LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
Data File : BG055072.D
Acq On : 4 Oct 2022 21:01
Operator : CG/JU
Sample : N4936-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-2-(10-16)

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-BG100322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055072.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.381	11	16	29	rVB	168293	278624	11.59%	2.223%
2	4.774	247	253	262	rVB	48314	72876	3.03%	0.581%
3	5.396	351	359	369	rVB	683522	1077034	44.81%	8.592%
4	5.860	430	438	452	rBV	555615	921601	38.34%	7.352%
5	6.495	539	546	555	rVB	45776	71527	2.98%	0.571%
6	7.470	704	712	722	rBV	645073	1092871	45.47%	8.719%
7	8.346	850	861	873	rVB	122752	213028	8.86%	1.699%
8	9.515	1052	1060	1068	rBV	372827	666610	27.73%	5.318%
9	10.913	1292	1298	1304	rBV	17809	28860	1.20%	0.230%
10	11.172	1335	1342	1349	rBV	170024	312155	12.99%	2.490%
11	13.581	1745	1752	1759	rVB	1139887	1699261	70.70%	13.556%
12	14.950	1978	1985	1992	rVB	285492	444164	18.48%	3.543%
13	16.425	2229	2236	2244	rBV	858849	1311638	54.57%	10.464%
14	17.682	2443	2450	2456	rBV	339657	512267	21.31%	4.087%
15	18.534	2589	2595	2601	rBV	55478	76409	3.18%	0.610%
16	19.474	2746	2755	2759	rBV3	22950	31714	1.32%	0.253%
17	19.791	2805	2809	2816	rBV3	28769	37656	1.57%	0.300%
18	20.261	2882	2889	2894	rBV	1826268	2403517	100.00%	19.175%
19	21.577	3108	3113	3122	rBV	39644	64494	2.68%	0.515%
20	21.977	3174	3181	3188	rBV	309757	548892	22.84%	4.379%
21	23.228	3388	3394	3400	rBV2	26212	52380	2.18%	0.418%
22	23.552	3443	3449	3452	rBV8	13562	31001	1.29%	0.247%
23	24.063	3530	3536	3541	rBV4	12424	25962	1.08%	0.207%
24	25.438	3759	3770	3784	rVB2	181376	560386	23.32%	4.471%

