LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020623\
Data File : BG056555.D
Acq On : 6 Feb 2023 15:02
Operator : CG/JU
Sample : 01442-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-01-SB02

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-BG012723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056555.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.372	6	14	24	rVB	53328	116064	3.39%	0.783%
2	5.311	337	344	352	rBV	156004	237264	6.94%	1.600%
3	5.799	419	427	436	rBV	641389	1009010	29.50%	6.804%
4	7.426	696	704	713	rBV	604886	1069130	31.25%	7.209%
5	8.272	842	848	856	rVB	111101	185342	5.42%	1.250%
6	9.453	1040	1049	1058	rVB	352568	625080	18.27%	4.215%
7	9.688	1061	1089	1093	rBV	239507	1141658	33.37%	7.698%
8	11.104	1322	1330	1339	rVB	142731	250728	7.33%	1.691%
9	13.519	1734	1741	1753	rVB	1294470	1948524	56.96%	13.139%
10	14.894	1966	1975	1985	rVB	261823	411405	12.03%	2.774%
11	16.234	2197	2203	2212	rBV	273595	381781	11.16%	2.574%
12	16.381	2221	2228	2237	rBV	1059798	1578184	46.14%	10.642%
13	16.798	2293	2299	2304	rBV	26242	41801	1.22%	0.282%
14	17.632	2434	2441	2450	rBV	371830	577797	16.89%	3.896%
15	18.478	2576	2585	2597	rBV	109687	174240	5.09%	1.175%
16	19.477	2749	2755	2763	rBV5	20580	50835	1.49%	0.343%
17	19.735	2795	2799	2809	rBV4	29167	45908	1.34%	0.310%
18	20.211	2874	2880	2886	rBV	2801689	3420785	100.00%	23.067%
19	20.482	2919	2926	2935	rVB3	31673	77650	2.27%	0.524%
20	20.699	2958	2963	2971	rVB4	24169	50487	1.48%	0.340%
21	21.504	3096	3100	3110	rVB2	82732	155252	4.54%	1.047%
22	21.927	3165	3172	3180	rBV2	394023	664046	19.41%	4.478%
23	25.347	3746	3754	3766	rBV2	205331	617083	18.04%	4.161%

