LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046712.D
Acq On : 25 Sep 2020 21:51
Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

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-BG092220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG046712.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.211	13	21	30	rBV4	120843	359493	8.68%	1.535%
2	3.293	30	35	40	rVV3	64917	129724	3.13%	0.554%
3	3.816	120	124	130	rBV	32121	53419	1.29%	0.228%
4	5.221	358	363	372	rBV2	43417	74303	1.79%	0.317%
5	5.685	434	442	451	rBV	1221201	1938965	46.81%	8.278%
6	7.271	703	712	723	rBV	1233215	2141251	51.69%	9.142%
7	7.706	780	786	792	rBV2	88425	144681	3.49%	0.618%
8	8.123	849	857	865	rBV	302654	508216	12.27%	2.170%
9	9.286	1045	1055	1064	rBV	806912	1436434	34.68%	6.133%
10	10.932	1327	1335	1343	rBV	383568	703155	16.97%	3.002%
11	13.370	1740	1750	1757	rBV	1979486	3038060	73.34%	12.970%
12	13.640	1790	1796	1802	rVB	158993	248713	6.00%	1.062%
13	14.187	1882	1889	1895	rBV	319491	486325	11.74%	2.076%
14	14.745	1976	1984	1992	rVB	613073	952254	22.99%	4.065%
15	16.225	2229	2236	2245	rBV	1580646	2374917	57.33%	10.139%
16	17.489	2444	2451	2456	rBV	713800	1109073	26.77%	4.735%
17	18.376	2596	2602	2611	rBV2	264818	425402	10.27%	1.816%
18	19.527	2794	2798	2803	rBV	89381	123799	2.99%	0.529%
19	19.639	2813	2817	2820	rBV3	90065	116414	2.81%	0.497%
20	20.091	2888	2894	2900	rBV	3090683	4142527	100.00%	17.686%
21	21.408	3114	3118	3129	rVB	300833	485826	11.73%	2.074%
22	21.766	3173	3179	3184	rBV	687209	1102804	26.62%	4.708%
23	22.618	3322	3324	3340	rVB6	92743	256590	6.19%	1.095%
24	25.050	3730	3738	3749	rVB2	383014	1070900	25.85%	4.572%