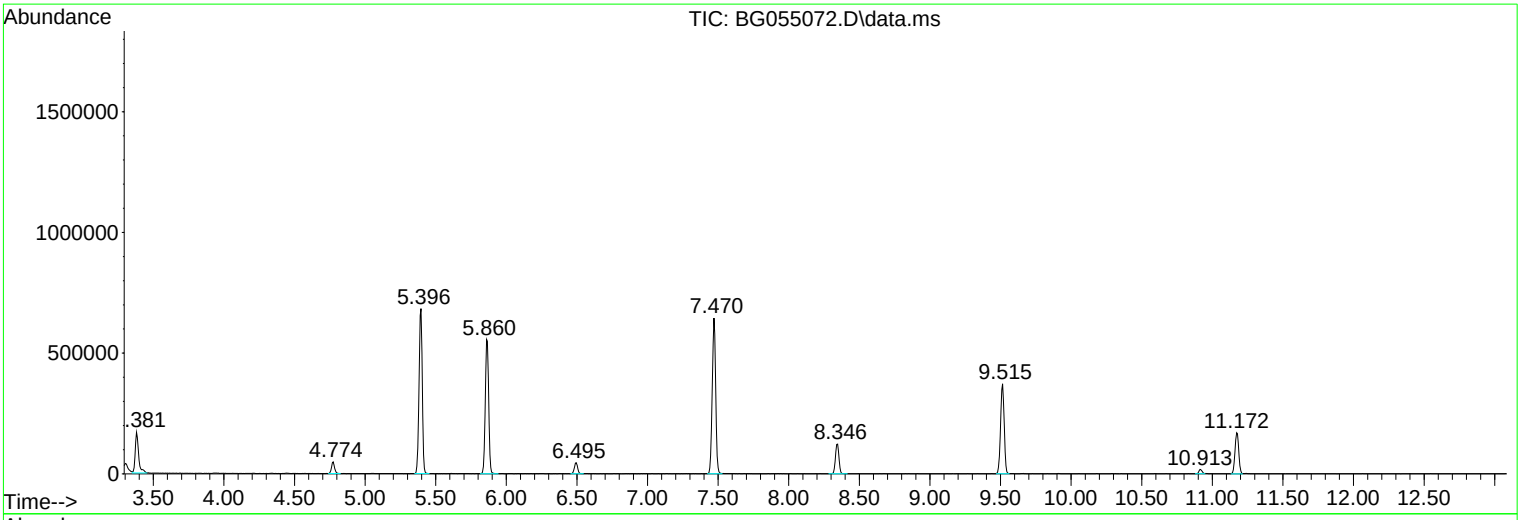
Sum of corrected areas: 12534927

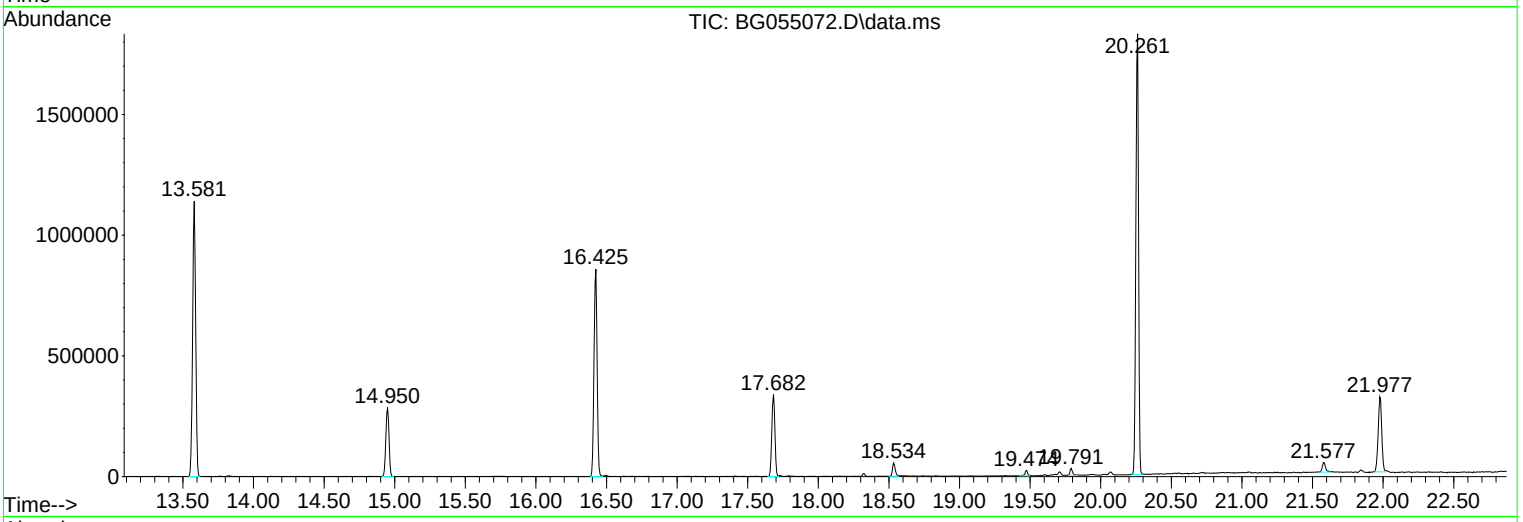
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
Data File : BG055072.D
Acq On : 4 Oct 2022 21:01
Operator : CG/JU
Sample : N4936-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

