LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055557.D
Acq On : 11 Nov 2022 3:09
Operator : CG/JU
Sample : N5494-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-17

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055557.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.330	3	7	24	rVB	249117	456656	16.32%	3.202%
2	4.710	235	242	249	rBV	38676	60650	2.17%	0.425%
3	5.327	340	347	356	rBV	292915	470316	16.81%	3.298%
4	5.792	419	426	439	rBV	726660	1197030	42.79%	8.393%
5	7.401	692	700	709	rBV	746244	1297207	46.37%	9.096%
6	8.265	840	847	853	rBV	167743	287218	10.27%	2.014%
7	9.434	1039	1046	1055	rBV	423223	752070	26.88%	5.273%
8	11.097	1320	1329	1336	rBV	228496	414421	14.81%	2.906%
9	13.512	1733	1740	1748	rVB	1100566	1753002	62.67%	12.292%
10	14.887	1967	1974	1983	rVB	378820	579240	20.71%	4.061%
11	16.362	2218	2225	2238	rBV	922223	1379519	49.31%	9.673%
12	17.625	2433	2440	2447	rBV	475107	738633	26.40%	5.179%
13	18.483	2582	2586	2597	rBV2	65482	100440	3.59%	0.704%
14	20.210	2874	2880	2886	rBV	2137145	2797362	100.00%	19.614%
15	21.532	3100	3105	3111	rBV	96412	150510	5.38%	1.055%
16	21.796	3146	3150	3156	rVB4	20784	33709	1.21%	0.236%
17	21.920	3165	3171	3180	rVB2	492662	836519	29.90%	5.865%
18	23.712	3471	3476	3483	rVB2	53720	104209	3.73%	0.731%
19	25.339	3743	3753	3767	rVB2	281575	853094	30.50%	5.982%