Sum of corrected areas: 23423245

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
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Misc :
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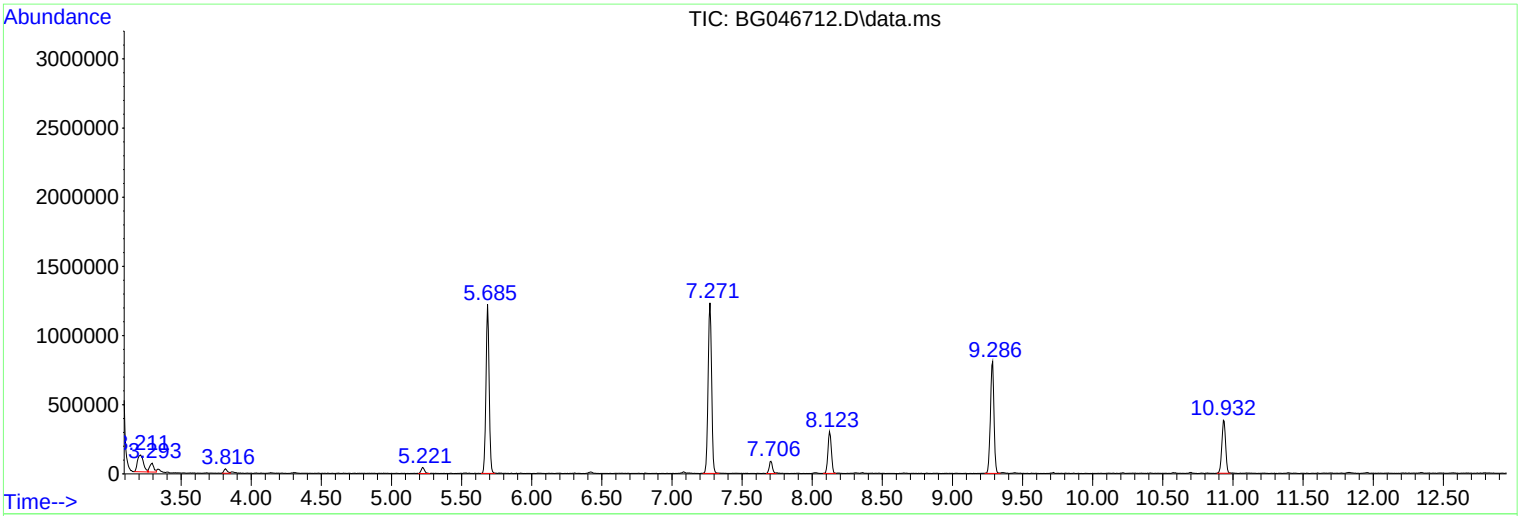
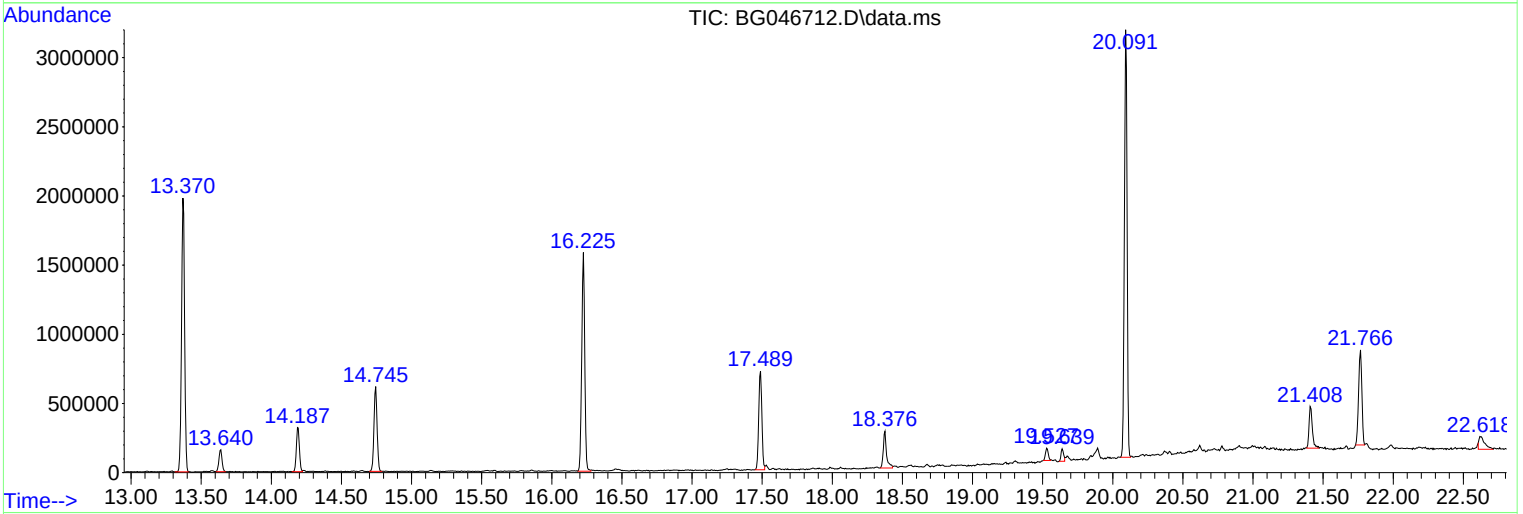
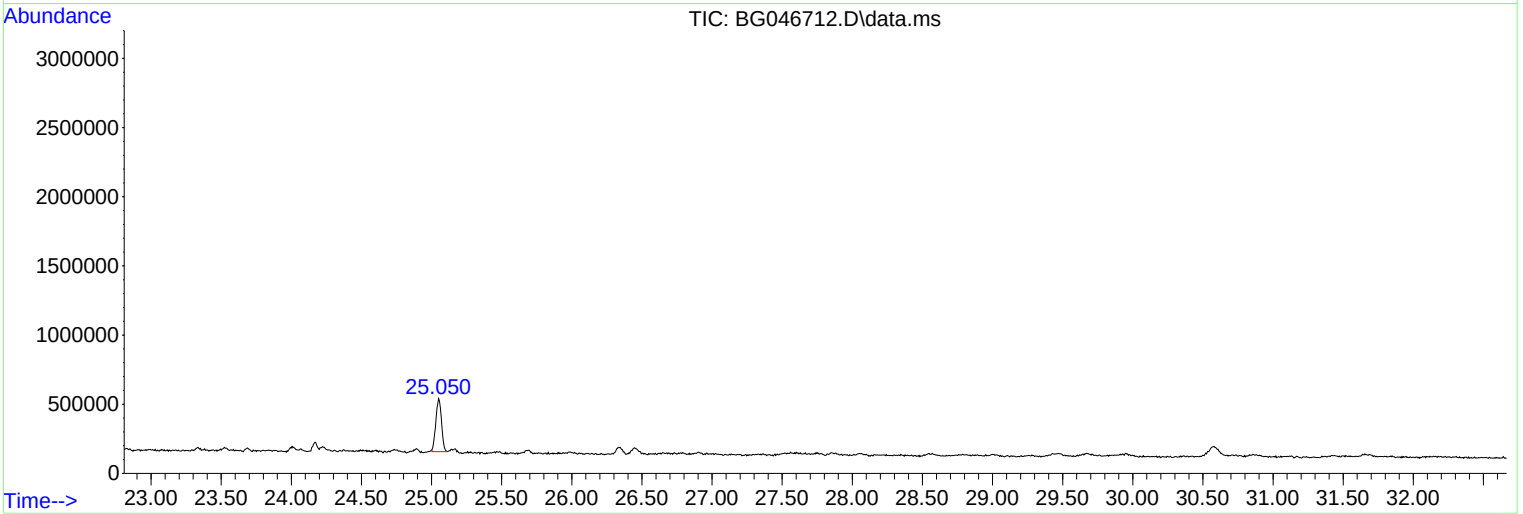
Instrument :
BNA_G
ClientSampleId :
FK-GF-02-061-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