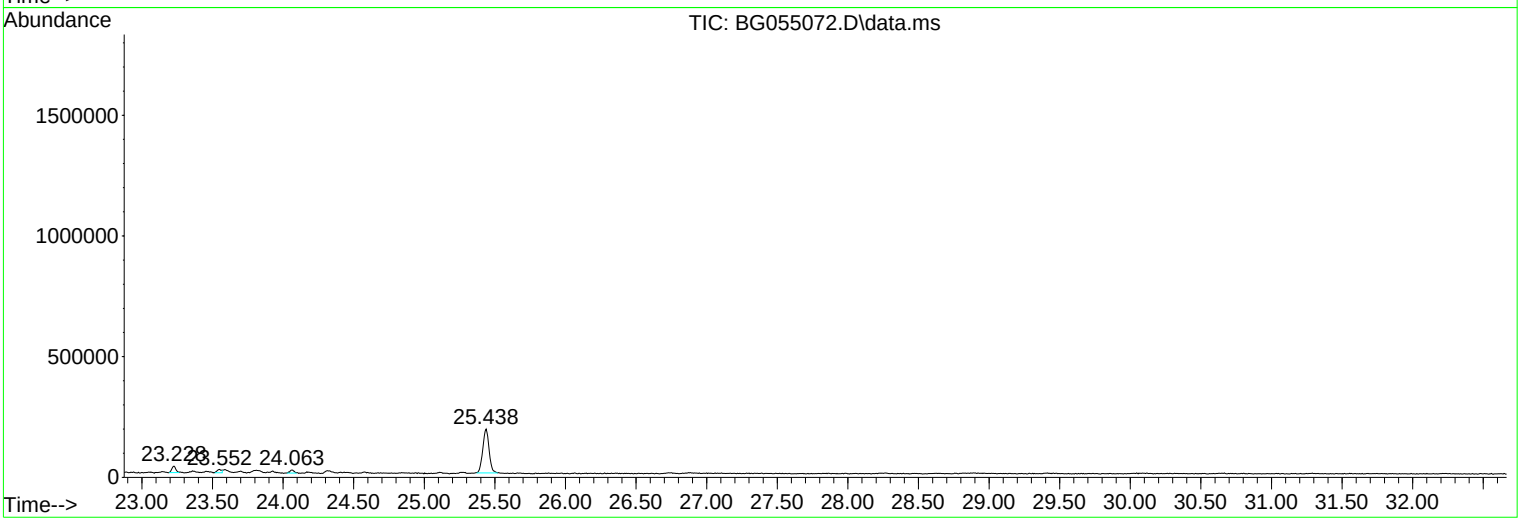
Instrument :
BNA_G
ClientSampleId :
SASP2-T-2-(10-16)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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\BG100422\
Data File : BG055072.D
Acq On : 4 Oct 2022 21:01
Operator : CG/JU
Sample : N4936-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-2-(10-16)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

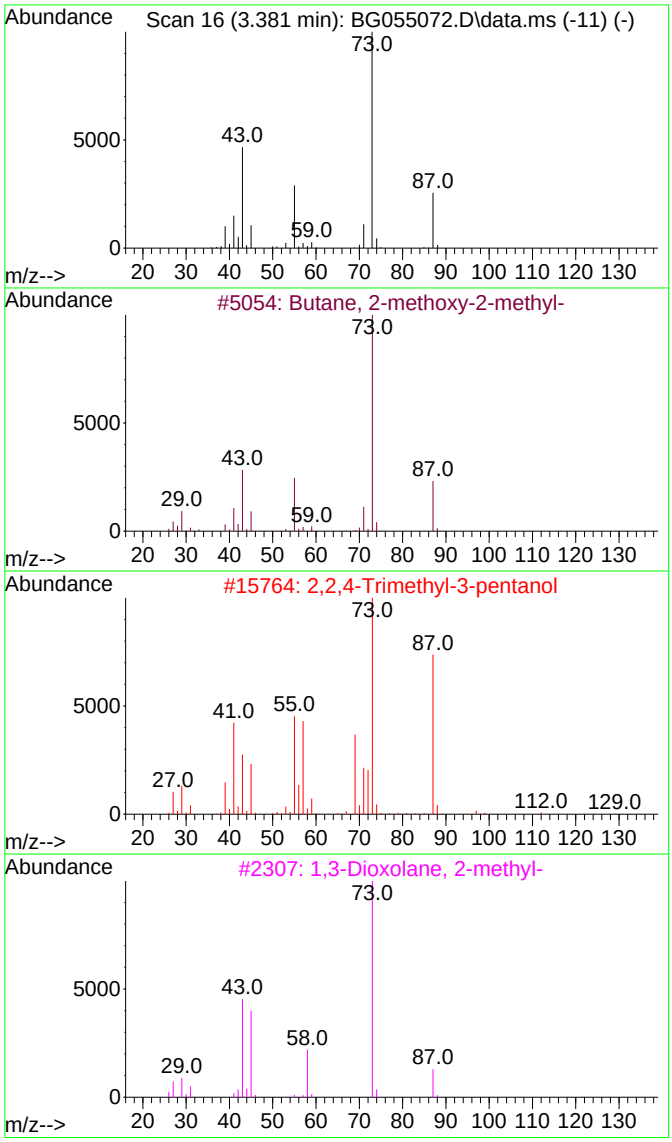
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