Sum of corrected areas: 14261805

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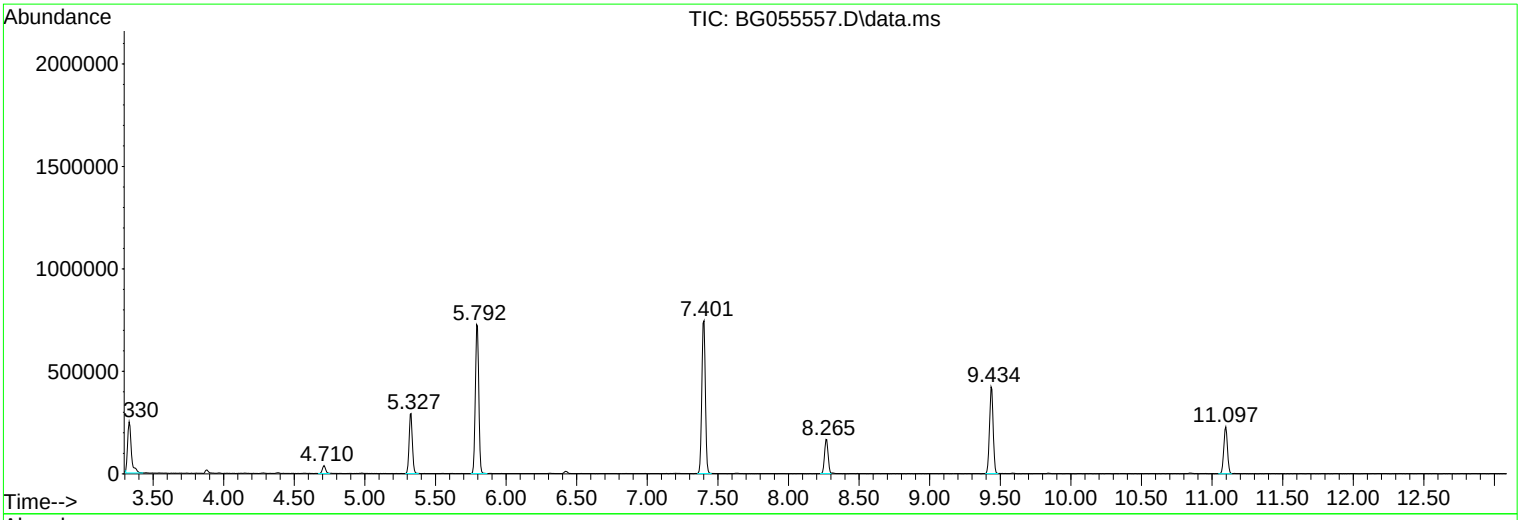
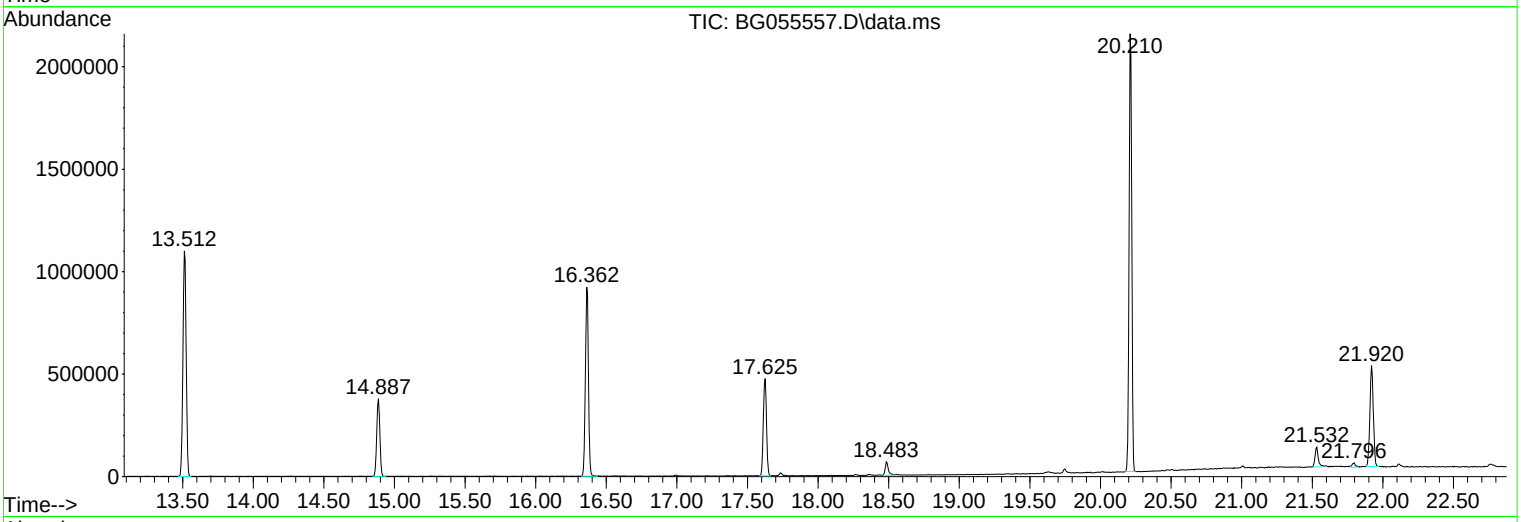
Misc :
ALS Vial : 17 Sample Multiplier: 1