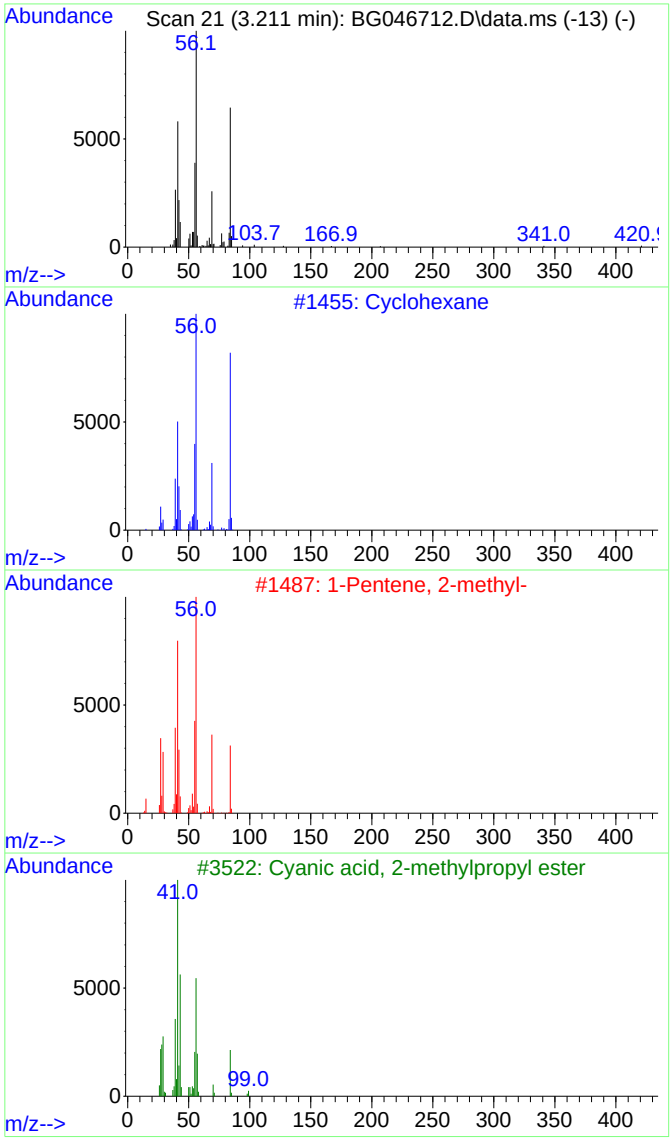
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

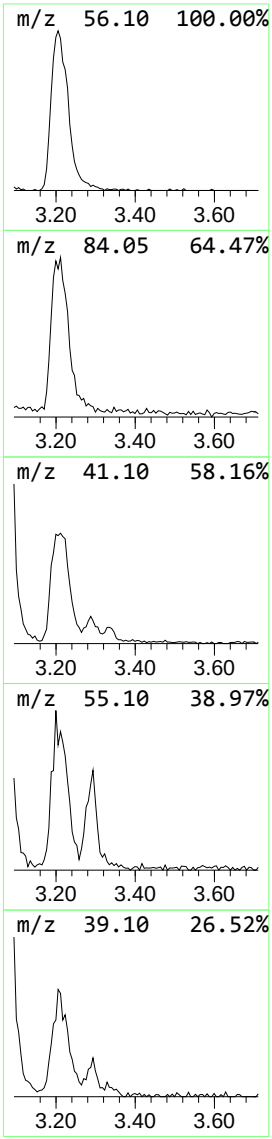
****

Peak Number 1 Cyclohexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.211	14.15 ng	359493	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	94
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	86
3	Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	72
4	Cyclobutane	56	C4H8	000287-23-0	46
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046712.D
Acq On : 25 Sep 2020 21:51
Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