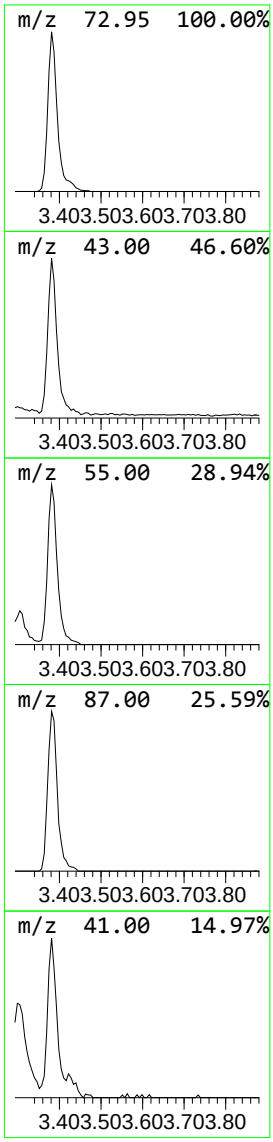
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.381	26.16 ng	278624	1,4-Dichlorobenzene-d4	8.346

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
Data File : BG055072.D
Acq On : 4 Oct 2022 21:01
Operator : CG/JU
Sample : N4936-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-2-(10-16)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

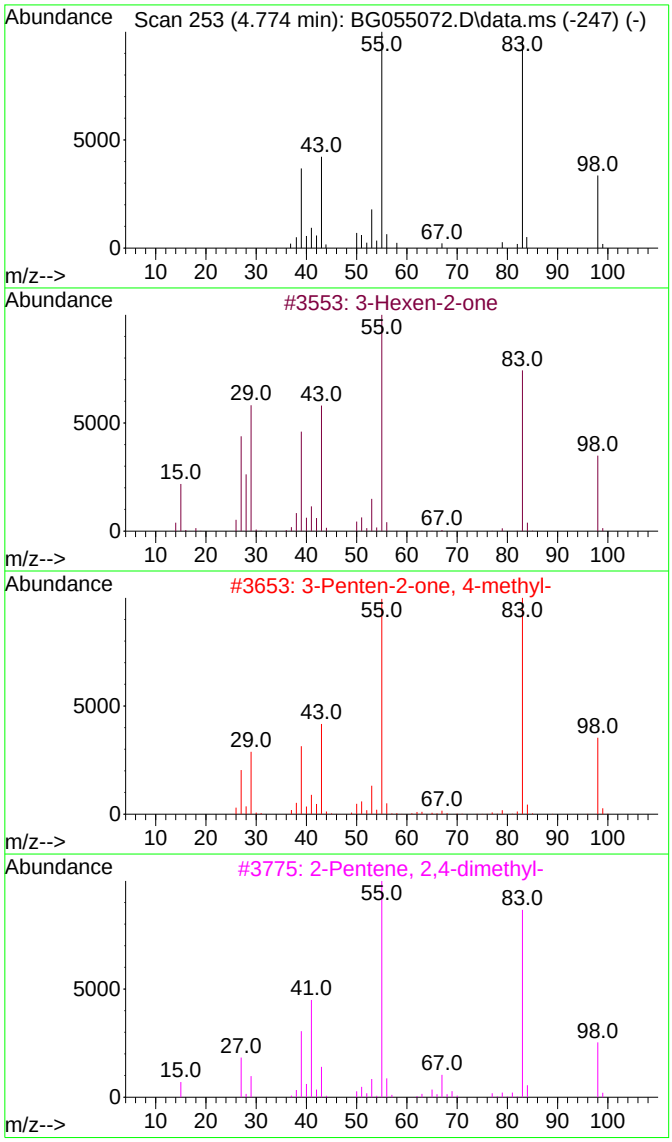
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

