LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060622\
Data File : BG053834.D
Acq On : 6 Jun 2022 18:23
Operator : CG/JU
Sample : N3143-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220425-AMENDED-COMP-E

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-BG060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053834.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.592	198	205	214	rBV	32036	56953	3.10%	0.693%
2	5.191	300	307	319	rVB	494045	812409	44.29%	9.888%
3	5.655	380	386	395	rVB	128685	217095	11.84%	2.642%
4	7.242	648	656	664	rBV	198868	356247	19.42%	4.336%
5	8.094	793	801	807	rBV	90814	162565	8.86%	1.979%
6	9.245	990	997	1007	rVB	227849	430415	23.46%	5.239%
7	9.610	1052	1059	1066	rBV2	14892	29735	1.62%	0.362%
8	10.896	1268	1278	1285	rBV	127052	244740	13.34%	2.979%
9	13.340	1687	1694	1704	rBV	707032	1168348	63.69%	14.221%
10	13.517	1718	1724	1732	rBV6	13150	30535	1.66%	0.372%
11	13.740	1755	1762	1770	rBV2	19771	40093	2.19%	0.488%
12	14.145	1826	1831	1837	rBV3	39643	60567	3.30%	0.737%
13	14.257	1846	1850	1856	rBV5	9639	19170	1.05%	0.233%
14	14.469	1881	1886	1891	rBV6	13350	26112	1.42%	0.318%
15	14.551	1896	1900	1906	rVB2	32461	50710	2.76%	0.617%
16	14.610	1906	1910	1919	rBV6	12611	27499	1.50%	0.335%
17	14.709	1919	1927	1935	rBV	217023	386320	21.06%	4.702%
18	15.509	2058	2063	2068	rVB3	22182	36188	1.97%	0.440%
19	16.196	2174	2180	2187	rBV	157501	272196	14.84%	3.313%
20	17.201	2347	2351	2360	rBV4	35974	68313	3.72%	0.831%
21	17.453	2388	2394	2399	rBV	285408	457786	24.96%	5.572%
22	17.494	2399	2401	2406	rVB	28427	34766	1.90%	0.423%
23	19.357	2715	2718	2725	rVB2	17284	26265	1.43%	0.320%
24	19.504	2739	2743	2748	rVB	63656	93629	5.10%	1.140%
25	19.862	2801	2804	2810	rVB	57270	90017	4.91%	1.096%
26	20.062	2832	2838	2845	rBV	1357344	1834293	100.00%	22.326%
27	21.372	3057	3061	3076	rVB2	92471	165746	9.04%	2.017%
28	21.731	3115	3122	3128	rBV	302124	557491	30.39%	6.786%
29	24.997	3670	3678	3690	rVB3	159866	459689	25.06%	5.595%

