LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061220\
Data File : BG045751.D
Acq On : 12 Jun 2020 22:05
Operator : CG/JU
Sample : L2993-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : AOC50MW002-200610

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-BG051520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.558	413	420	432	rBV	269027	475049	12.15%	2.816%
2	6.950	651	657	665	rBV	34054	62277	1.59%	0.369%
3	7.179	689	696	710	rBV	166452	324623	8.30%	1.925%
4	7.473	739	746	754	rBV	199907	350086	8.95%	2.076%
5	7.890	809	817	821	rBV2	115953	208535	5.33%	1.236%
6	7.949	821	827	835	rVB	197224	358448	9.17%	2.125%
7	8.272	874	882	890	rBV	686924	1199354	30.68%	7.111%
8	9.112	1017	1025	1033	rBV	543540	1024066	26.19%	6.071%
9	10.751	1296	1304	1311	rBV	261531	491947	12.58%	2.917%
10	11.661	1449	1459	1465	rBV	29150	60076	1.54%	0.356%
11	13.212	1714	1723	1734	rBV	1619890	2570925	65.76%	15.242%
12	14.040	1858	1864	1876	rBV	208260	331102	8.47%	1.963%
13	14.592	1950	1958	1968	rBV	422652	676599	17.31%	4.011%
14	16.090	2206	2213	2229	rBV	1259262	2027981	51.87%	12.023%
15	17.342	2419	2426	2438	rBV	514126	829696	21.22%	4.919%
16	18.240	2574	2579	2588	rBV2	58186	100215	2.56%	0.594%
17	19.956	2864	2871	2883	rBV	2782106	3909527	100.00%	23.178%
18	21.248	3086	3091	3099	rBV2	83482	159246	4.07%	0.944%
19	21.601	3144	3151	3165	rBV	464304	866138	22.15%	5.135%
20	24.749	3676	3687	3706	rBV	250793	841172	21.52%	4.987%

Sum of corrected areas: 16867062

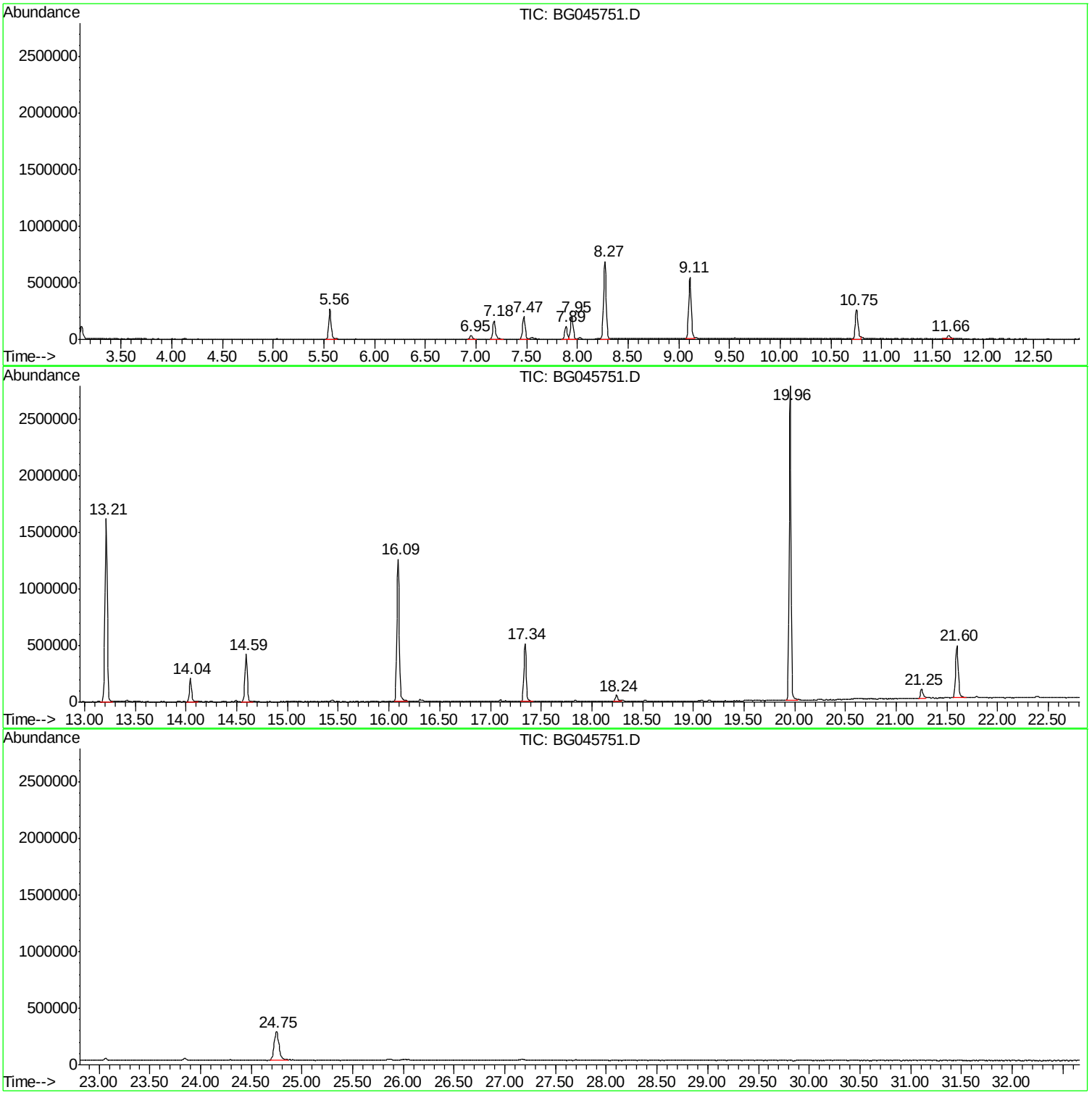
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061220\
Data File : BG045751.D
Acq On : 12 Jun 2020 22:05
Operator : CG/JU
Sample : L2993-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : AOC50MW002-200610