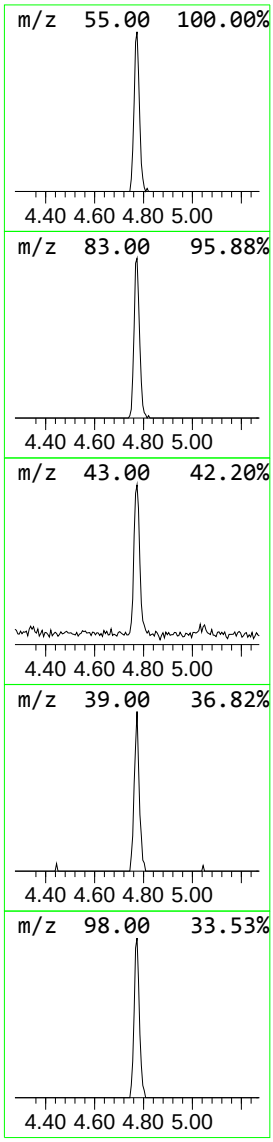
****

Peak Number 2 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.774	6.84 ng	72876	1,4-Dichlorobenzene-d4	8.346

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
Data File : BG055072.D
Acq On : 4 Oct 2022 21:01
Operator : CG/JU
Sample : N4936-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-2-(10-16)

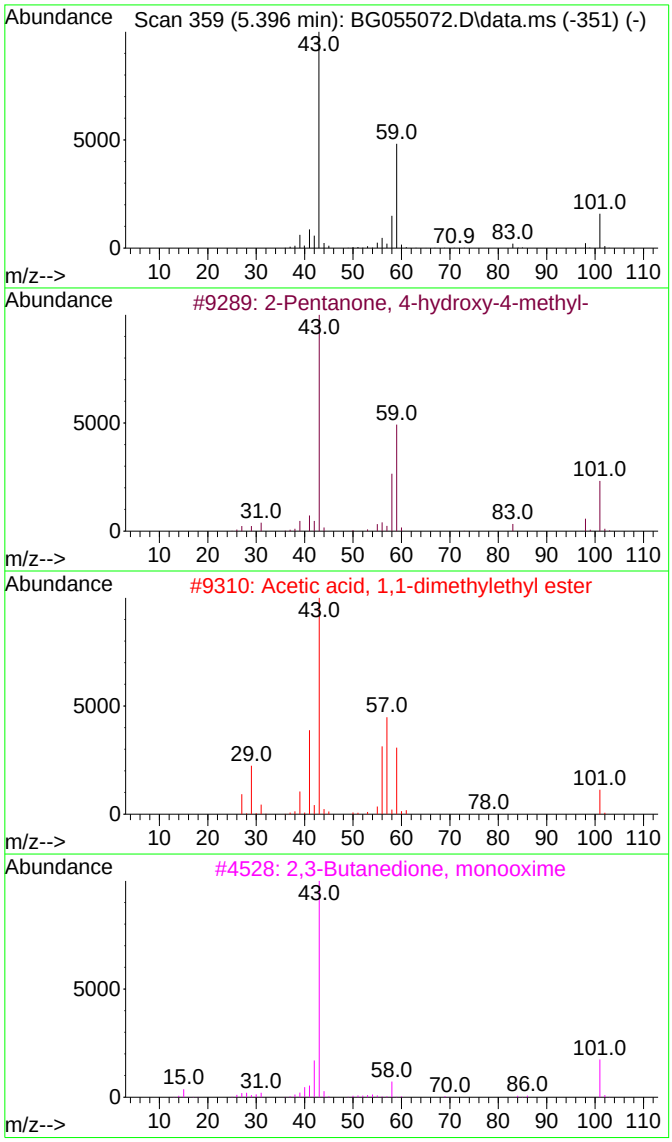
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

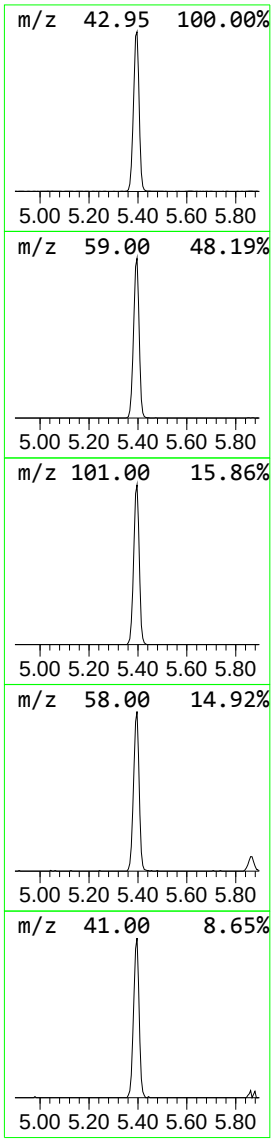
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.396	101.12 ng	1077030	1,4-Dichlorobenzene-d4	8.346