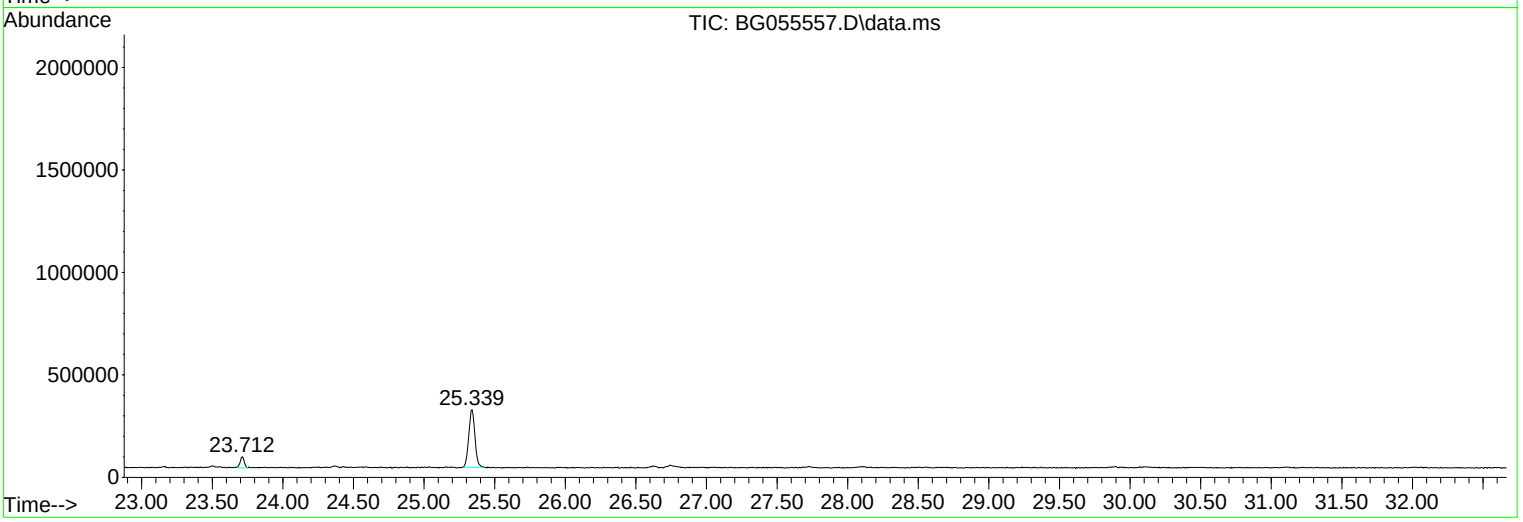
Instrument :
BNA_G
ClientSampleId :
SB-17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

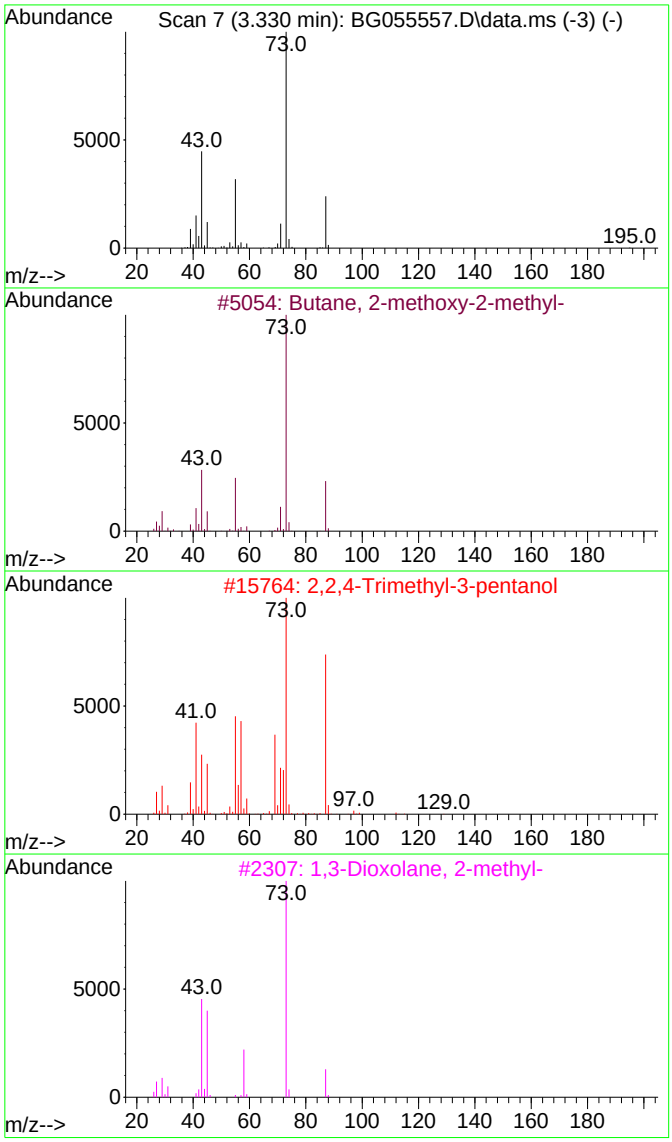
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