Sum of corrected areas: 8215892

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060622\
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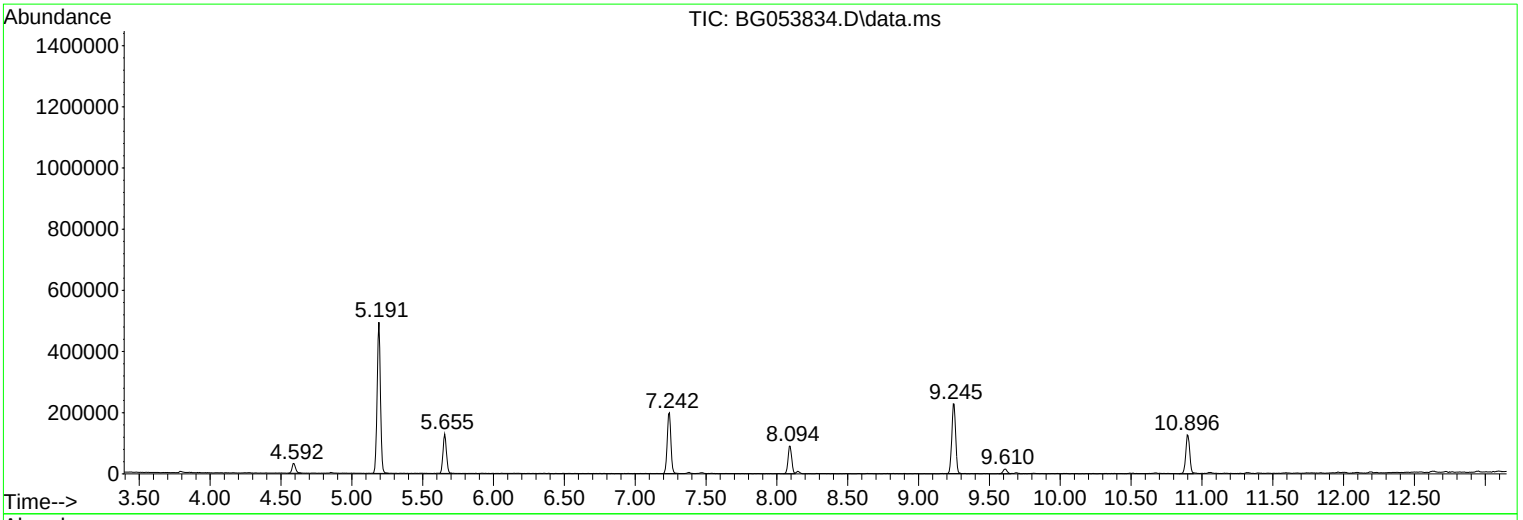
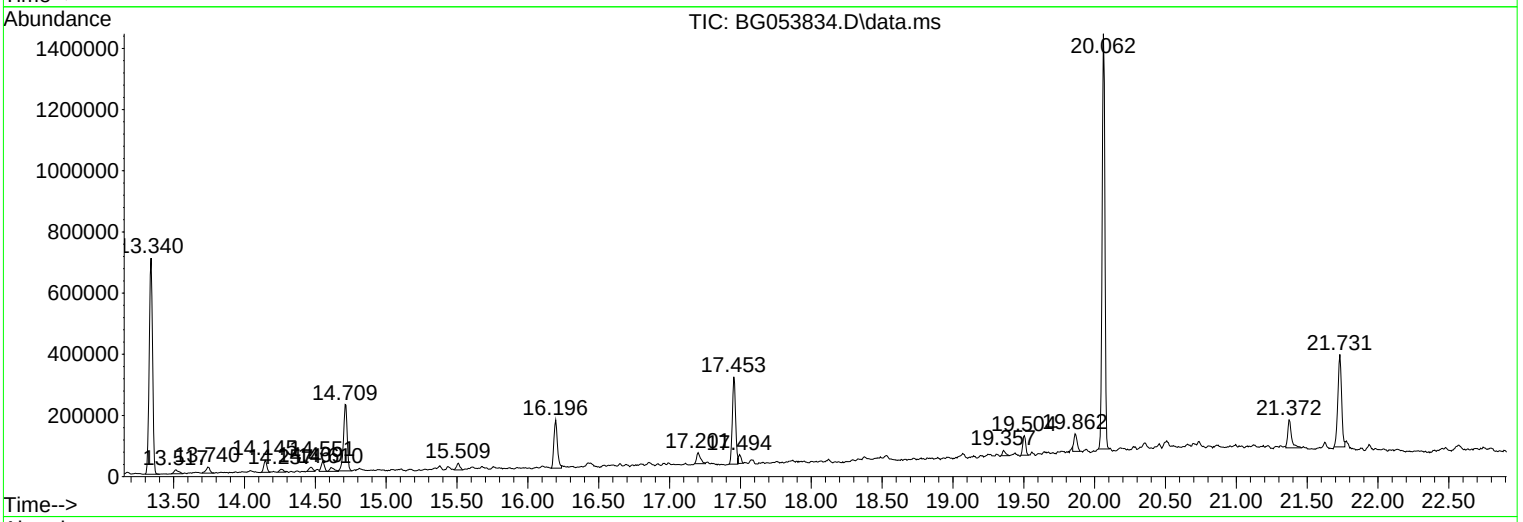
Misc :
ALS Vial : 12 Sample Multiplier: 1

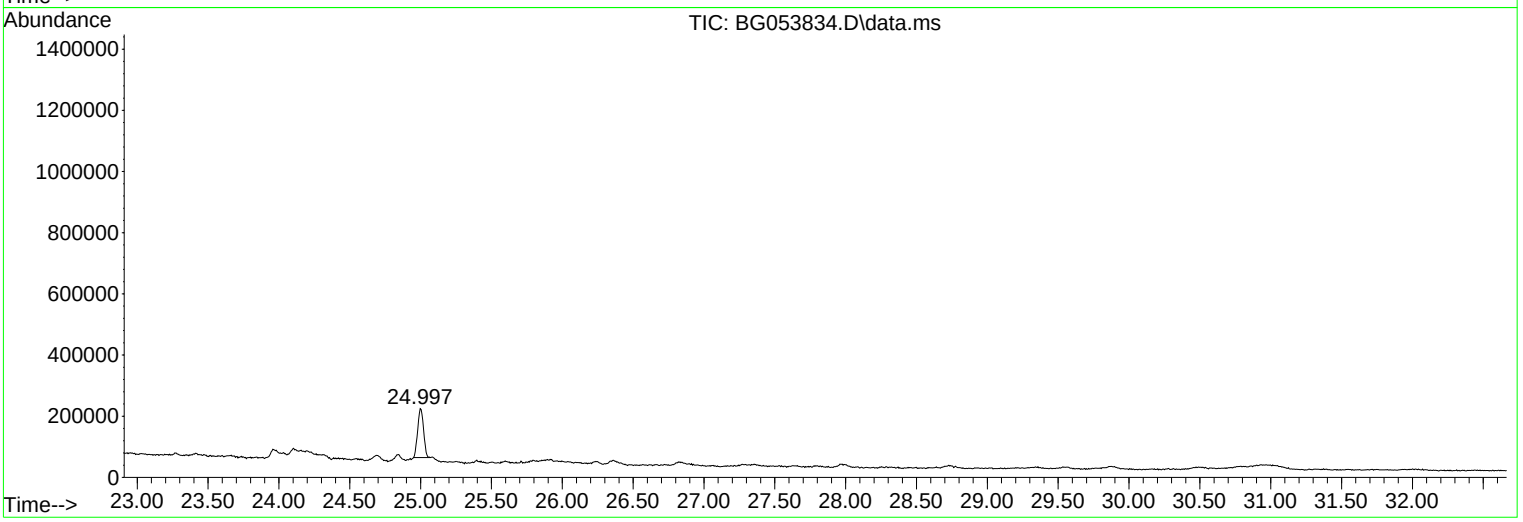
Instrument :
BNA_G
ClientSampleId :
20220425-AMENDED-COMP-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.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\BG060622\
Data File : BG053834.D
Acq On : 6 Jun 2022 18:23
Operator : CG/JU
Sample : N3143-03
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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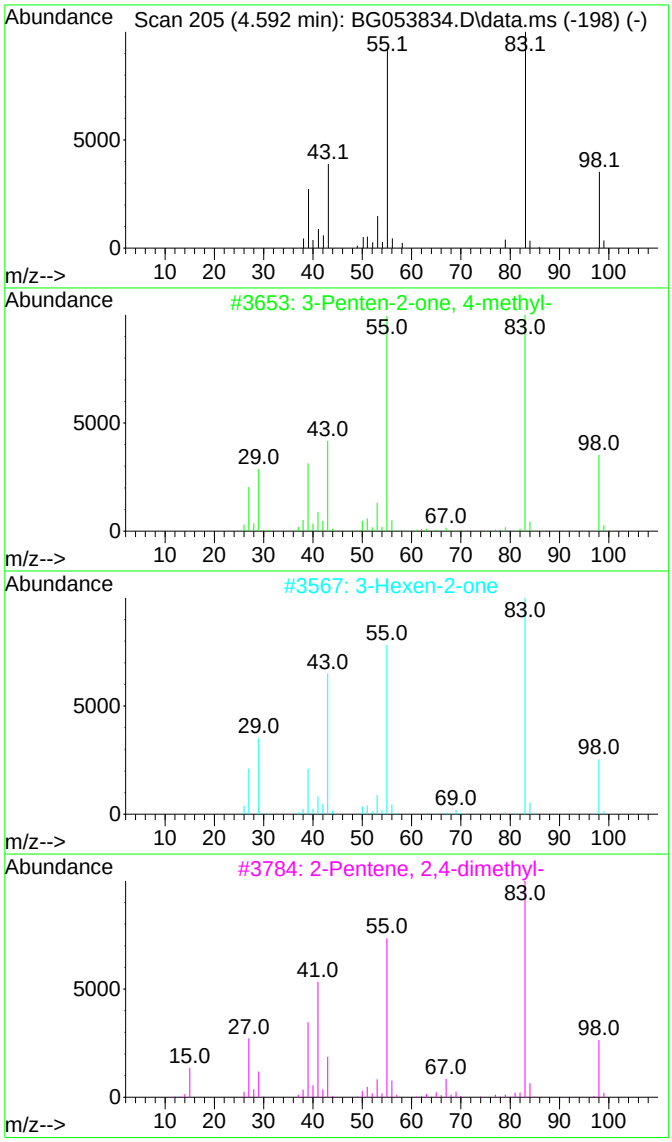
TIC Integration Parameters: LSCINT.P