Sum of corrected areas: 14830054

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020623\
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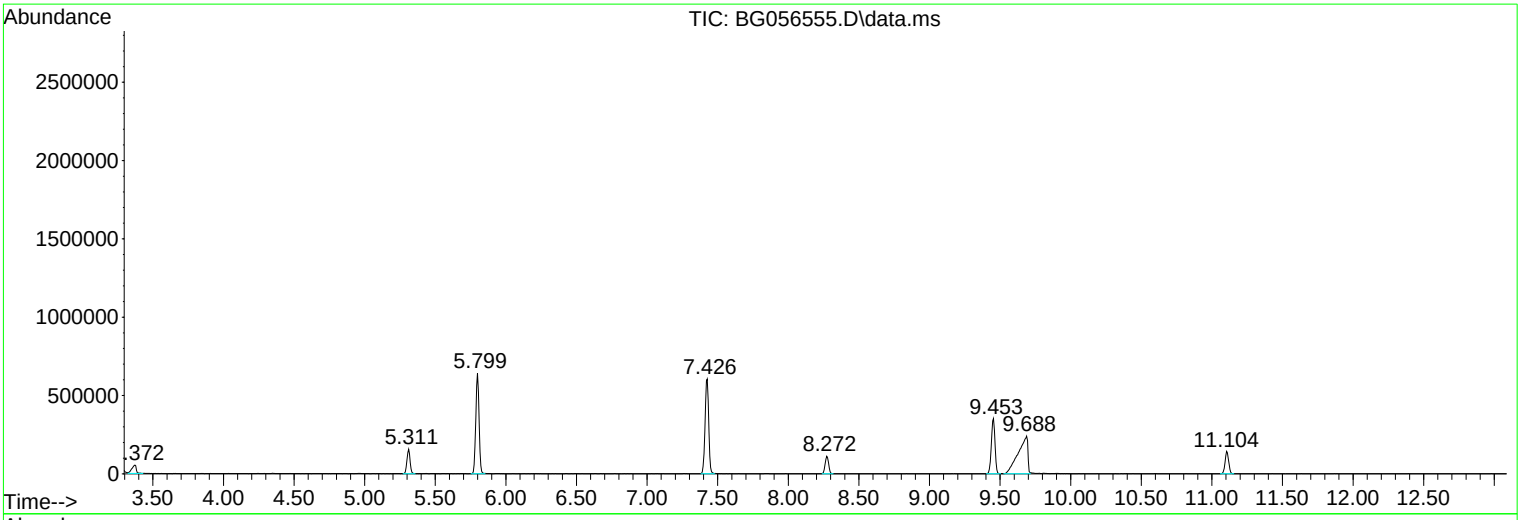
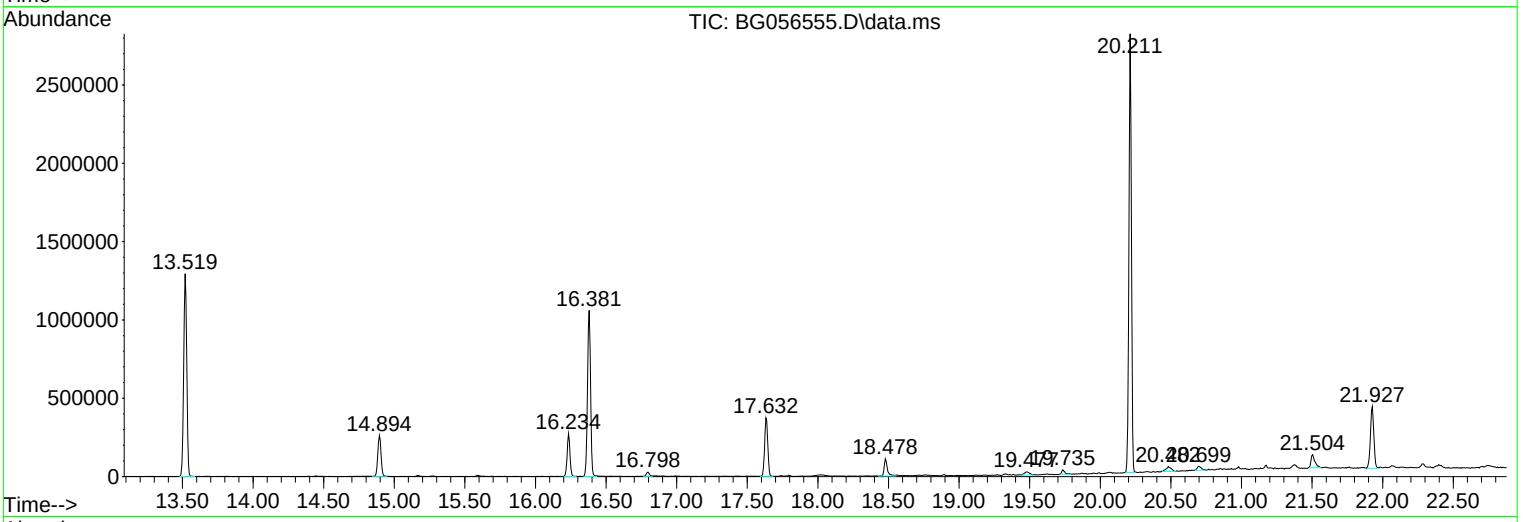
Sample : 01442-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

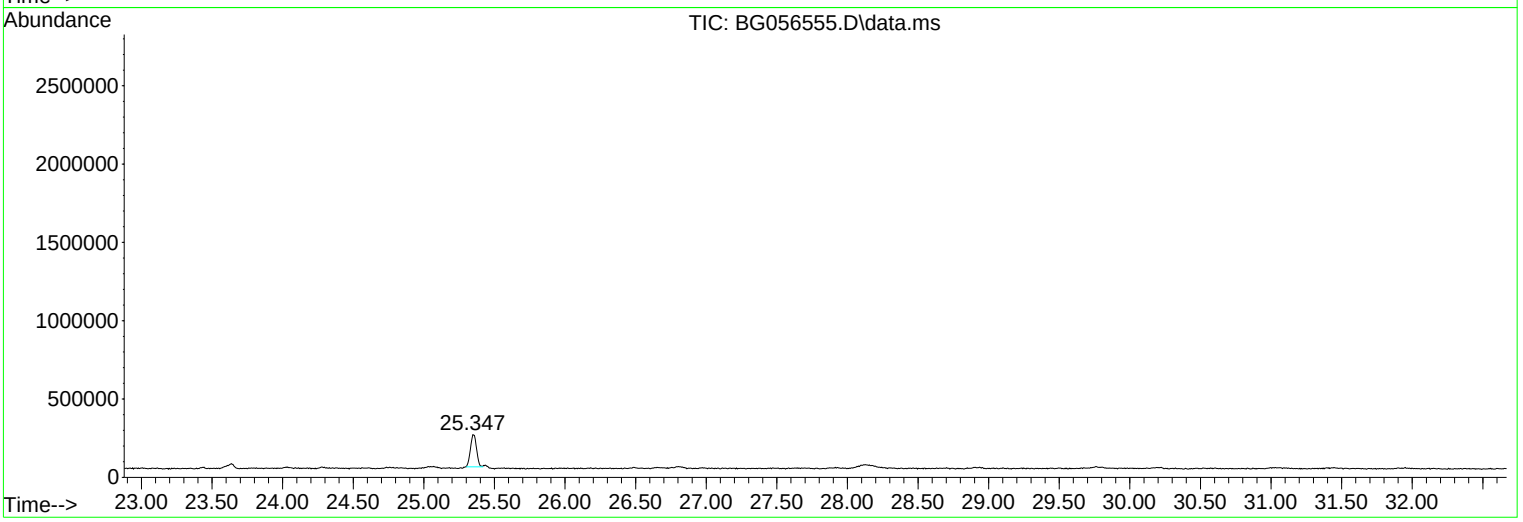
Instrument :
BNA_G
ClientSampleId :
B-01-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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\BG020623\
Data File : BG056555.D
Acq On : 6 Feb 2023 15:02
Operator : CG/JU
Sample : 01442-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