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061220\
Data File : BG045751.D
Acq On : 12 Jun 2020 22:05
Operator : CG/JU
Sample : L2993-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : AOC50MW002-200610

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

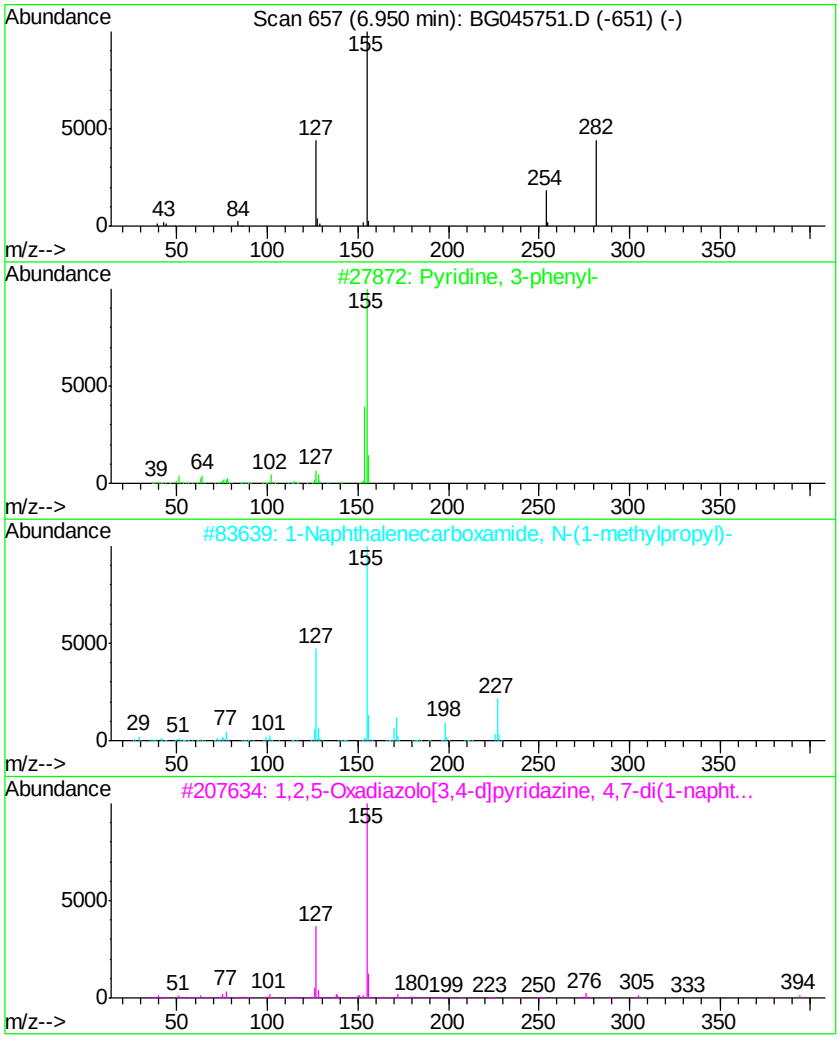
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