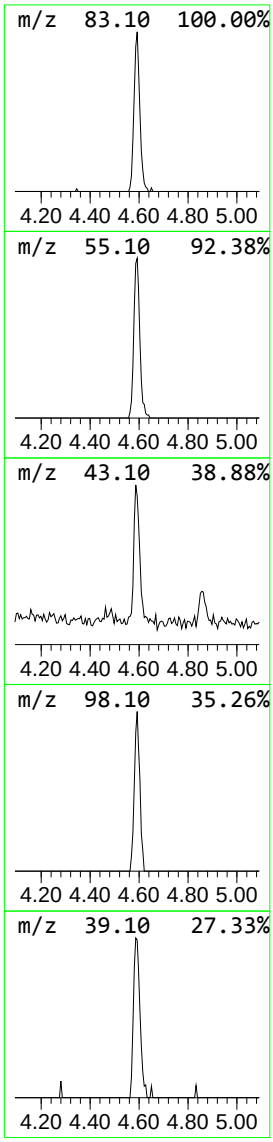
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.592	7.01 ng	56953	1,4-Dichlorobenzene-d4	8.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72





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Data File : BG053834.D
Acq On : 6 Jun 2022 18:23
Operator : CG/JU
Sample : N3143-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220425-AMENDED-COMP-E

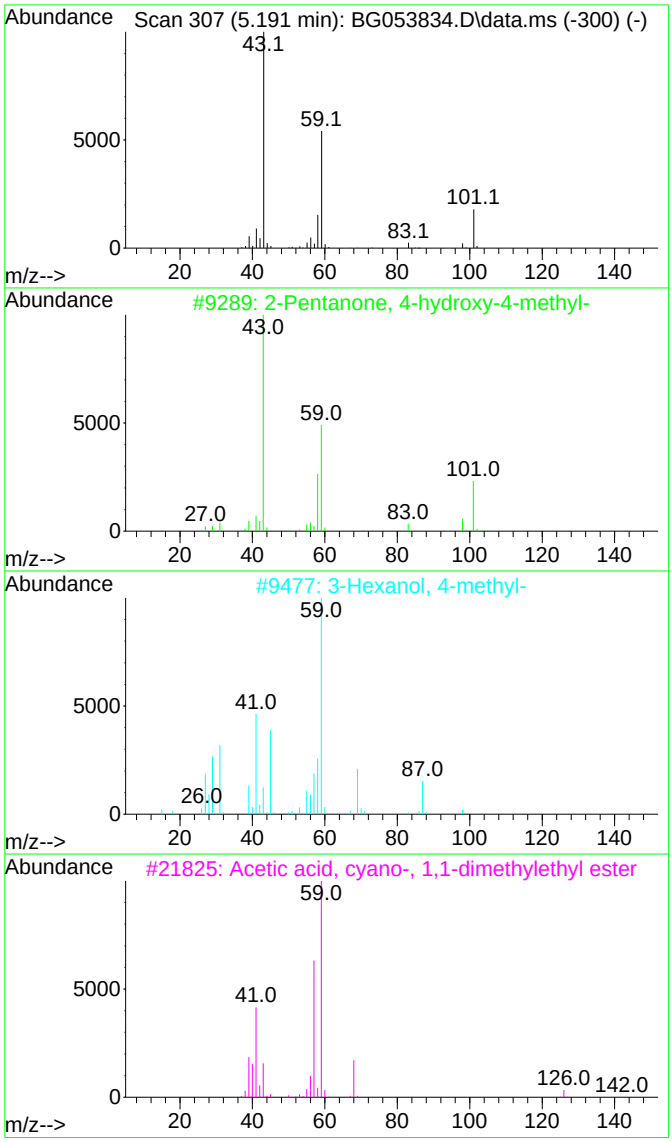
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