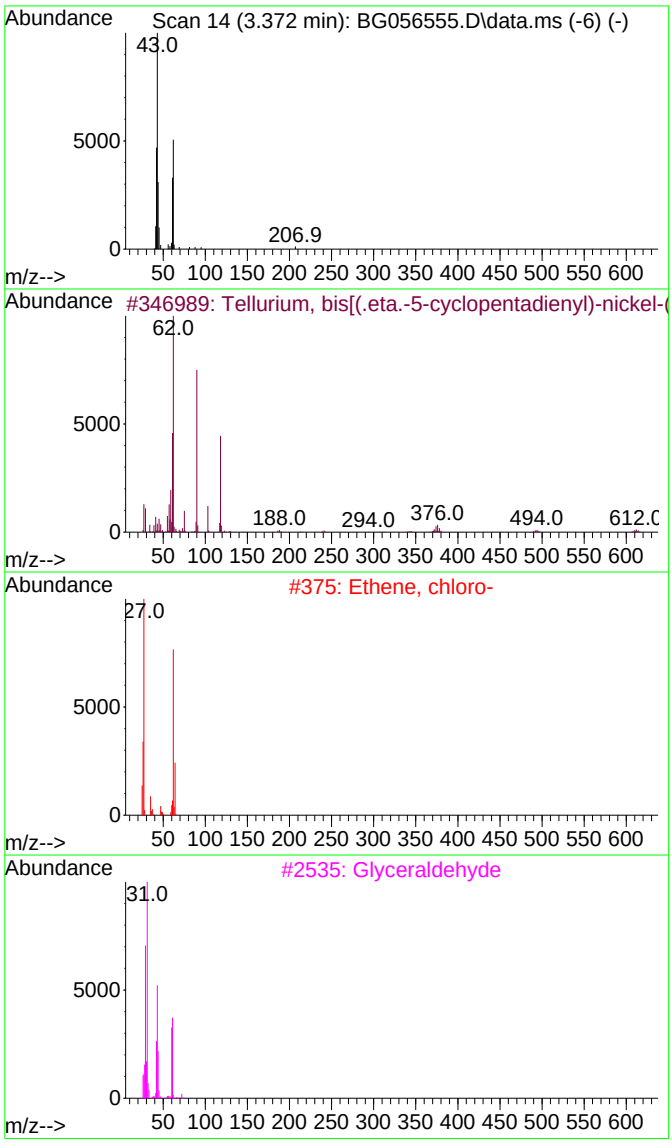
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

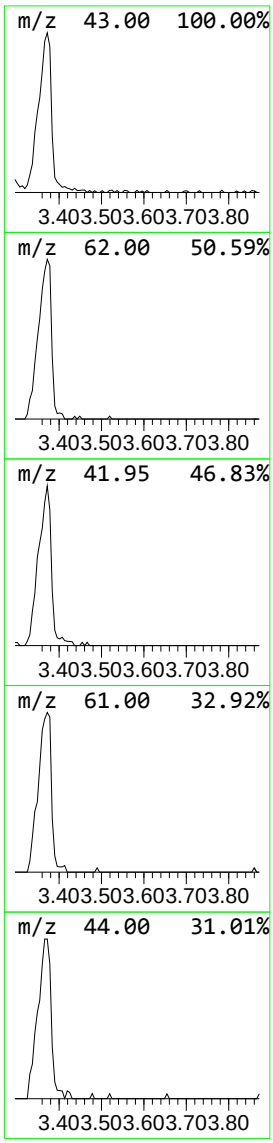
****

Peak Number 1 unknown3.372 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.372	12.52 ng	116064	1,4-Dichlorobenzene-d4	8.272

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tellurium, bis[(.eta.-5-cyclopen...	612	C22H40Ni2P2Te	1000161-69-8	33
2	Ethene, chloro-	62	C2H3Cl	000075-01-4	9
3	Glyceraldehyde	90	C3H6O3	000056-82-6	9
4	Propane, 1-[(1-methylethyl)thio]-	118	C6H14S	005008-73-1	9
5	Ethanethiol	62	C2H6S	000075-08-1	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020623\
Data File : BG056555.D
Acq On : 6 Feb 2023 15:02
Operator : CG/JU
Sample : 01442-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-01-SB02