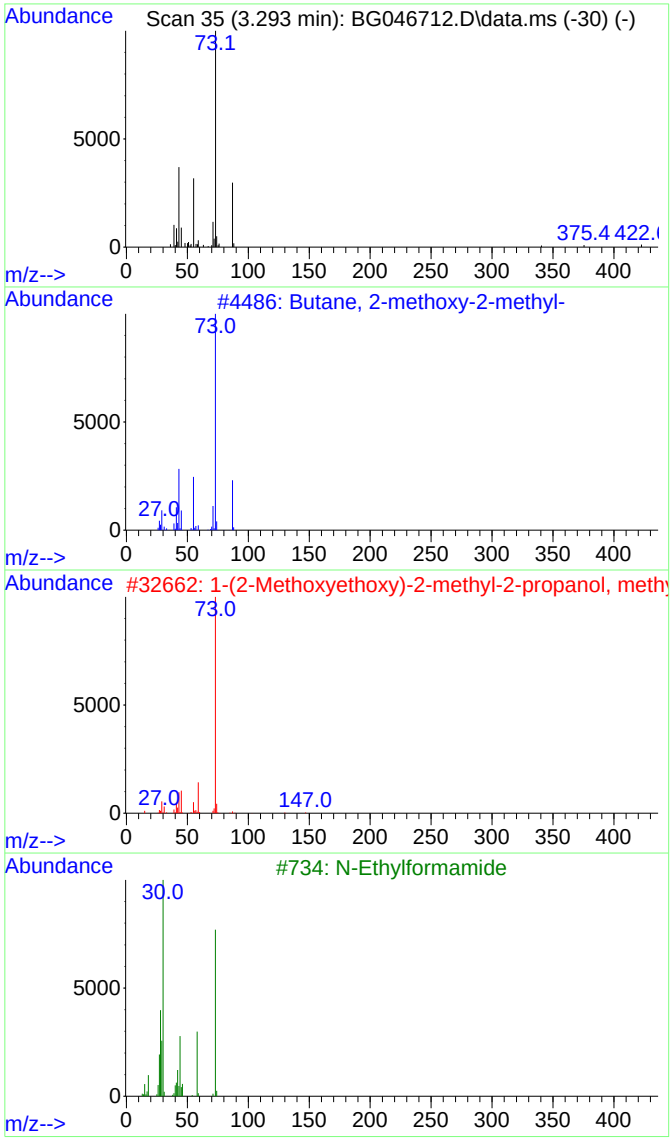
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