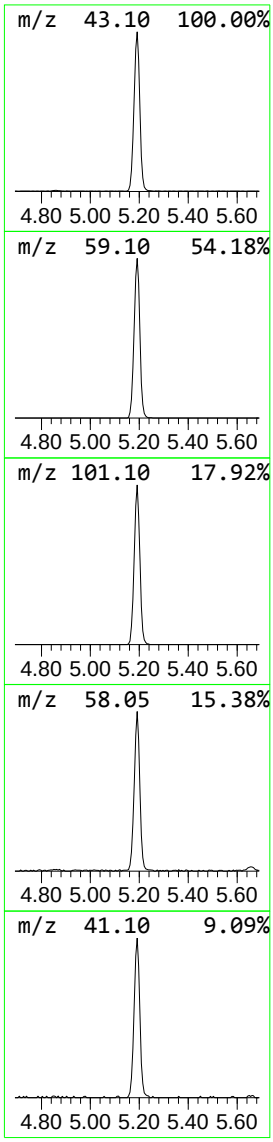
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	99.95 ng	812409	1,4-Dichlorobenzene-d4	8.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Sample : N3143-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220425-AMENDED-COMP-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

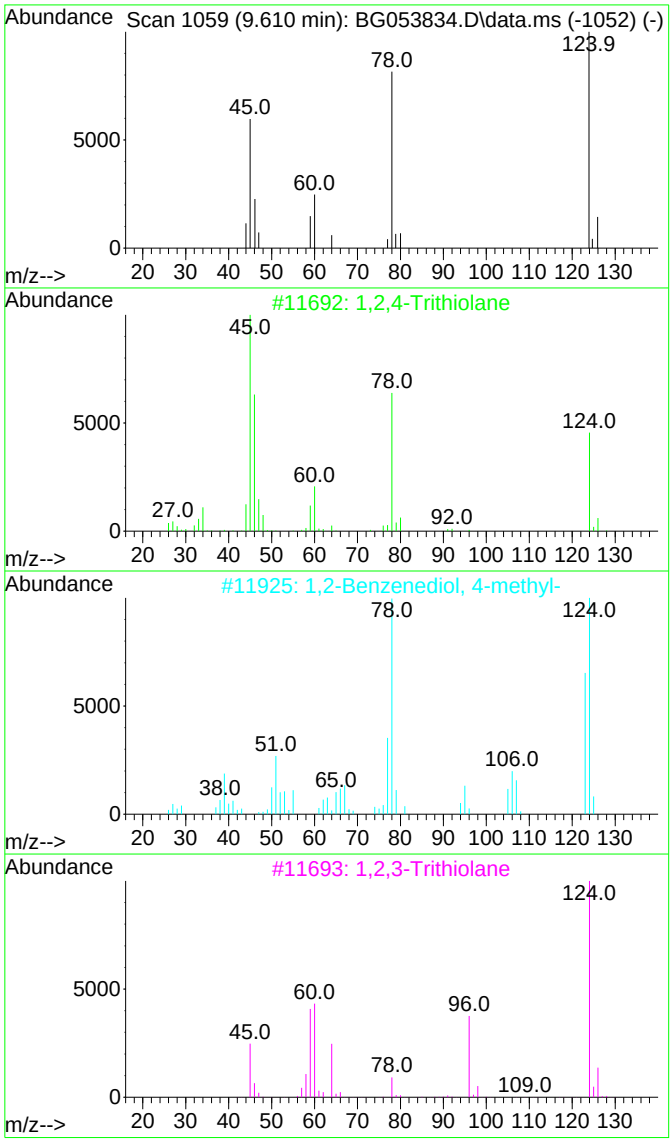
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

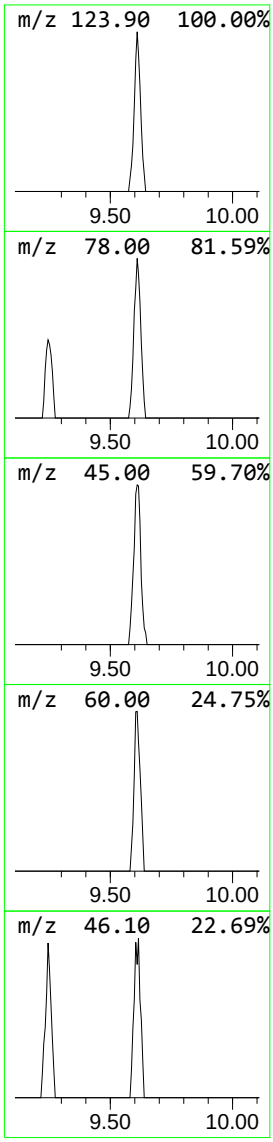
****

Peak Number 3 unknown9.610 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.610	2.43 ng	29735	Naphthalene-d8	10.896