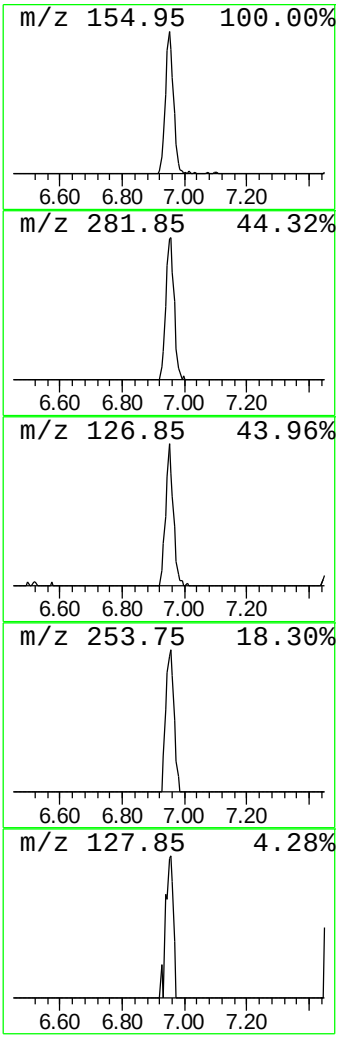
****

Peak Number 1 unknown6.95 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	3.47 ng	62277	1,4-Dichlorobenzene-d4	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 3-phenyl-	155	C11H9N	001008-88-4	9
2	1-Naphthalenecarboxamide, N-(1-m...	227	C15H17NO	031609-18-4	9
3	1,2,5-Oxadiazolo[3,4-d]pyridazin...	390	C24H14N4O2	1000276-89-8	9
4	1-Naphthalenecarboxamide, N-(1-m...	241	C16H19NO	053463-12-0	9
5	1-Naphthalen-1-yl-2-(1-phenyl-1H...	346	C19H14N4OS	1000295-34-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061220\
Data File : BG045751.D
Acq On : 12 Jun 2020 22:05
Operator : CG/JU
Sample : L2993-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : AOC50MW002-200610

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

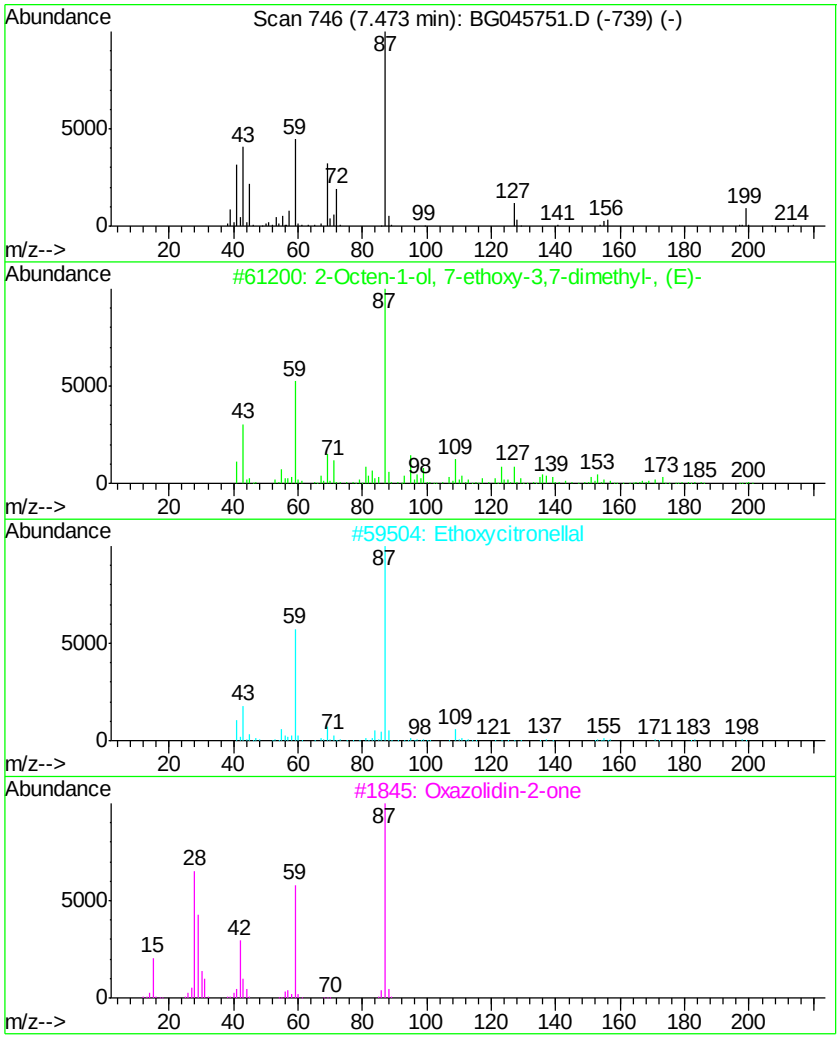
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