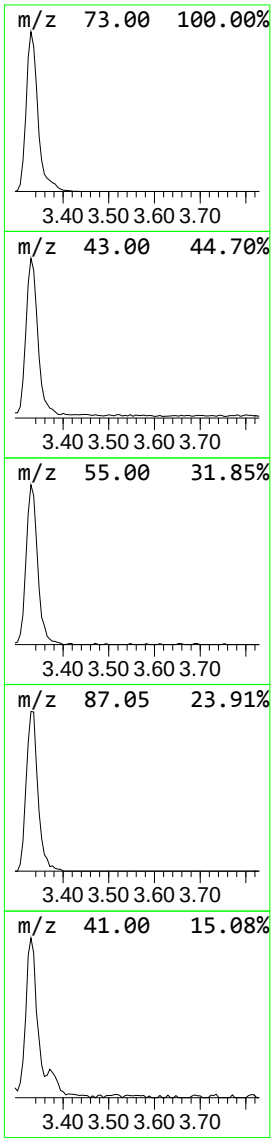
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.330	31.80 ng	456656	1,4-Dichlorobenzene-d4	8.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Data File : BG055557.D
Acq On : 11 Nov 2022 3:09
Operator : CG/JU
Sample : N5494-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

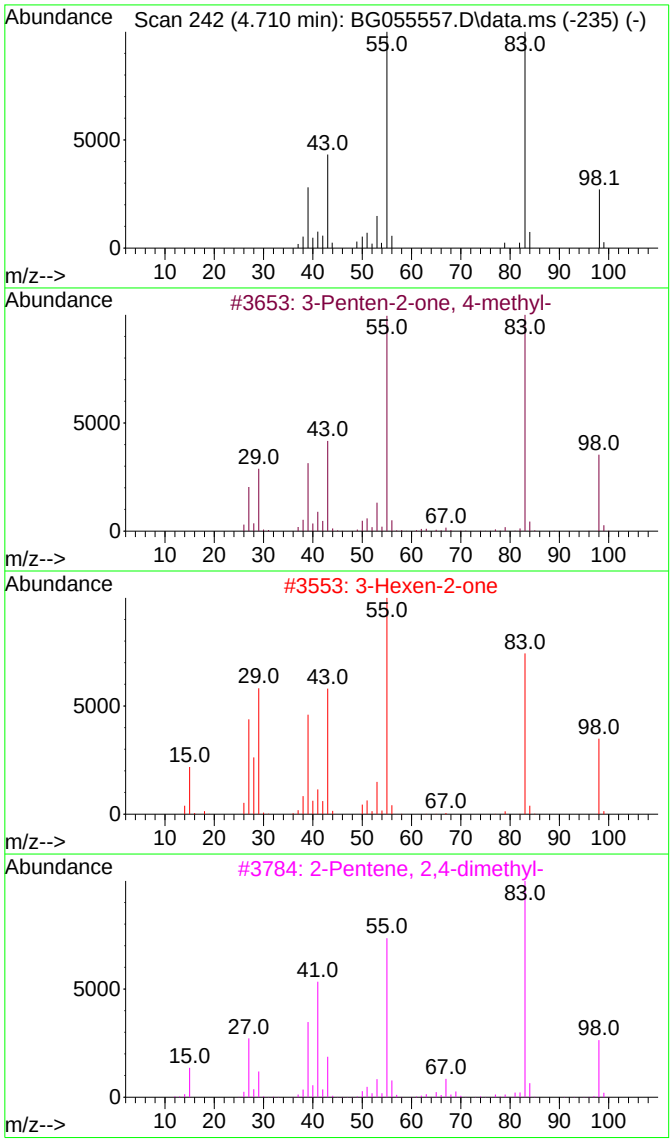
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