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
Data File : BG055072.D
Acq On : 4 Oct 2022 21:01
Operator : CG/JU
Sample : N4936-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-2-(10-16)

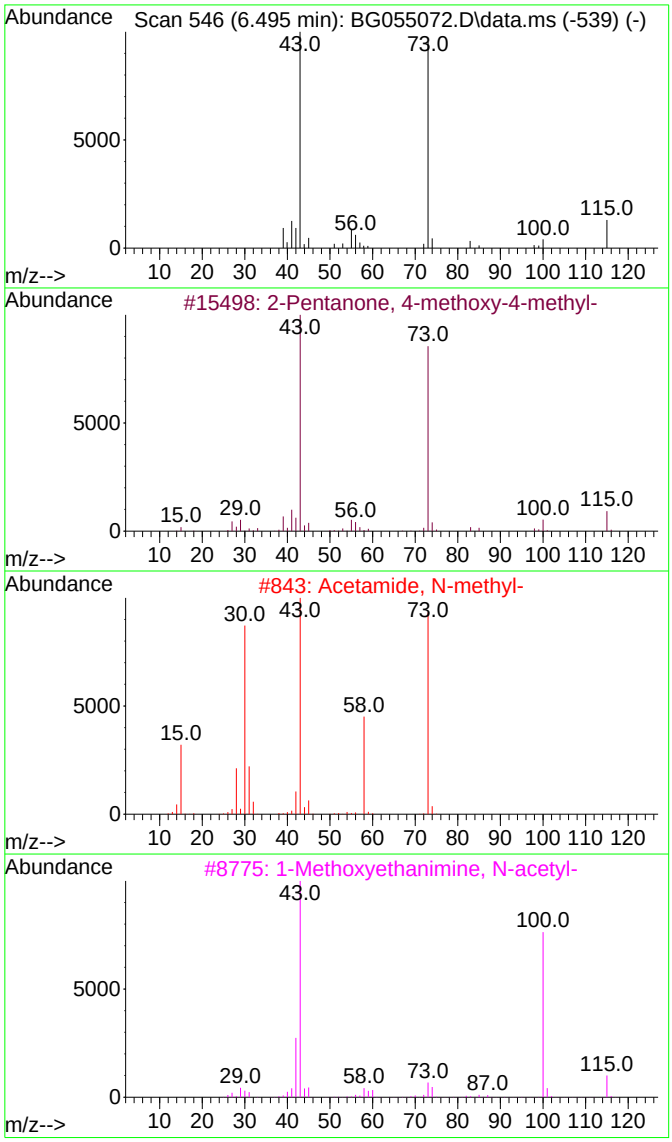
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

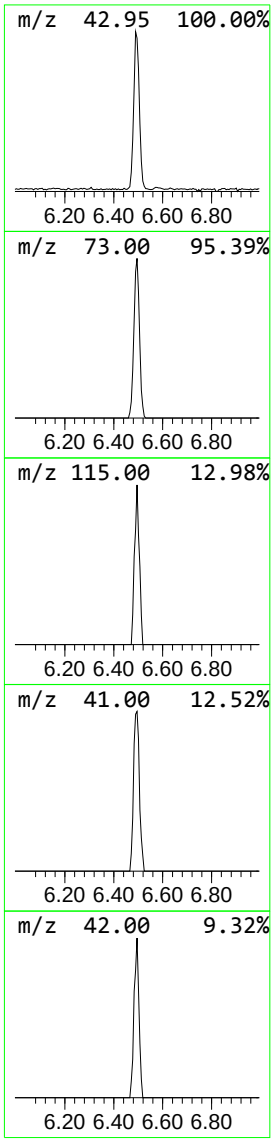
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.495	6.72 ng	71527	1,4-Dichlorobenzene-d4	8.346