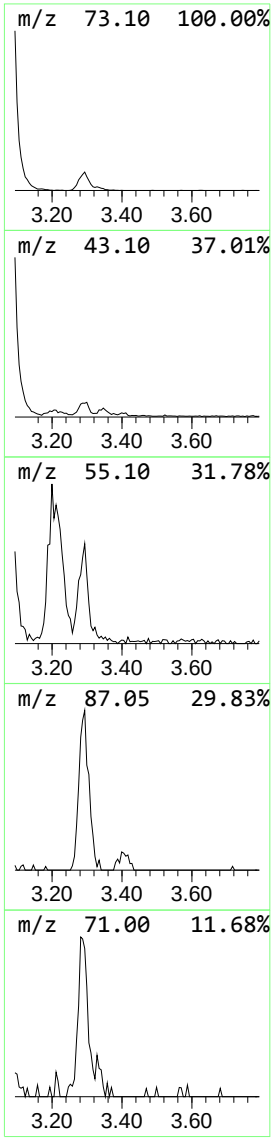
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.293	5.11 ng	129724	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	10
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046712.D
Acq On : 25 Sep 2020 21:51
Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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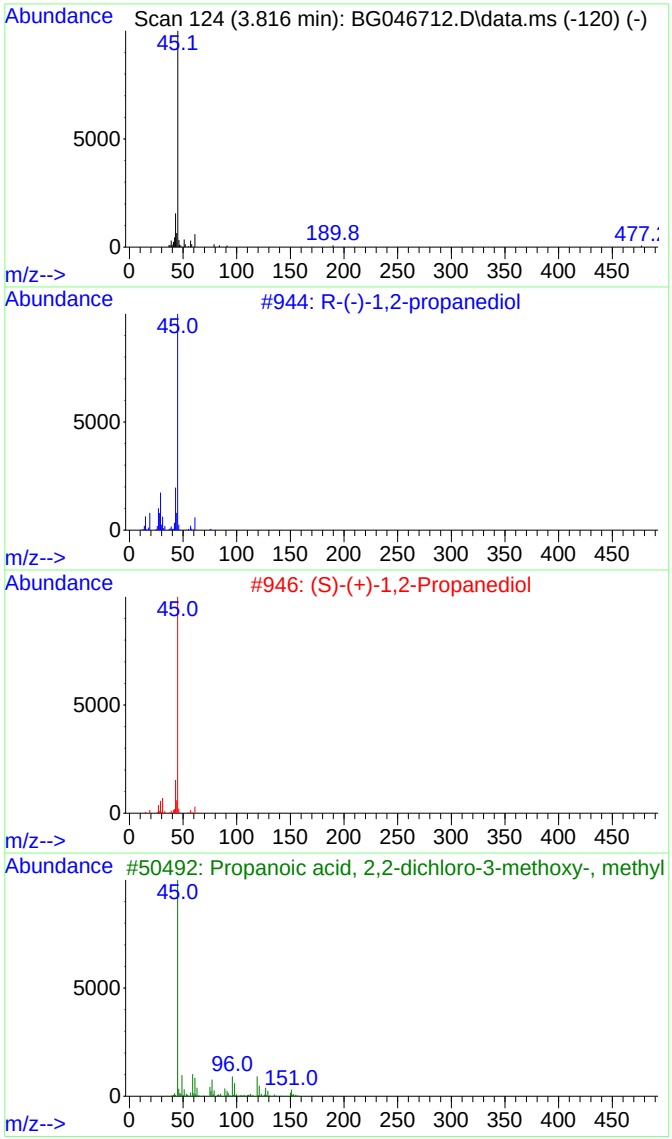
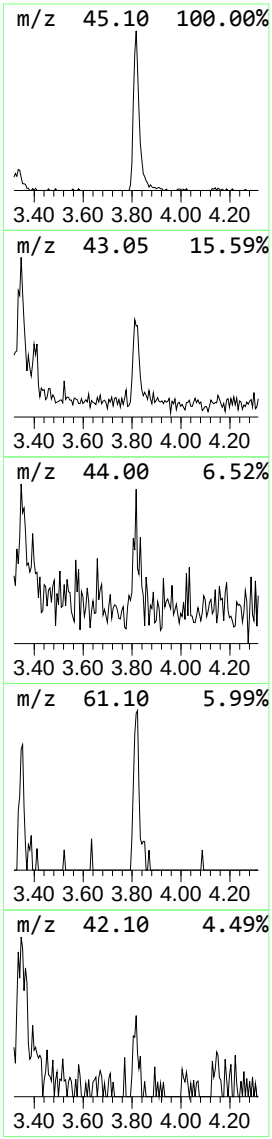
****

Peak Number 3 unknown3.816 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	2.10 ng	53419	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3	Propanoic acid, 2,2-dichloro-3-m...	186	C5H8Cl2O3	027579-25-5	39
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	39
5	2-Propanol, 1-chloro-	94	C3H7ClO	000127-00-4	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046712.D
Acq On : 25 Sep 2020 21:51
Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-061-B

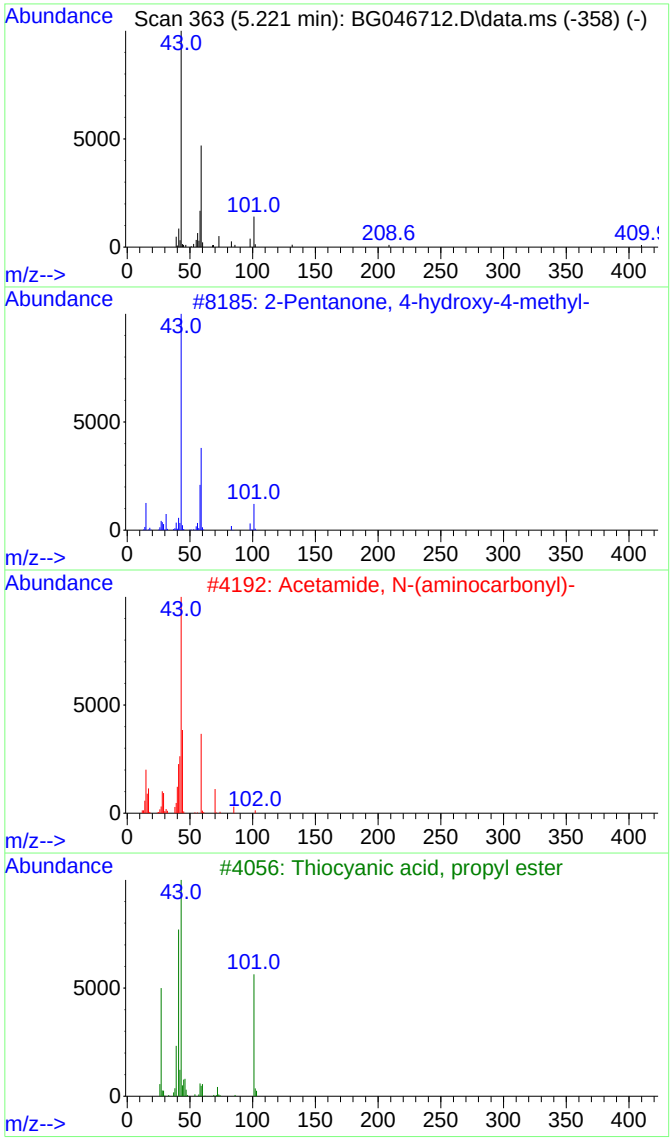
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