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	39
2	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	7
3	1,2,3-Trithiolane	124	C2H4S3	006669-39-2	7
4	2-(2-Methylvinyl)thiophene	124	C7H8S	023229-68-7	5
5	2-Cyclopropylthiophene	124	C7H8S	029481-22-9	5





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Acq On : 6 Jun 2022 18:23
Operator : CG/JU
Sample : N3143-03
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Instrument :
BNA_G
ClientSampleId :
20220425-AMENDED-COMP-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

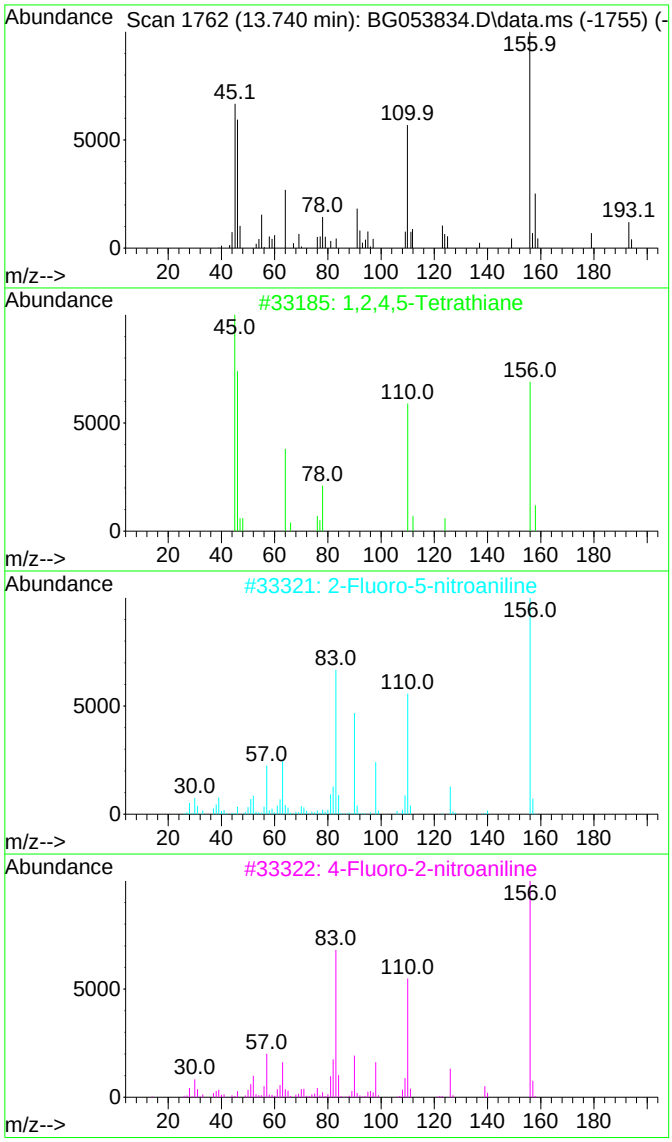
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

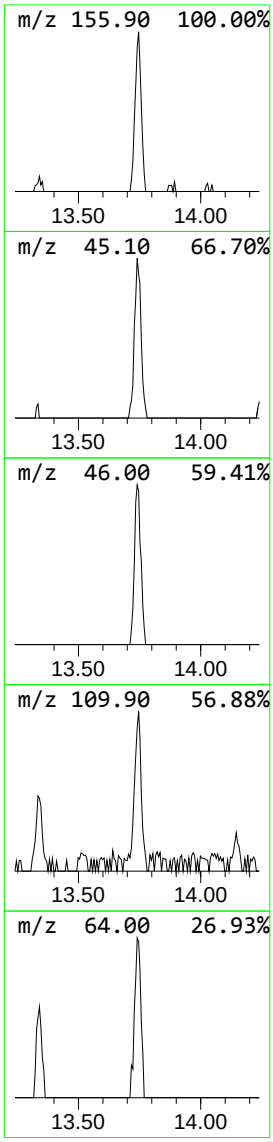
****

Peak Number 4 1,2,4,5-Tetrathiane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.740	2.08 ng	40093	Acenaphthene-d10	14.715

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	91
2	2-Fluoro-5-nitroaniline	156	C6H5FN2O2	000369-36-8	35
3	4-Fluoro-2-nitroaniline	156	C6H5FN2O2	000364-78-3	30
4	1,2-Benzenedithiol, 4-methyl-	156	C7H8S2	000496-74-2	27
5	4(1H)-Pyrimidinone, 5-methyl-2-(...	156	C6H8N2OS	020651-30-3	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060622\
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Operator : CG/JU
Sample : N3143-03
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220425-AMENDED-COMP-E