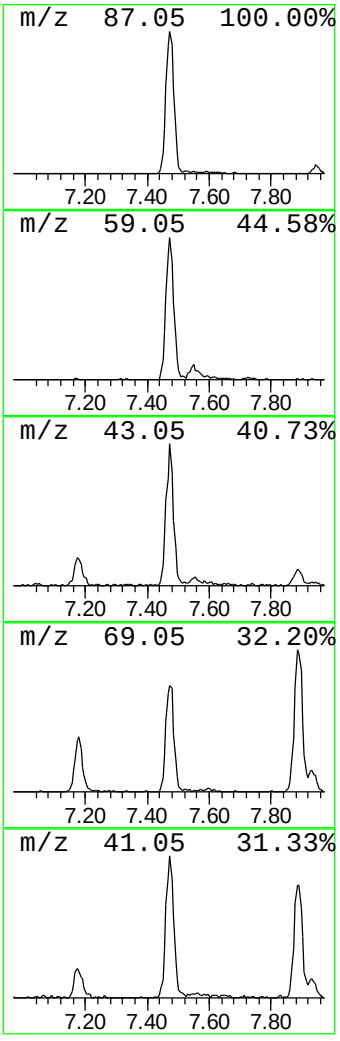
****

Peak Number 2 2-Octen-1-ol, 7-ethoxy-3,7-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	19.53 ng	350086	1,4-Dichlorobenzene-d4	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octen-1-ol, 7-ethoxy-3,7-dimet...	200	C12H24O2	1000132-19-5	53
2	Ethoxycitronellal	198	C12H22O2	1000132-02-6	50
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	50
4	N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	47
5	2-[2-[2-[2-(2-Methoxyethoxy)etho...	294	C13H26O7	1000351-91-3	45





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061220\
Data File : BG045751.D
Acq On : 12 Jun 2020 22:05
Operator : CG/JU
Sample : L2993-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : AOC50MW002-200610

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

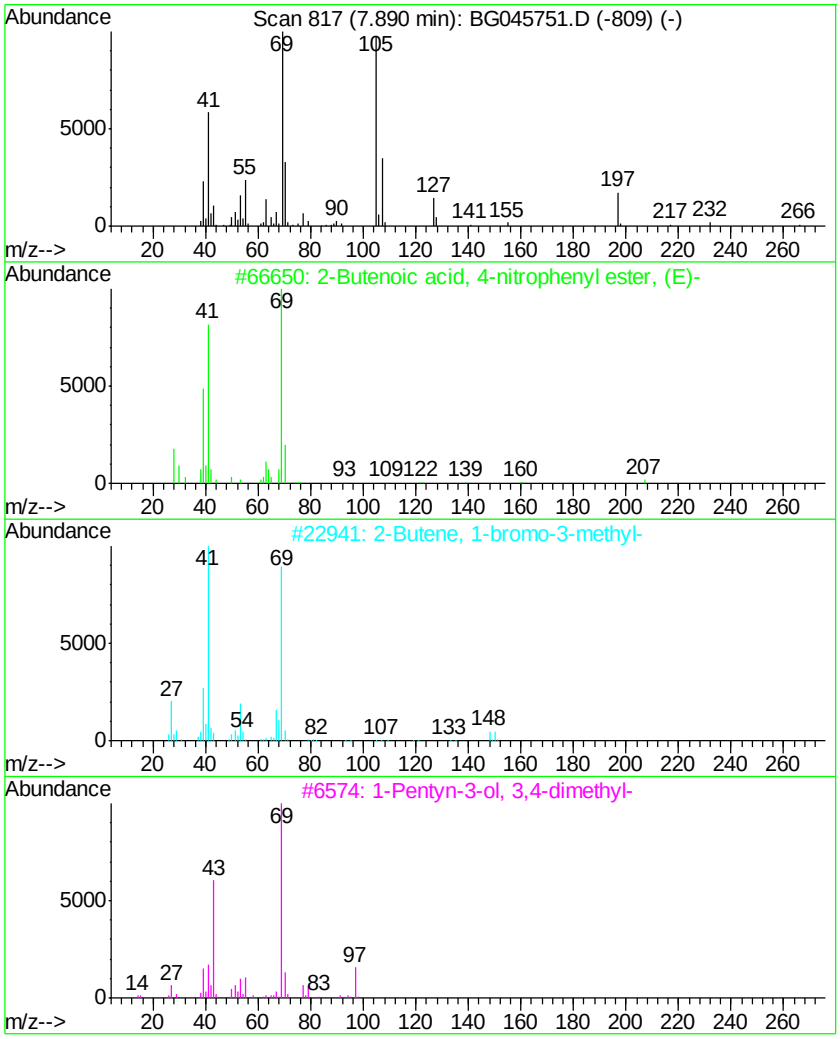
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