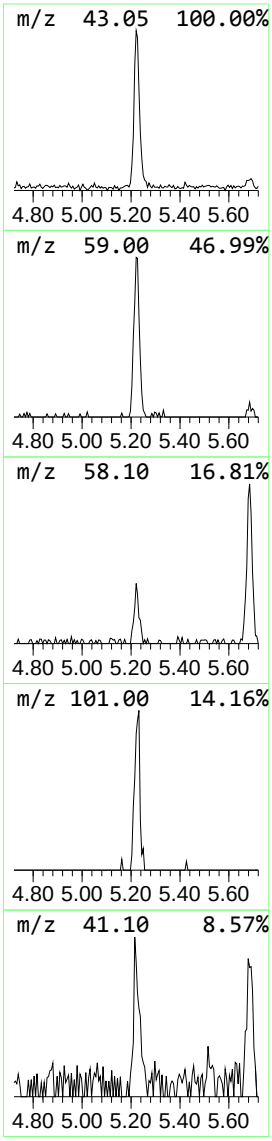
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.221	2.92 ng	74303	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
3	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046712.D
Acq On : 25 Sep 2020 21:51
Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

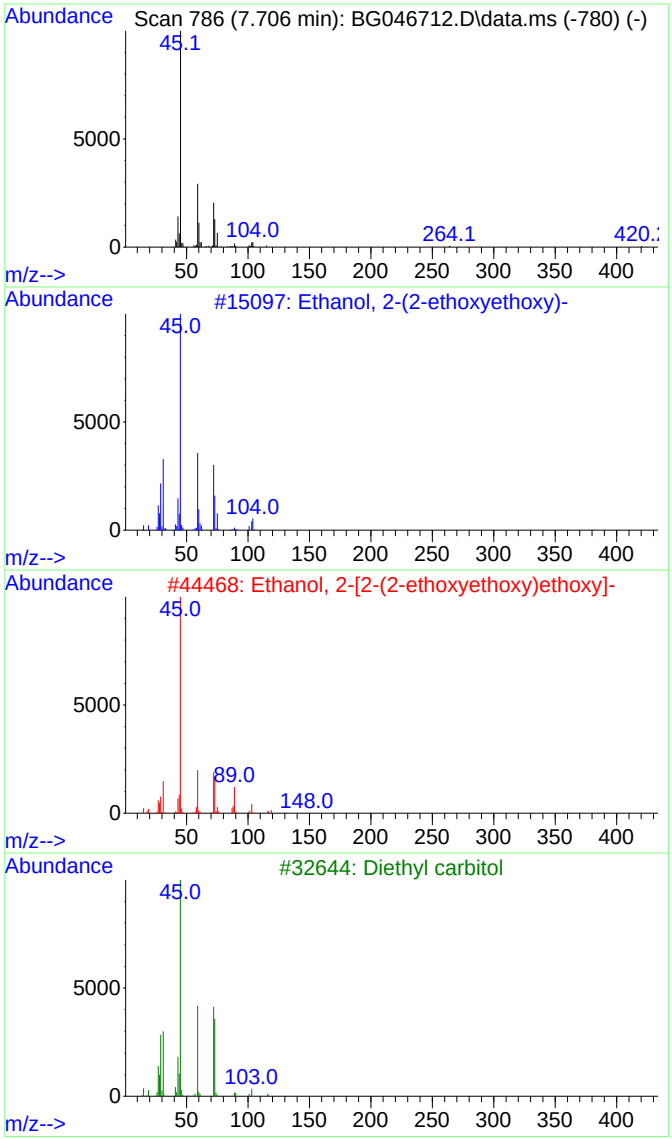
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