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	37
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	37
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	10
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
Data File : BG055072.D
Acq On : 4 Oct 2022 21:01
Operator : CG/JU
Sample : N4936-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-2-(10-16)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

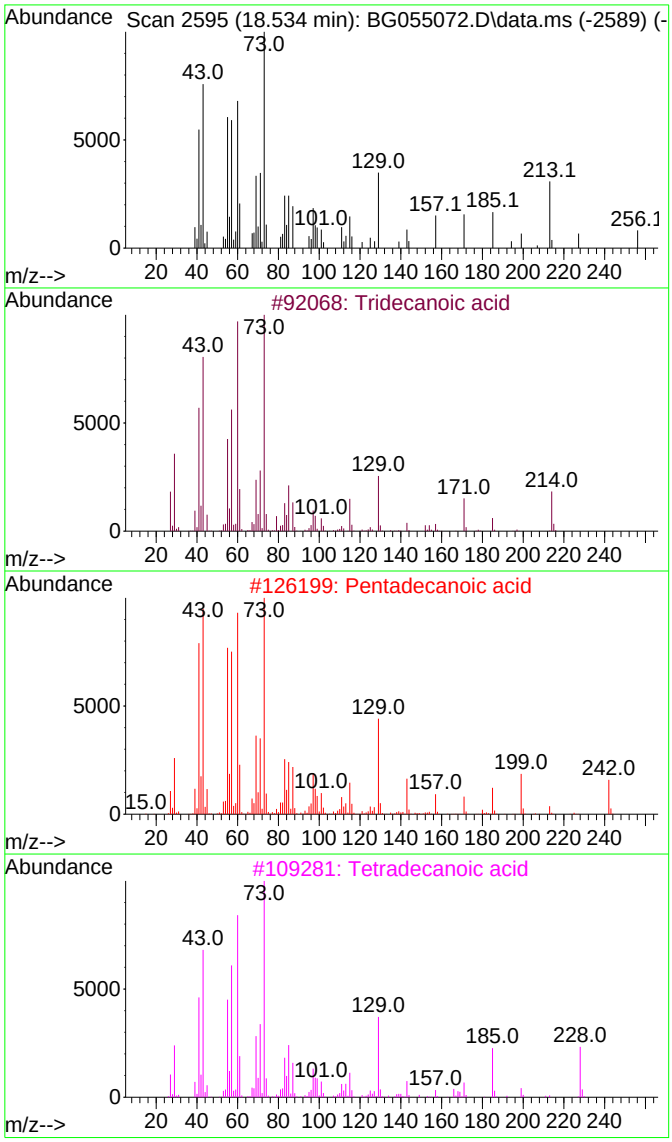
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

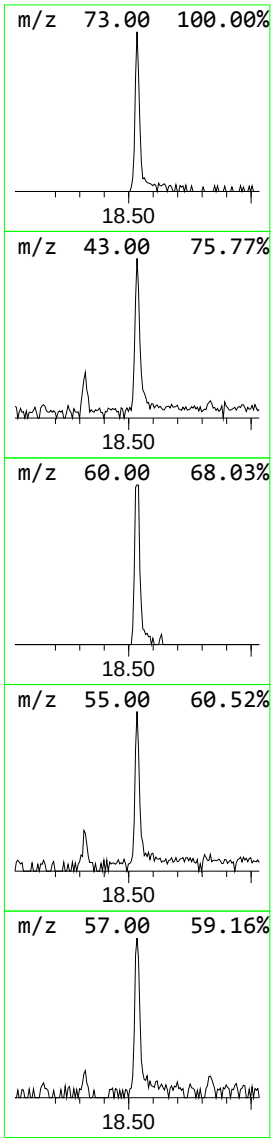
****

Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.534	2.98 ng	76409	Phenanthrene-d10	17.682

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
Data File : BG055072.D
Acq On : 4 Oct 2022 21:01
Operator : CG/JU
Sample : N4936-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-2-(10-16)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