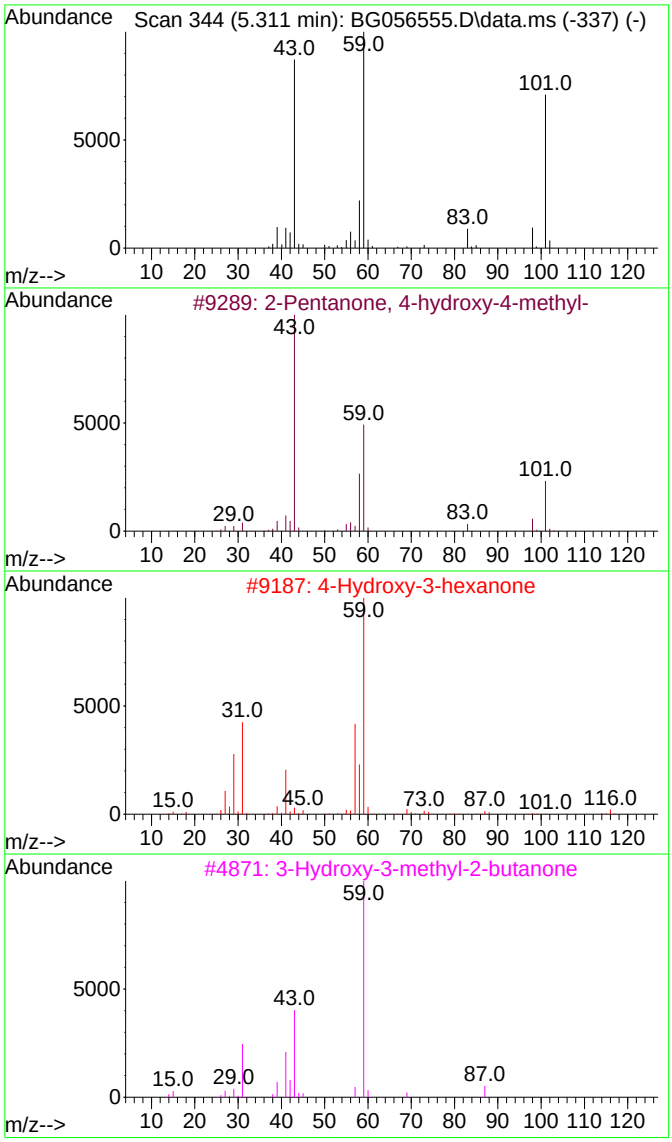
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

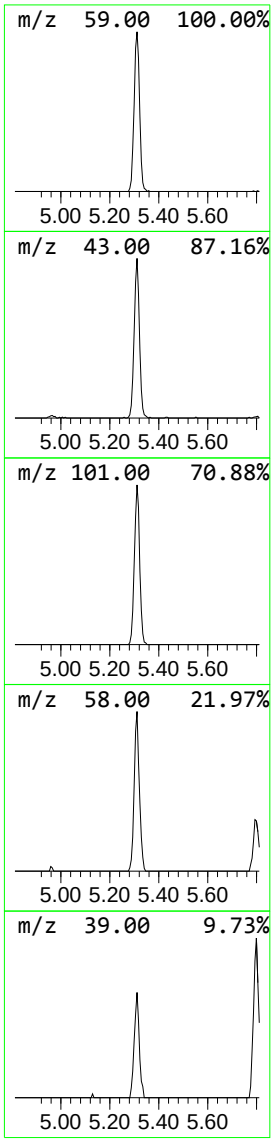
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.311	25.60 ng	237264	1,4-Dichlorobenzene-d4	8.272

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5	1,2-Butanediol	90	C4H10O2	000584-03-2	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020623\
Data File : BG056555.D
Acq On : 6 Feb 2023 15:02
Operator : CG/JU
Sample : 01442-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-01-SB02