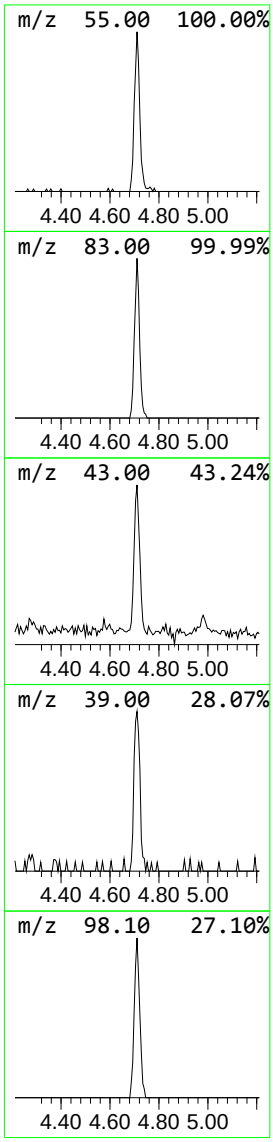
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.710	4.22 ng	60650	1,4-Dichlorobenzene-d4	8.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	86
5	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	86





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Data File : BG055557.D
Acq On : 11 Nov 2022 3:09
Operator : CG/JU
Sample : N5494-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-17

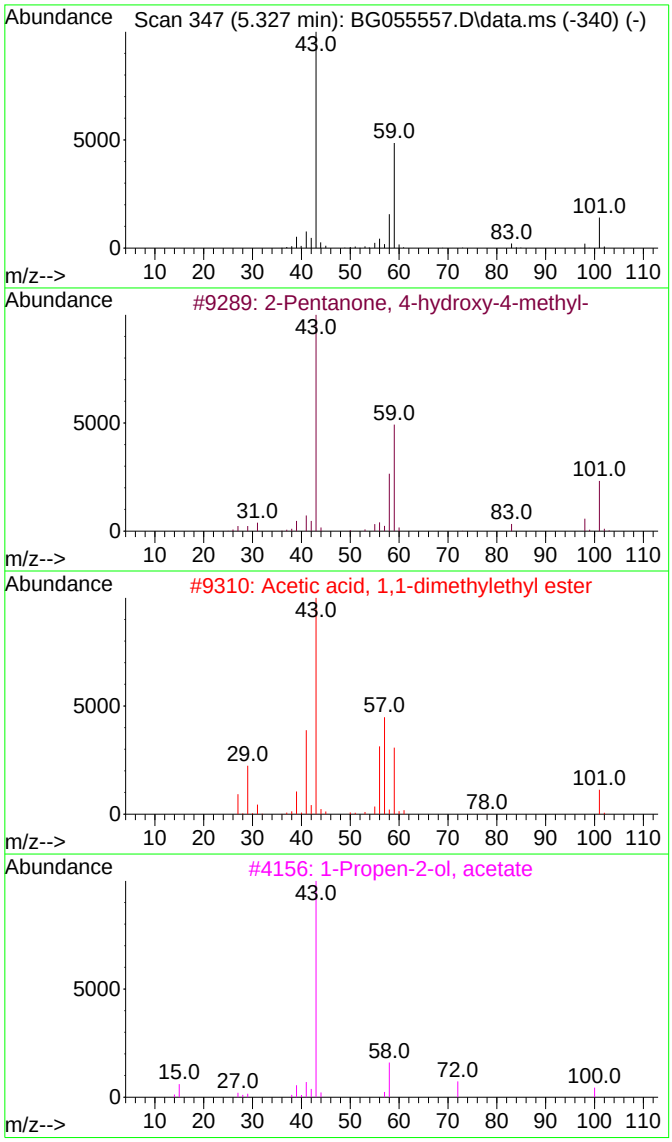
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