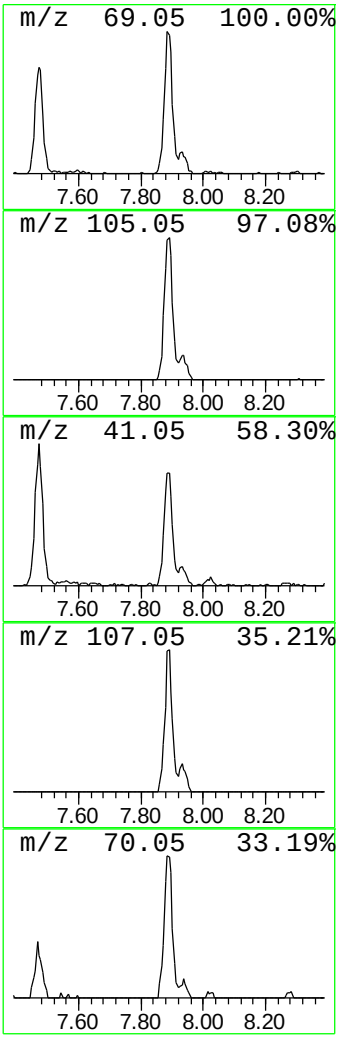
****

Peak Number 3 unknown7.89 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.89	11.64 ng	208535	1,4-Dichlorobenzene-d4	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	014617-88-0	38
2	2-Butene, 1-bromo-3-methyl-	148	C5H9Br	000870-63-3	35
3	1-Pentyn-3-ol, 3,4-dimethyl-	112	C7H12O	001482-15-1	23
4	2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	035665-90-8	17
5	1,2,4-Triazole, 3-trifluromethyl...	197	C5H6F3N3S	054770-35-3	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061220\
Data File : BG045751.D
Acq On : 12 Jun 2020 22:05
Operator : CG/JU
Sample : L2993-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : AOC50MW002-200610