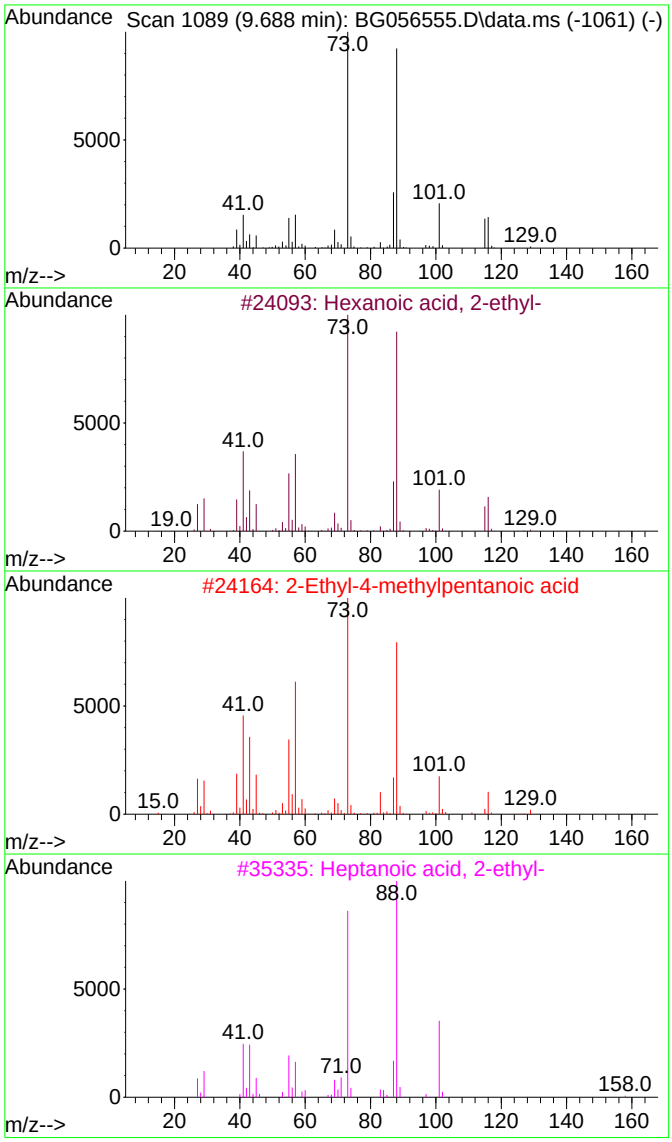
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

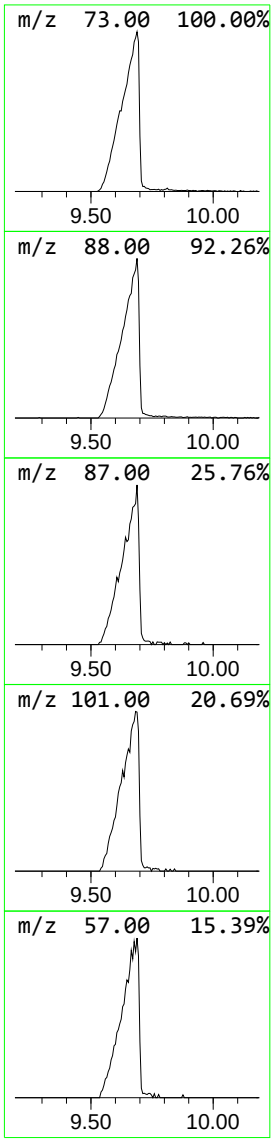
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.688	123.19 ng	1141660	1,4-Dichlorobenzene-d4	8.272

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	64
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
4	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	50
5	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020623\
Data File : BG056555.D
Acq On : 6 Feb 2023 15:02
Operator : CG/JU
Sample : 01442-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-01-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

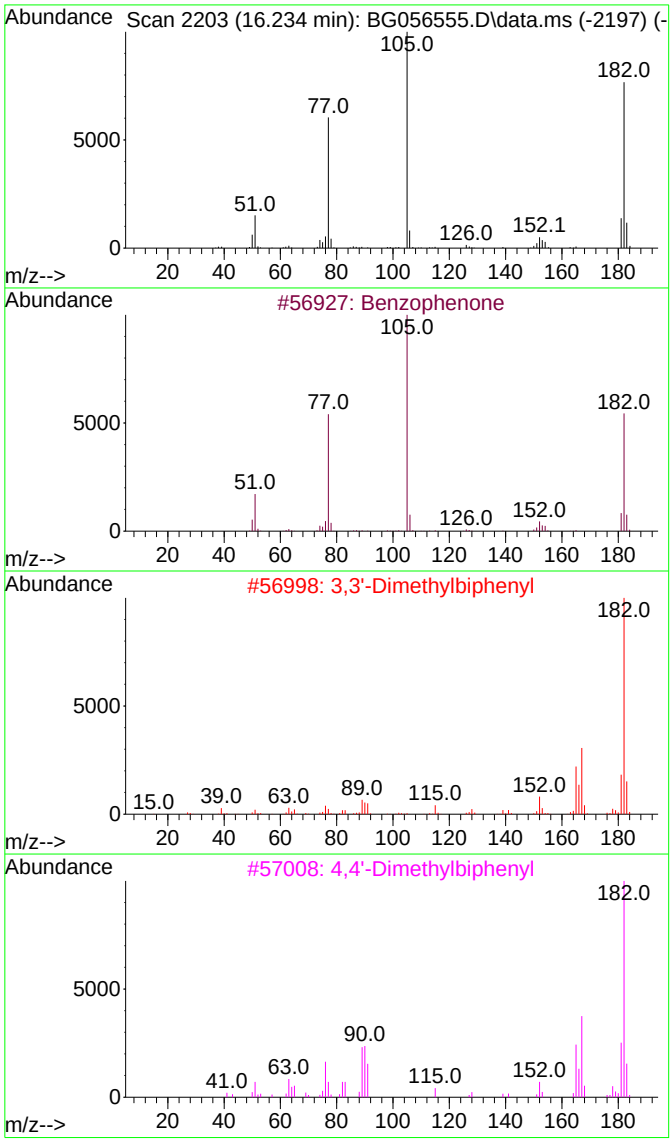
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