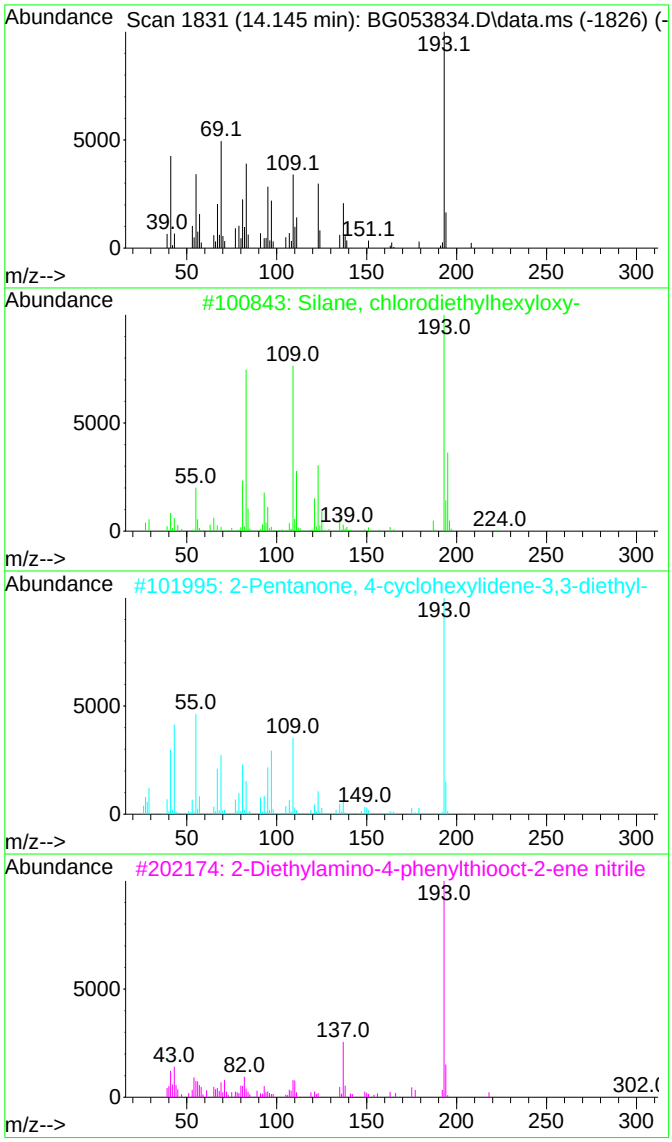
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

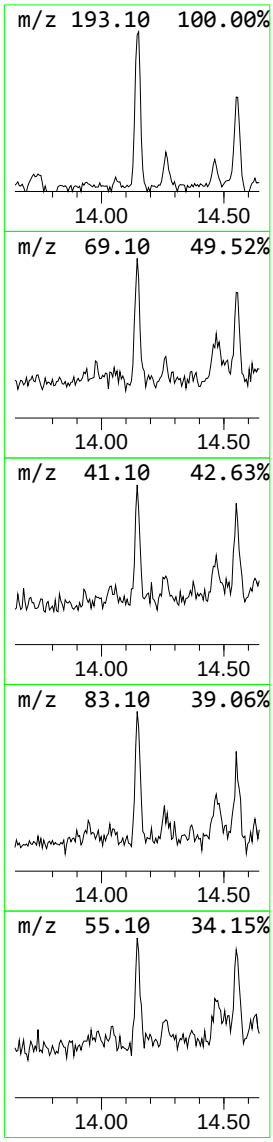
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Silane, chlorodiethylhexyloxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.145	3.14 ng	60567	Acenaphthene-d10	14.715

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	53
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	49
3	2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	38
4	benzoxazole, 5,6-dimethoxy-2-met...	193	C10H11NO3	1000395-98-9	35
5	Toxoflavin	193	C7H7N5O2	000084-82-2	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060622\
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Sample : N3143-03
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Instrument :
BNA_G
ClientSampleId :
20220425-AMENDED-COMP-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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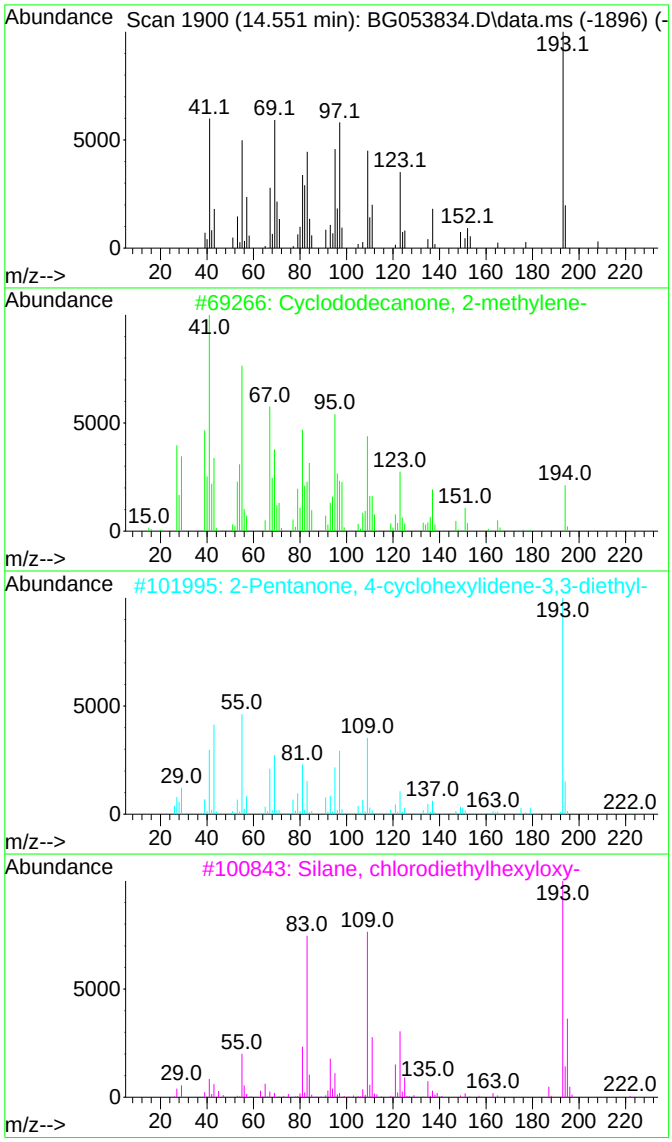
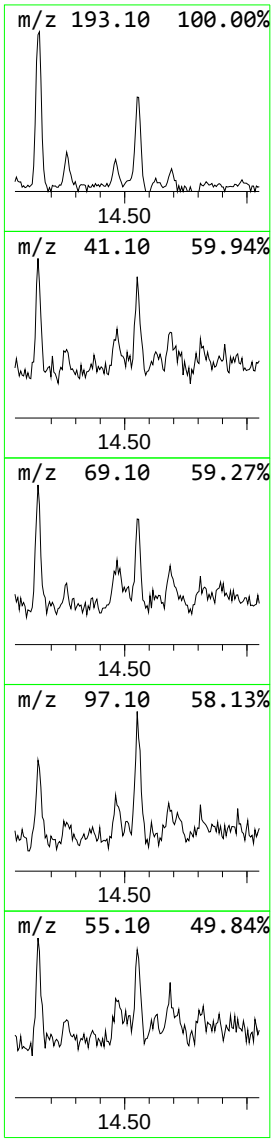
****