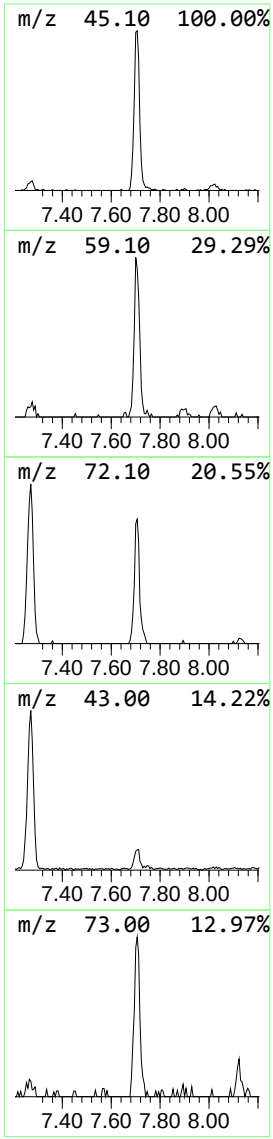
****

Peak Number 5 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.706	5.69 ng	144681	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39
3	Diethyl carbitol	162	C8H18O3	000112-36-7	38
4	Methoxyacetic acid, 2-methylprop...	146	C7H14O3	1000282-40-9	38
5	.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046712.D
Acq On : 25 Sep 2020 21:51
Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
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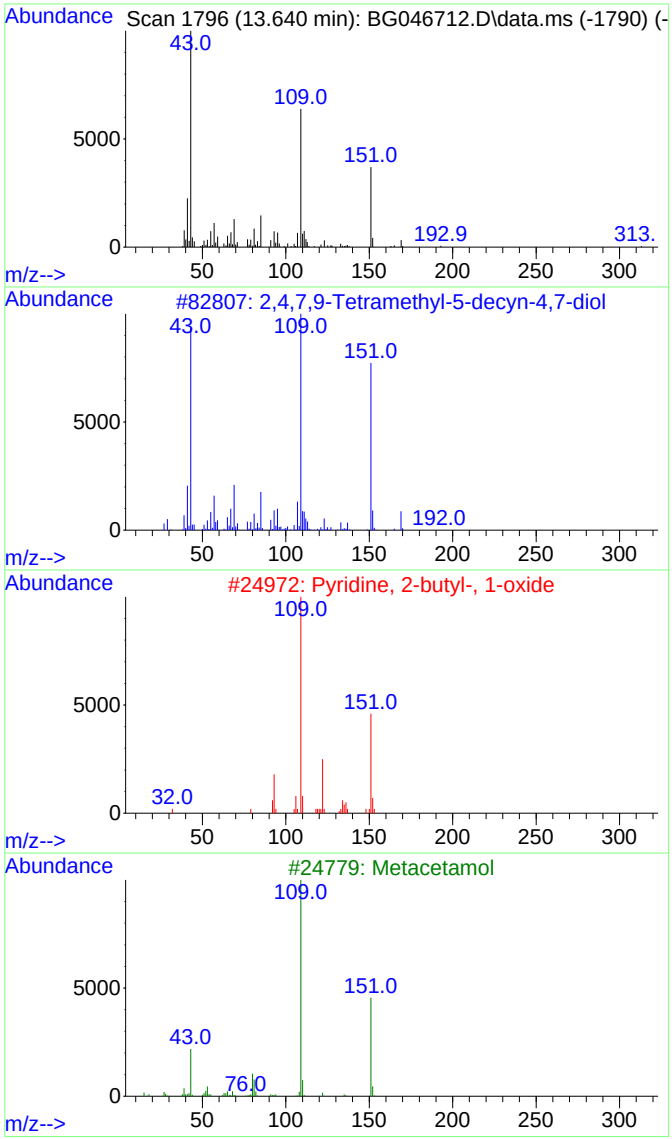
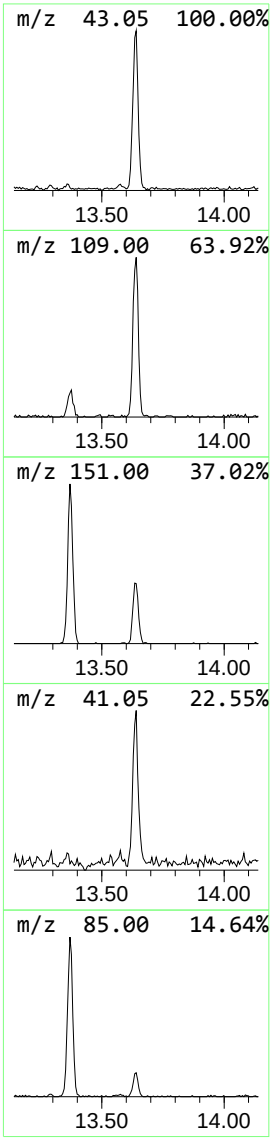
****
Peak Number 6 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.640	5.22 ng	248713	Acenaphthene-d10	14.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	83
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3	Metacetamol	151	C8H9NO2	000621-42-1	49
4	Acetaminophen	151	C8H9NO2	000103-90-2	47
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	47