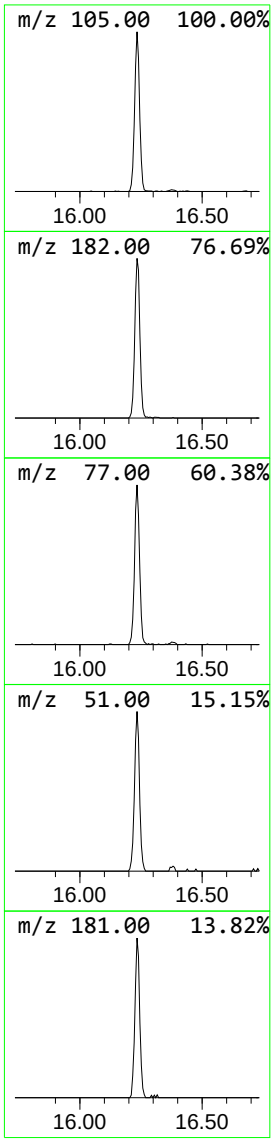
****

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.234	18.56 ng	381781	Acenaphthene-d10	14.894

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	47
3	4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	46
4	3,4-Dimethoxy-5-hydroxybenzaldehyde	182	C9H10O4	029865-90-5	43
5	2-Methyl-1H-perimidine	182	C12H10N2	005157-10-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020623\
Data File : BG056555.D
Acq On : 6 Feb 2023 15:02
Operator : CG/JU
Sample : 01442-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-01-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

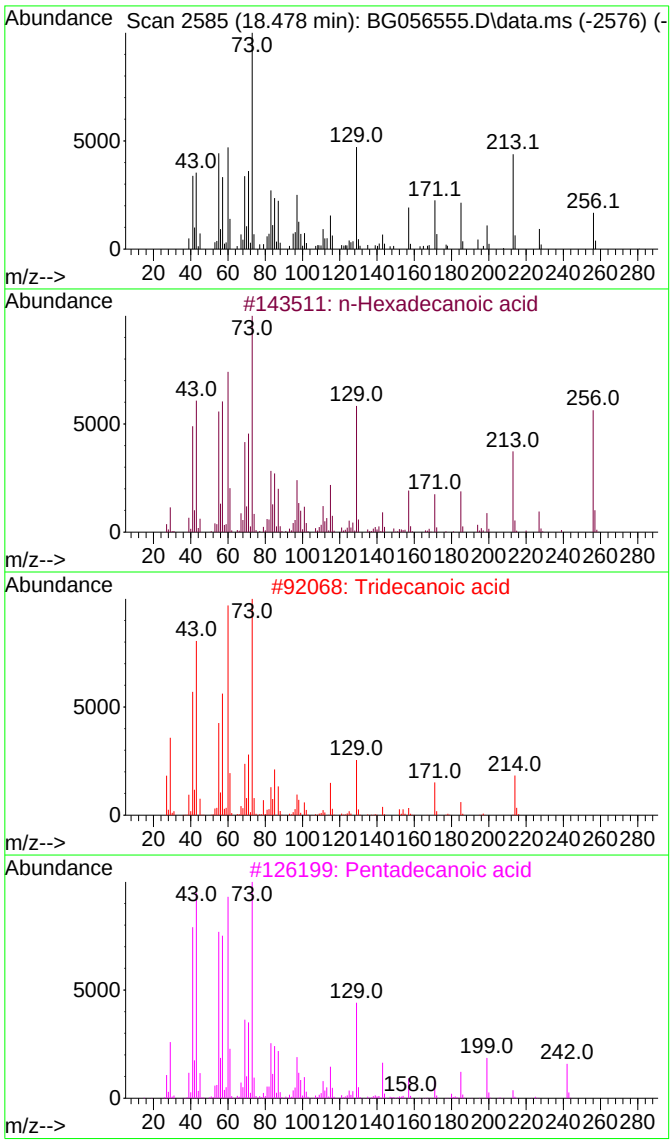
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