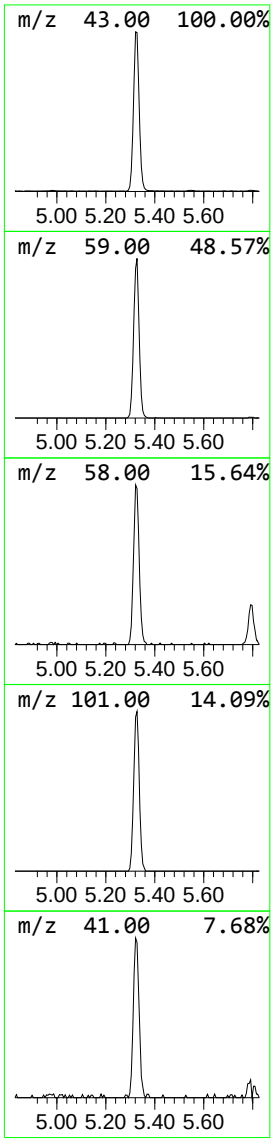
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.327	32.75 ng	470316	1,4-Dichlorobenzene-d4	8.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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Sample : N5494-05
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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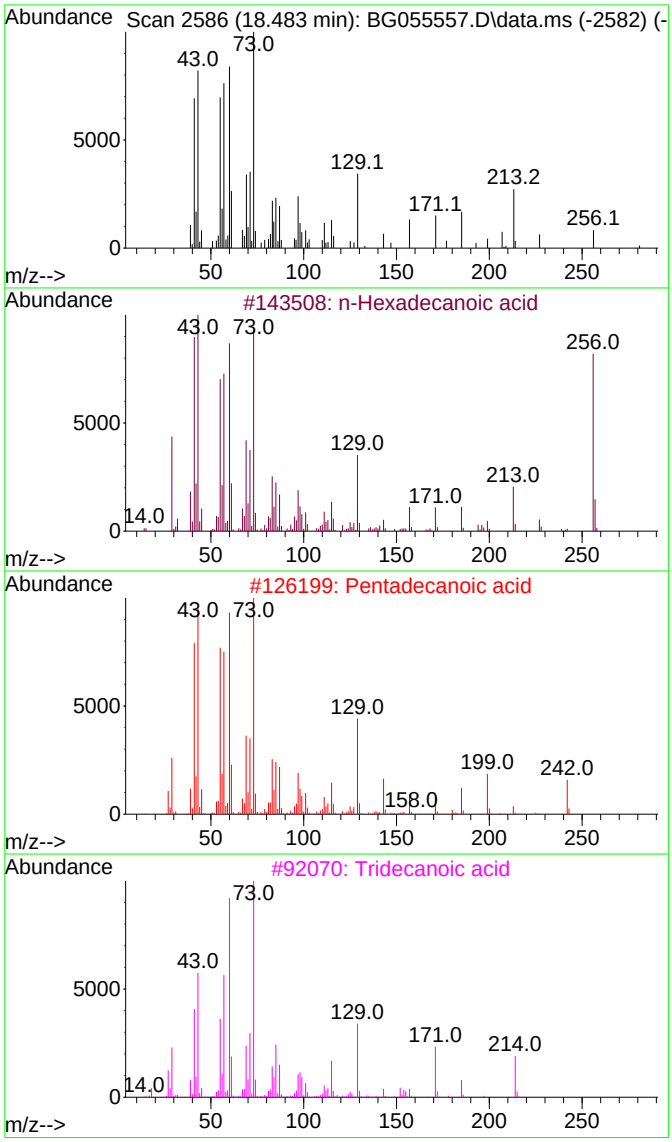
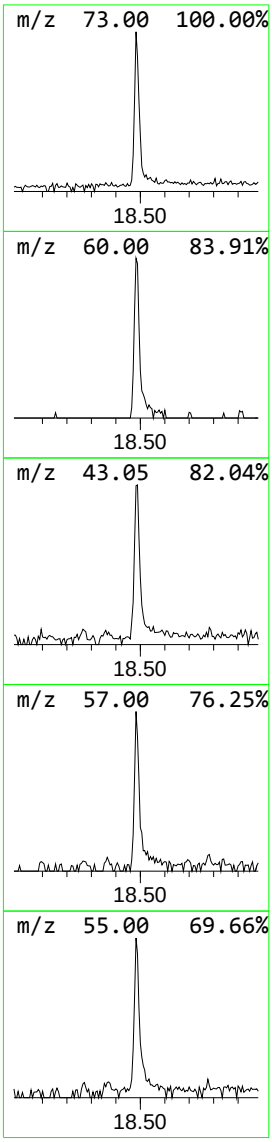
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.483	2.72 ng	100440	Phenanthrene-d10	17.625