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

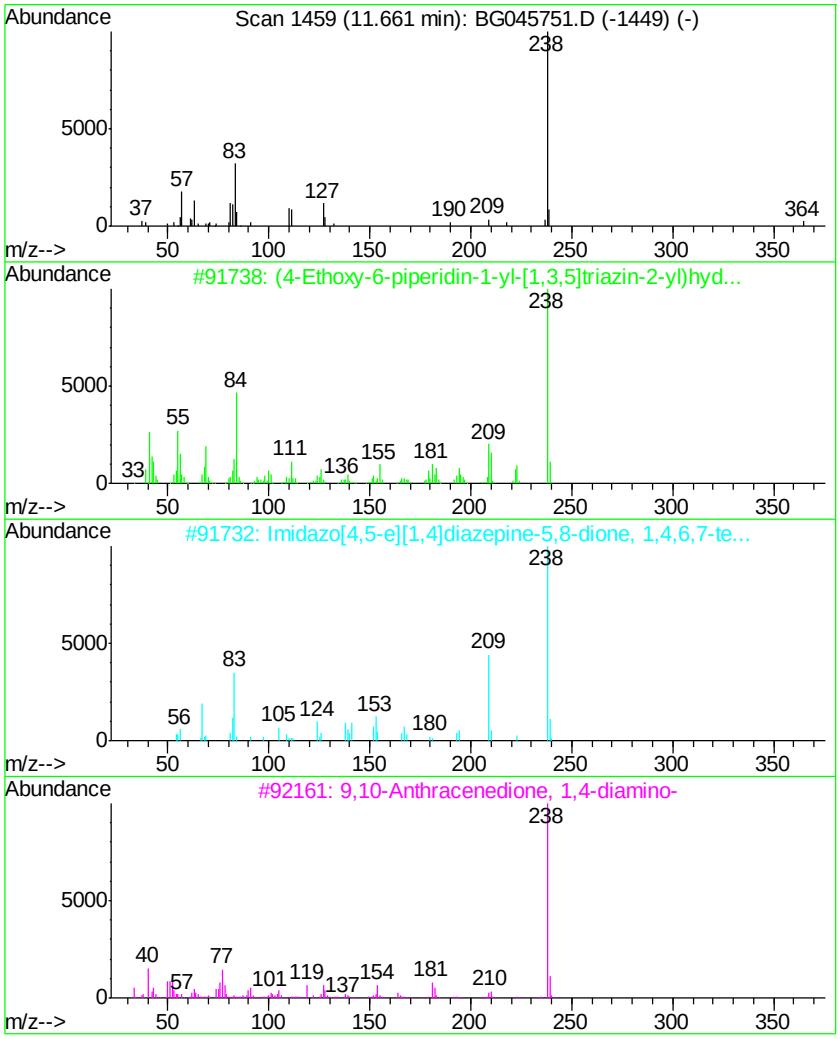
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

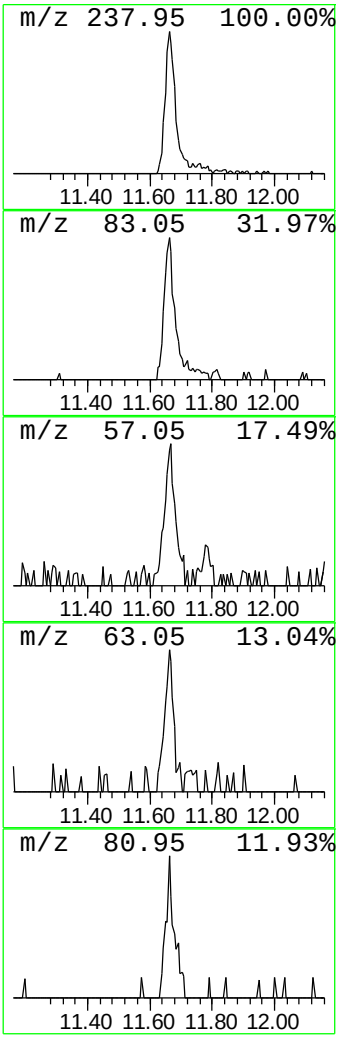
****

Peak Number 5 unknown11.66 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	2.44 ng	60076	Naphthalene-d8	10.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4-Ethoxy-6-piperidin-1-yl-[1,3,...	238	C10H18N6O	1000302-56-6	9
2	Imidazo[4,5-e][1,4]diazepine-5,8...	238	C10H14N4O3	077246-18-5	9
3	9,10-Anthracenedione, 1,4-diamino-	238	C14H10N2O2	000128-95-0	9
4	5-Iodofuran-2-carboxylic acid	238	C5H3IO3	1000311-58-2	9
5	5-Iodouracil	238	C4H3IN2O2	000696-07-1	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061220\
Data File : BG045751.D
Acq On : 12 Jun 2020 22:05
Operator : CG/JU
Sample : L2993-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : AOC50MW002-200610