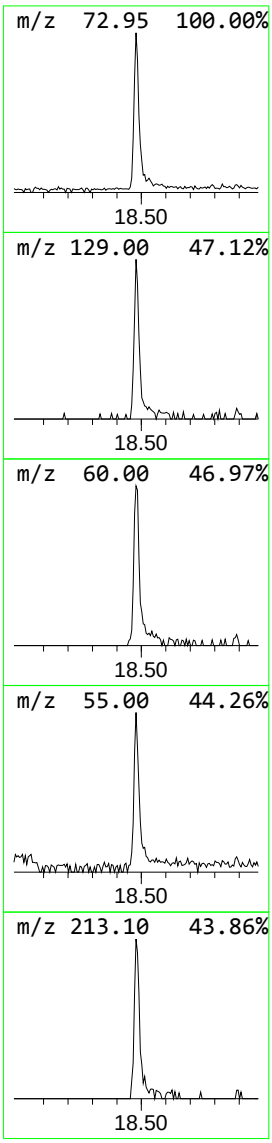
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.478	6.03 ng	174240	Phenanthrene-d10	17.632

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	40
5	Dodecanoic acid	200	C12H24O2	000143-07-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020623\
Data File : BG056555.D
Acq On : 6 Feb 2023 15:02
Operator : CG/JU
Sample : 01442-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-01-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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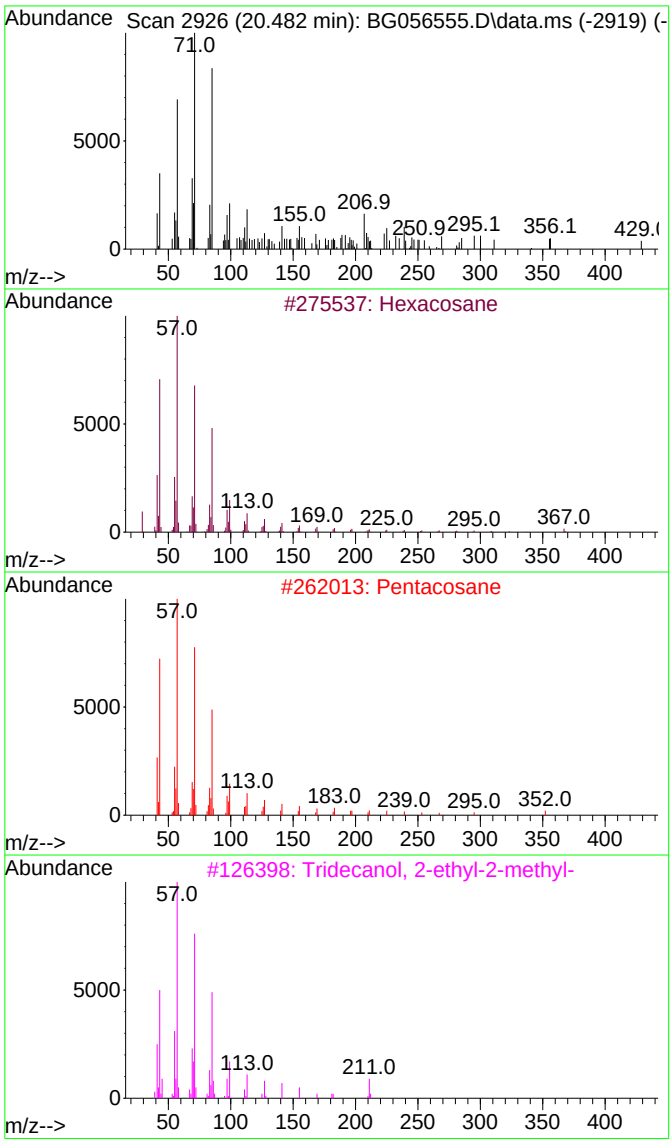
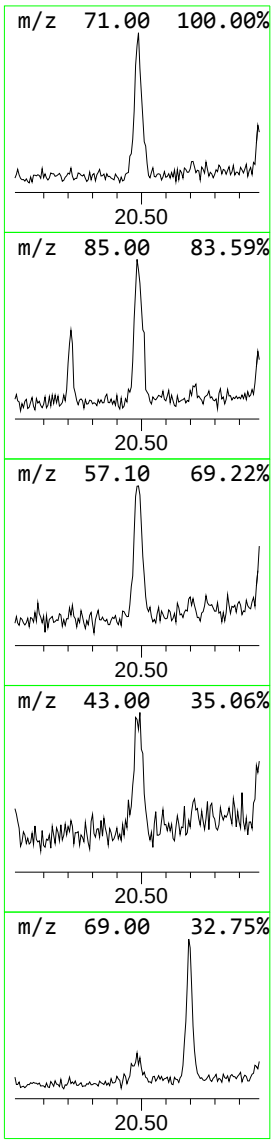
****