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	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	50





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Sample : N5494-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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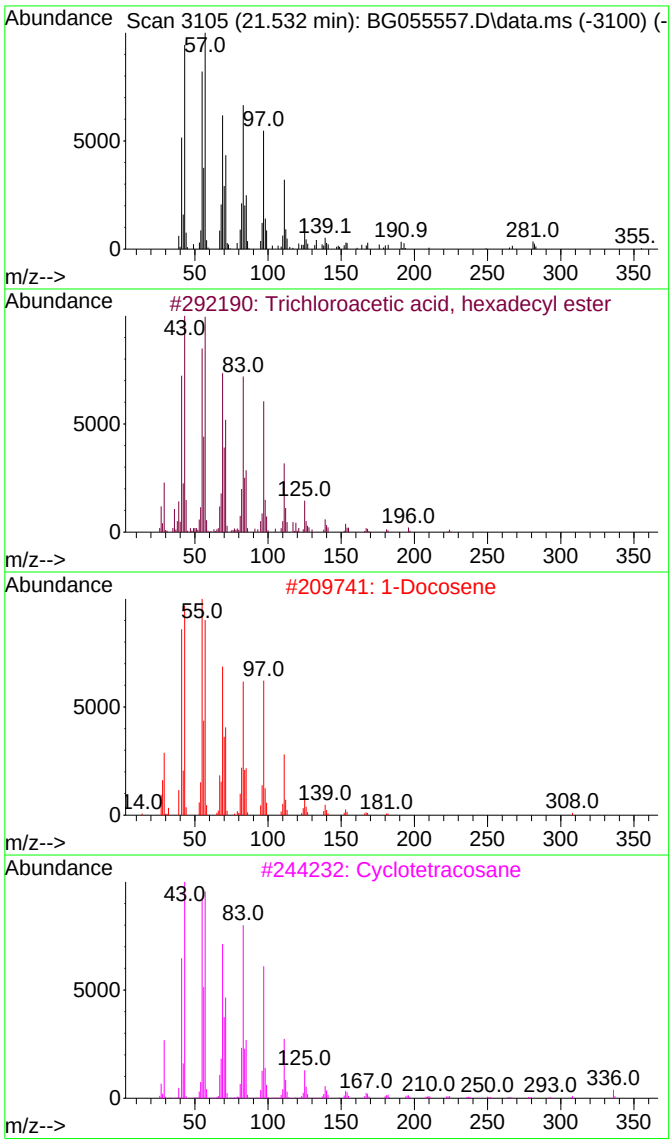
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

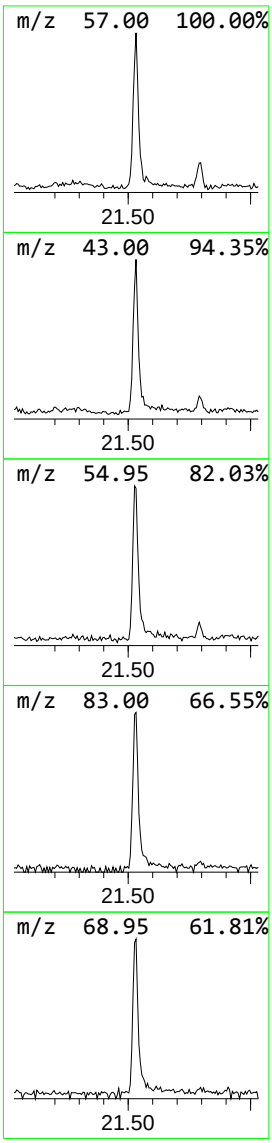
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.532	3.60 ng	150510	Chrysene-d12	21.920

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2	1-Docosene	308	C22H44	001599-67-3	95
3	Cyclotetracosane	336	C24H48	000297-03-0	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