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

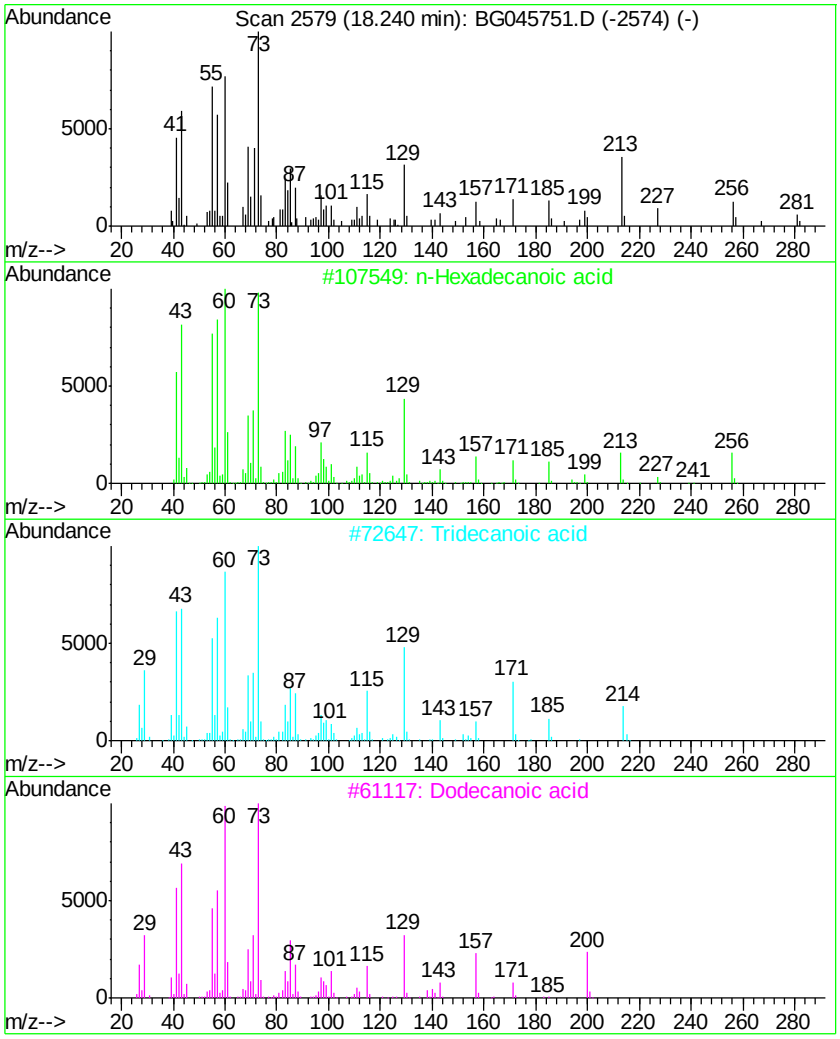
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

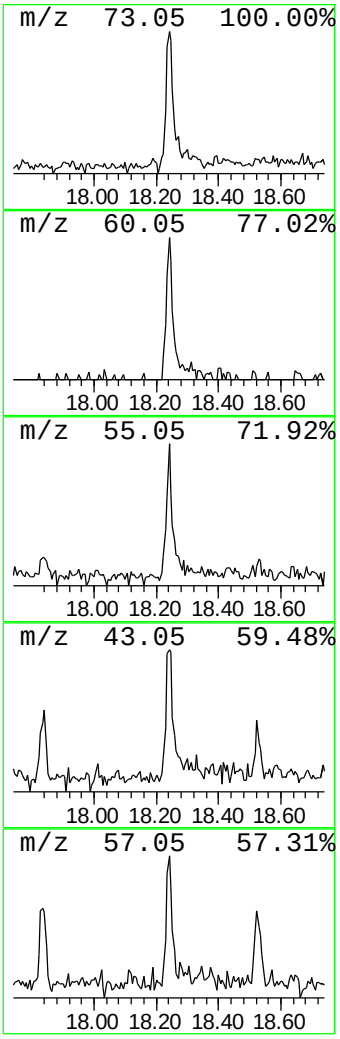
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	2.42 ng	100215	Phenanthrene-d10	17.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Dodecanoic acid	200	C12H24O2	000143-07-7	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061220\
Data File : BG045751.D
Acq On : 12 Jun 2020 22:05
Operator : CG/JU
Sample : L2993-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : AOC50MW002-200610