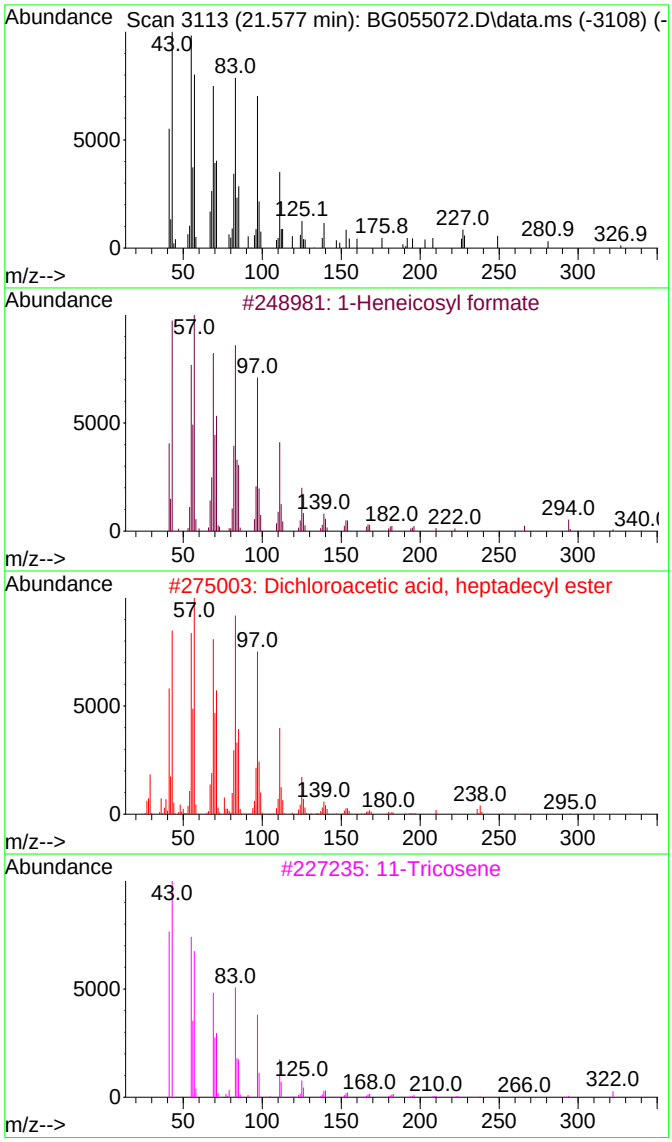
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

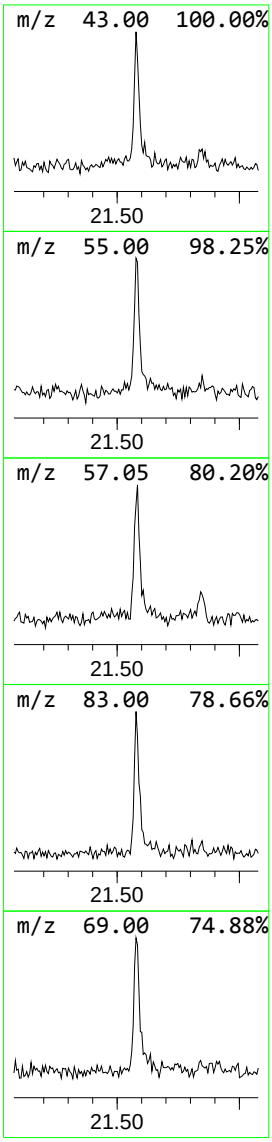
****

Peak Number 6 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.577	2.35 ng	64494	Chrysene-d12	21.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
3	11-Tricosene	322	C23H46	052078-56-5	91
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
5	1-Octadecanol	270	C18H38O	000112-92-5	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
Data File : BG055072.D
Acq On : 4 Oct 2022 21:01
Operator : CG/JU
Sample : N4936-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-2-(10-16)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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...	3.381	26.2	ng	278624	1	8.346	213028	20.0
3-Hexen-2-one	4.774	6.8	ng	72876	1	8.346	213028	20.0
2-Pentanone, 4-...	5.396	101.1	ng	1077030	1	8.346	213028	20.0
2-Pentanone, 4-...	6.495	6.7	ng	71527	1	8.346	213028	20.0
Tridecanoic acid	18.534	3.0	ng	76409	4	17.682	512267	20.0
1-Heneicosyl fo...	21.577	2.4	ng	64494	5	21.977	548892	20.0