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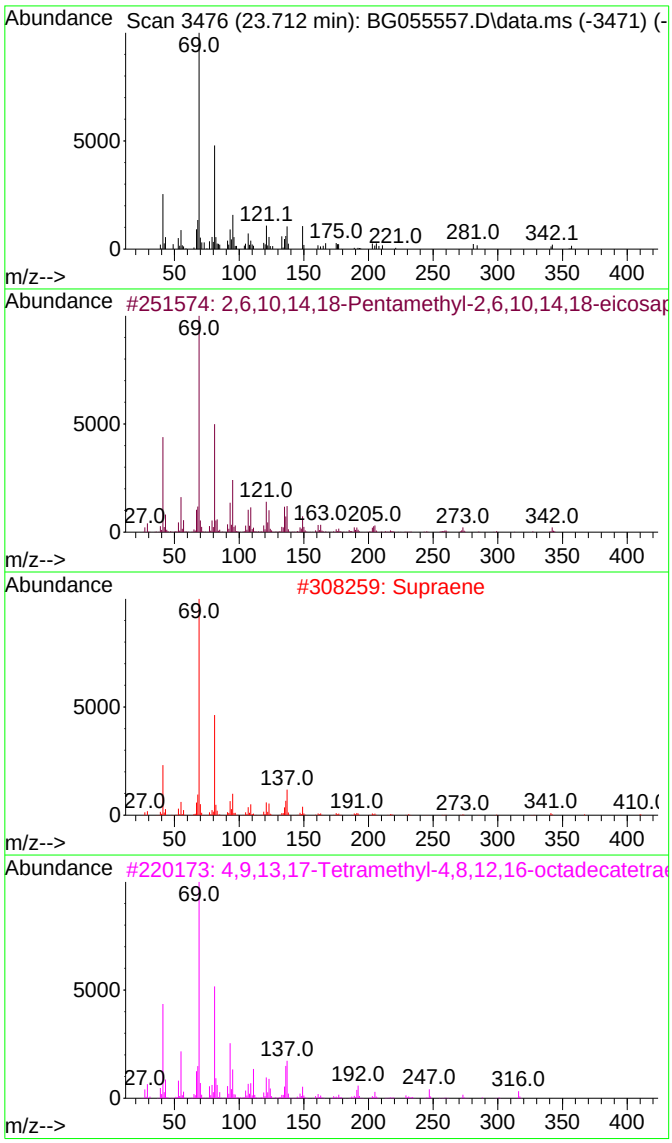
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

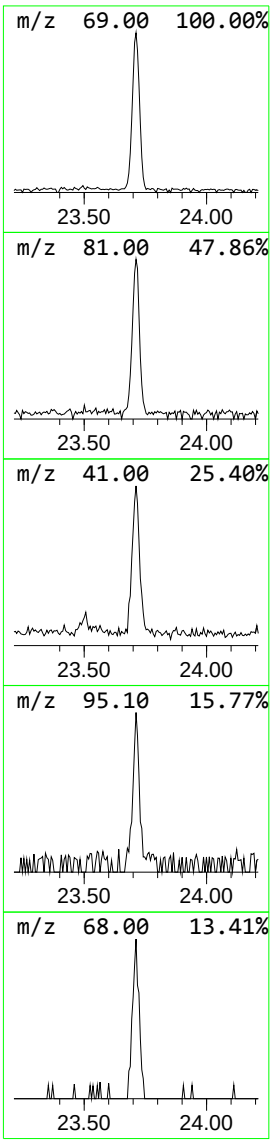
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2,6,10,14,18-Pentamethyl-2,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.712	2.44 ng	104209	Perylene-d12	25.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	87
2	Supraene	410	C30H50	007683-64-9	72
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
4	5-Bromo-1-pentanol	166	C5H11BrO	034626-51-2	53
5	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	53





Tentatively Identified Compound (LSC) summary

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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...	3.330	31.8	ng	456656	1	8.271	287218	20.0
3-Penten-2-one,...	4.710	4.2	ng	60650	1	8.271	287218	20.0
2-Pentanone, 4-...	5.327	32.8	ng	470316	1	8.271	287218	20.0
n-Hexadecanoic ...	18.483	2.7	ng	100440	4	17.625	738633	20.0
Trichloroacetic...	21.532	3.6	ng	150510	5	21.920	836519	20.0
2,6,10,14,18-Pe...	23.712	2.4	ng	104209	6	25.339	853094	20.0