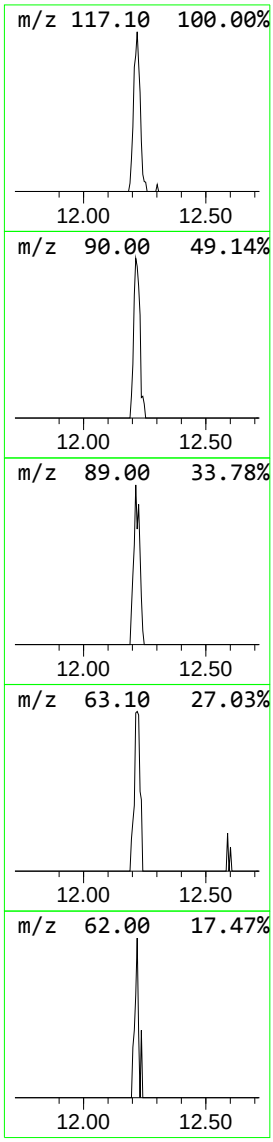
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-isocyano-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	2.09 ng	24497	Naphthalene-d8	10.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-isocyano-2-methyl-	117	C8H7N	010468-64-1	86
2	Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	86
3	Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	86
4	Indolizine	117	C8H7N	000274-40-8	64
5	Indole	117	C8H7N	000120-72-9	64





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Sample : P2354-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
V359

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

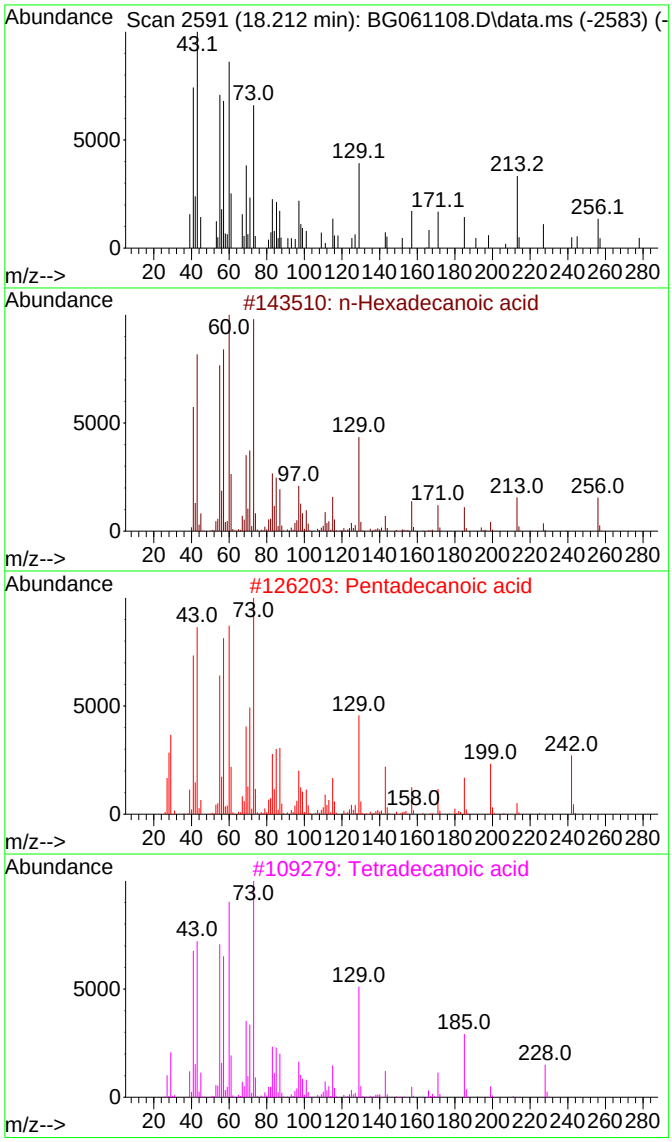
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

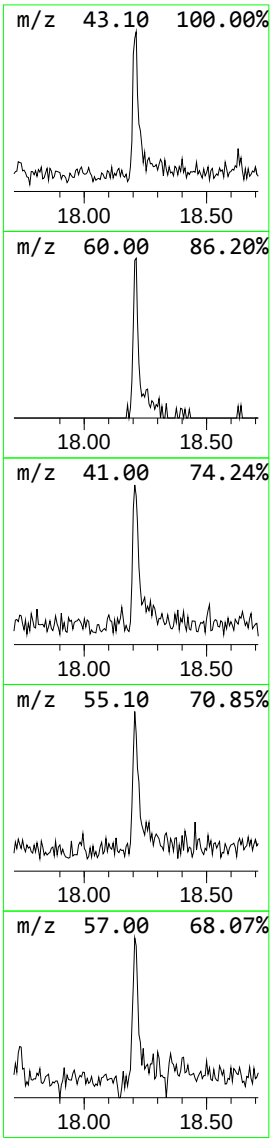
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.212	3.31 ng	69896	Phenanthrene-d10	17.313

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061108.D
Acq On : 3 May 2024 16:09
Operator : MA/JU
Sample : P2354-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
V359

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
1-Pentene, 2-me...	3.071	3.1	ng	26571	1	7.936	171320	20.0
Butane, 2-metho...	3.153	41.2	ng	352988	1	7.936	171320	20.0
2-Pentanone, 4-...	5.057	15.9	ng	135967	1	7.936	171320	20.0
Ethanol, 2-(2-b...	10.498	2.6	ng	30579	2	10.727	234124	20.0
Benzene, 1-isoc...	12.219	2.1	ng	24497	2	10.727	234124	20.0
n-Hexadecanoic ...	18.212	3.3	ng	69896	4	17.313	421805	20.0