Peak Number 6 unknown14.551 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.551	2.63 ng	50710	Acenaphthene-d10	14.715

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	43
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	40
3	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	32
4	[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	22
5	4-Cyano-4'-methylbiphenyl	193	C14H11N	050670-50-3	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060622\
Data File : BG053834.D
Acq On : 6 Jun 2022 18:23
Operator : CG/JU
Sample : N3143-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220425-AMENDED-COMP-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

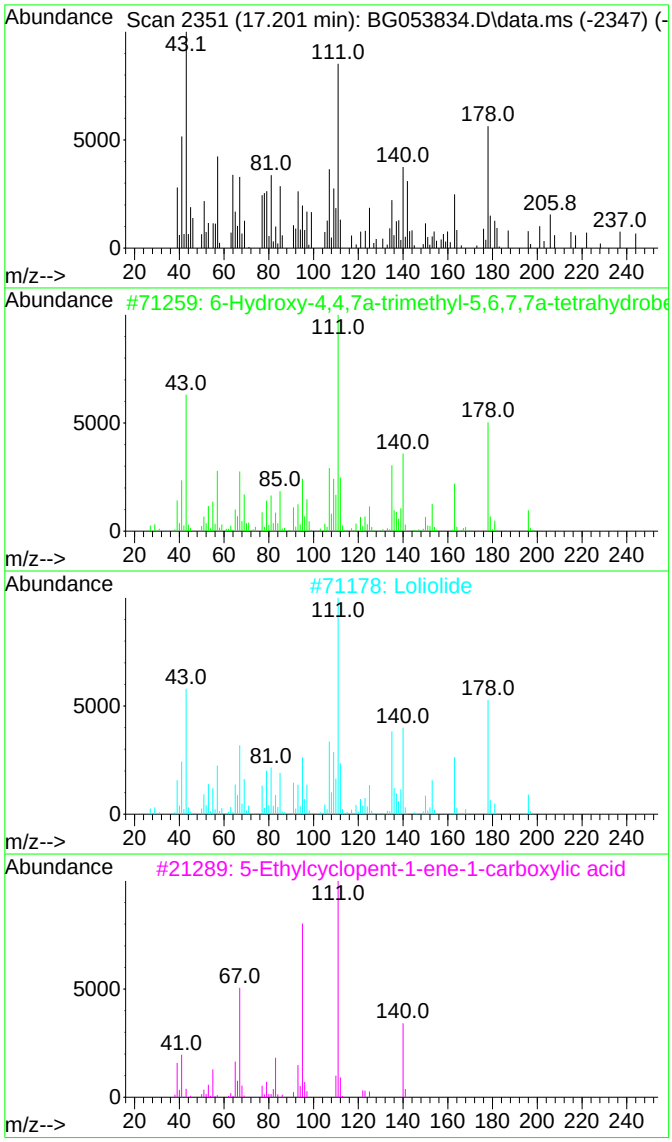
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

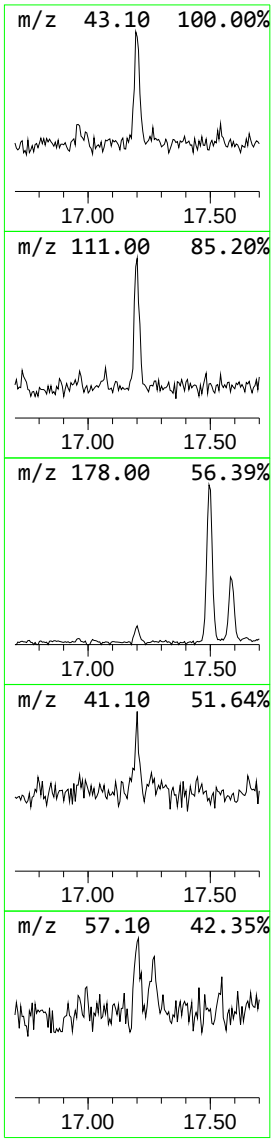
****

Peak Number 7 6-Hydroxy-4,4,7a-trimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.201	2.98 ng	68313	Phenanthrene-d10	17.453