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

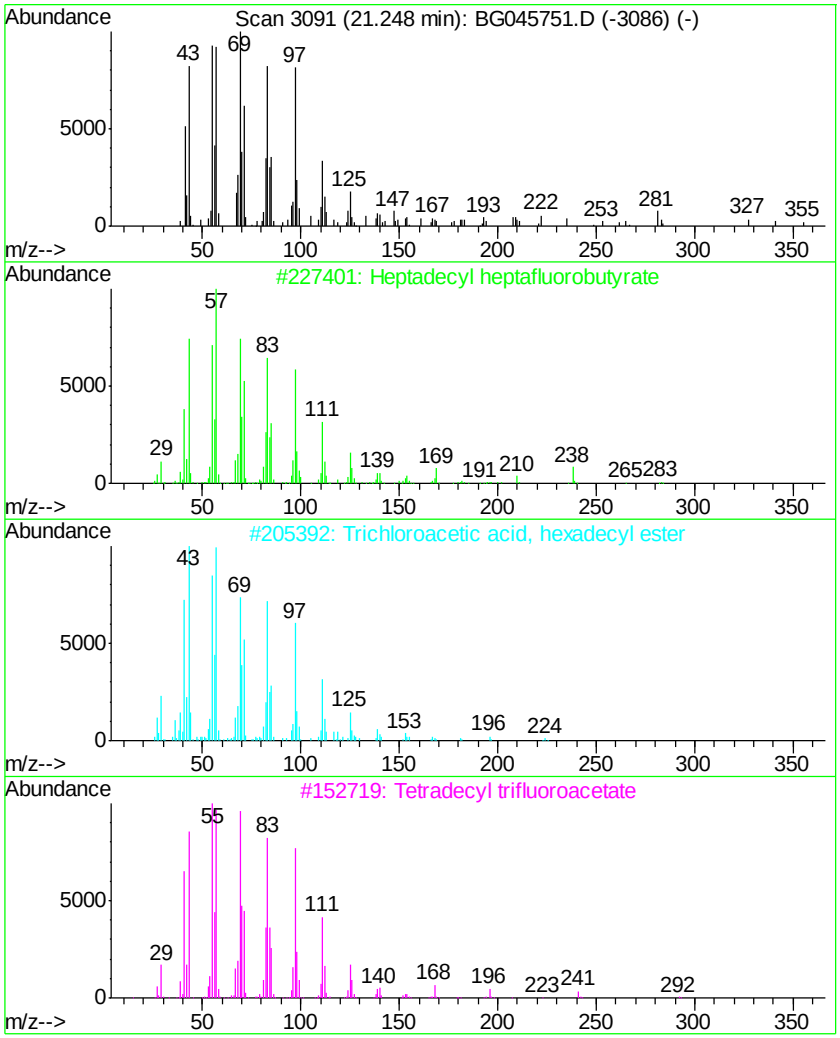
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

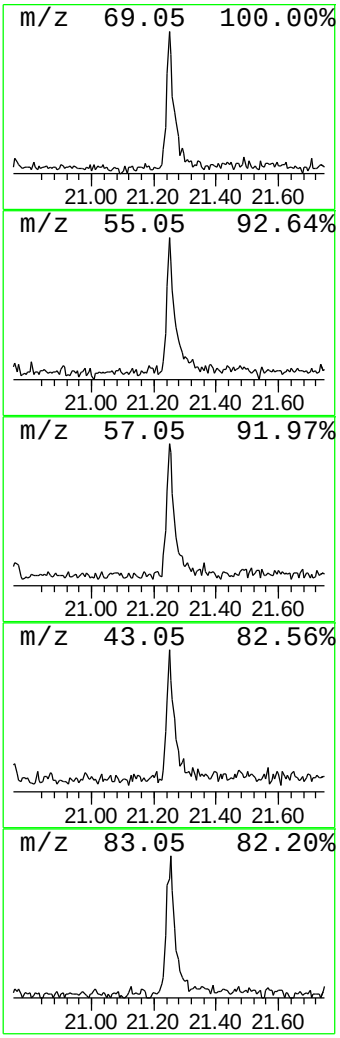
****

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.25	3.68 ng	159246	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG061220\
Data File : BG045751.D
Acq On : 12 Jun 2020 22:05
Operator : CG/JU
Sample : L2993-02
Misc :
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Instrument : BNA_G
ClientSampleId : AOC50MW002-200610

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.95	6.95	3.5	ng	62277	1	7.95	358448	20.0
2-Octen-1-ol, 7-e...	7.47	19.5	ng	350086	1	7.95	358448	20.0
unknown7.89	7.89	11.6	ng	208535	1	7.95	358448	20.0
unknown11.66	11.66	2.4	ng	60076	2	10.76	491947	20.0
n-Hexadecanoic acid	18.24	2.4	ng	100215	4	17.34	829696	20.0
Heptadecyl heptaf...	21.25	3.7	ng	159246	5	21.60	866138	20.0