Peak Number 6 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.482	2.34 ng	77650	Chrysene-d12	21.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	72
2	Pentacosane	352	C25H52	000629-99-2	72
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	72
4	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	64
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	64





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Data File : BG056555.D
Acq On : 6 Feb 2023 15:02
Operator : CG/JU
Sample : 01442-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-01-SB02

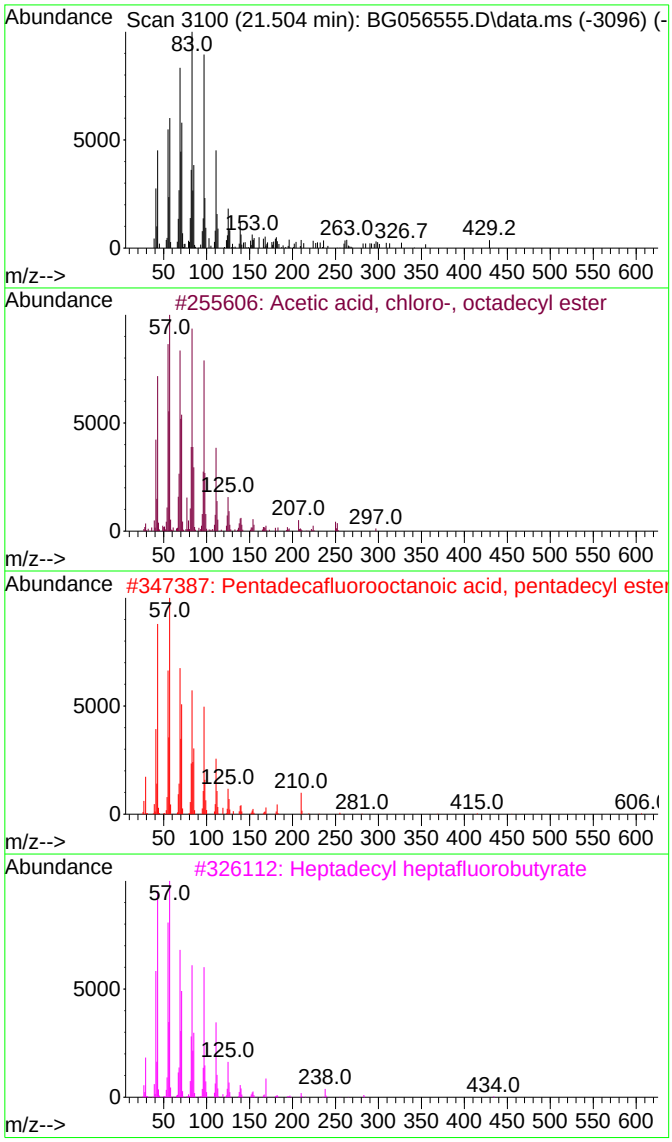
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

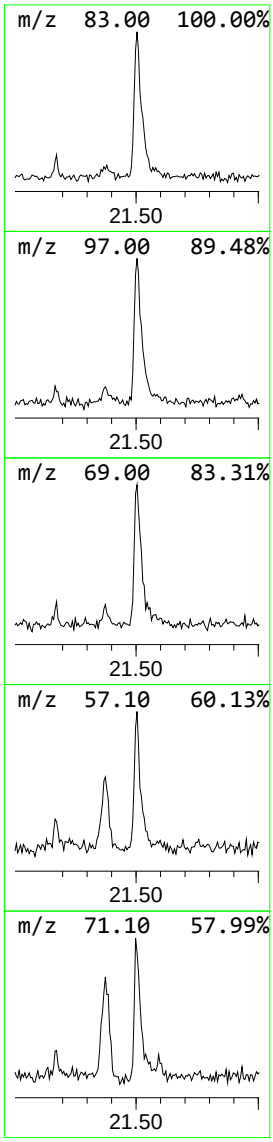
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Acetic acid, chloro-, octad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.504	4.68 ng	155252	Chrysene-d12	21.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	87
2	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	83
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
4	1-Docosene	308	C22H44	001599-67-3	76
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020623\
Data File : BG056555.D
Acq On : 6 Feb 2023 15:02
Operator : CG/JU
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Misc :
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Instrument :
BNA_G
ClientSampleId :
B-01-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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
unknown3.372	3.372	12.5	ng	116064	1	8.272	185342	20.0
2-Pentanone, 4-...	5.311	25.6	ng	237264	1	8.272	185342	20.0
Hexanoic acid, ...	9.688	123.2	ng	1141660	1	8.272	185342	20.0
Benzophenone	16.234	18.6	ng	381781	3	14.894	411405	20.0
n-Hexadecanoic ...	18.478	6.0	ng	174240	4	17.632	577797	20.0
Hexacosane	20.482	2.3	ng	77650	5	21.927	664046	20.0
Acetic acid, ch...	21.504	4.7	ng	155252	5	21.927	664046	20.0