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Hydroxy-4,4,7a-trimethyl-5,6,7...	196	C11H16O3	073410-02-3	81
2	Loliolide	196	C11H16O3	005989-02-6	81
3	5-Ethylcyclopent-1-ene-1-carboxy...	140	C8H12O2	036258-07-8	30
4	Cyclohexanebutanal, 2-methyl-3-o...	182	C11H18O2	092485-93-3	25
5	11-Oxa-tricyclo[4.4.1.0(1,6)]und...	168	C10H16O2	1000186-25-5	22





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

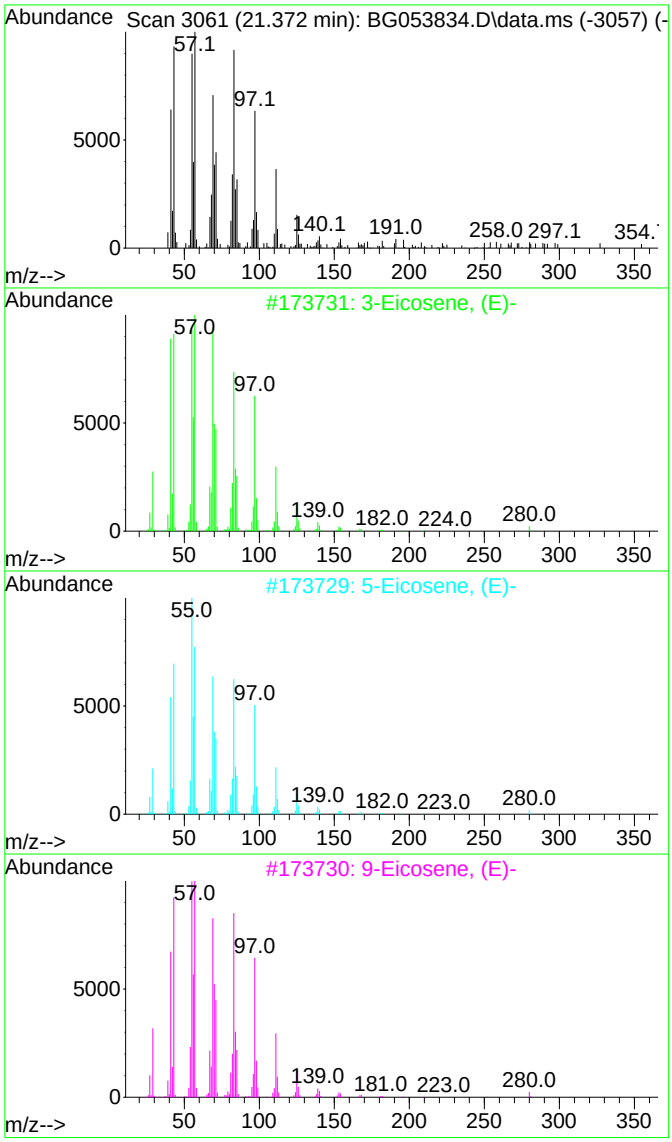
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

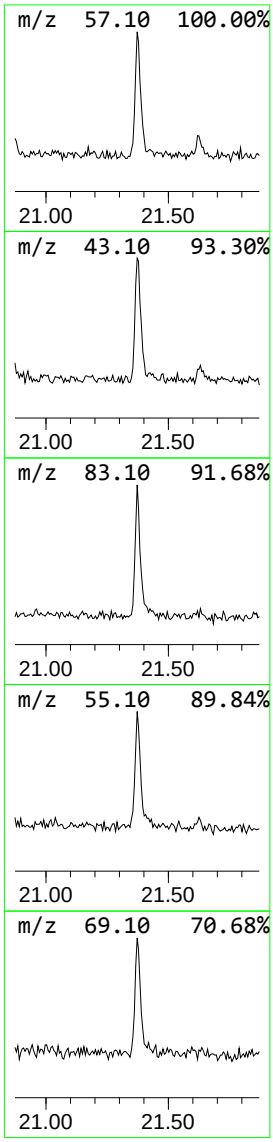
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.372	5.95 ng	165746	Chrysene-d12	21.731

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060622\
Data File : BG053834.D
Acq On : 6 Jun 2022 18:23
Operator : CG/JU
Sample : N3143-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220425-AMENDED-COMP-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.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
3-Penten-2-one,...	4.592	7.0	ng	56953	1	8.094	162565	20.0
2-Pentanone, 4-...	5.191	100.0	ng	812409	1	8.094	162565	20.0
unknown9.610	9.610	2.4	ng	29735	2	10.896	244740	20.0
1,2,4,5-Tetrath...	13.740	2.1	ng	40093	3	14.715	386320	20.0
Silane, chlorod...	14.145	3.1	ng	60567	3	14.715	386320	20.0
unknown14.551	14.551	2.6	ng	50710	3	14.715	386320	20.0
6-Hydroxy-4,4,7...	17.201	3.0	ng	68313	4	17.453	457786	20.0
3-Eicosene, (E)-	21.372	6.0	ng	165746	5	21.731	557491	20.0