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Data File : BG046712.D
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Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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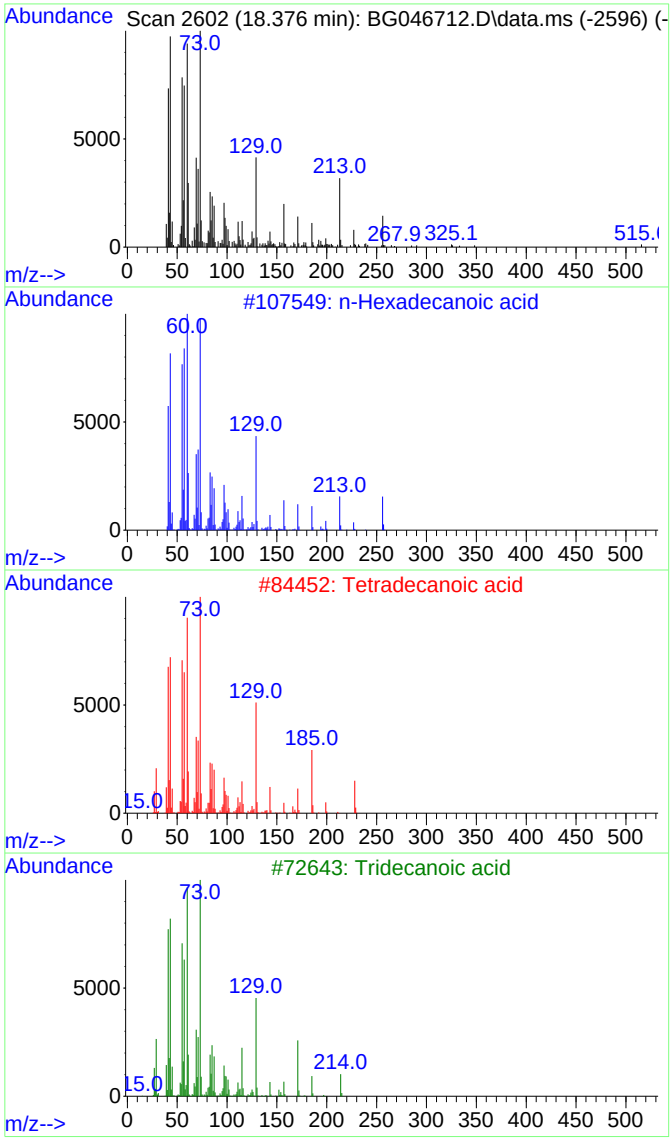
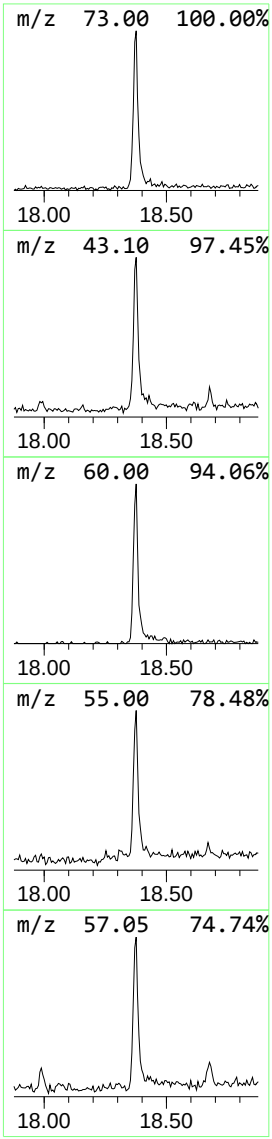
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.376	7.67 ng	425402	Phenanthrene-d10	17.489

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	83





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Misc :
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Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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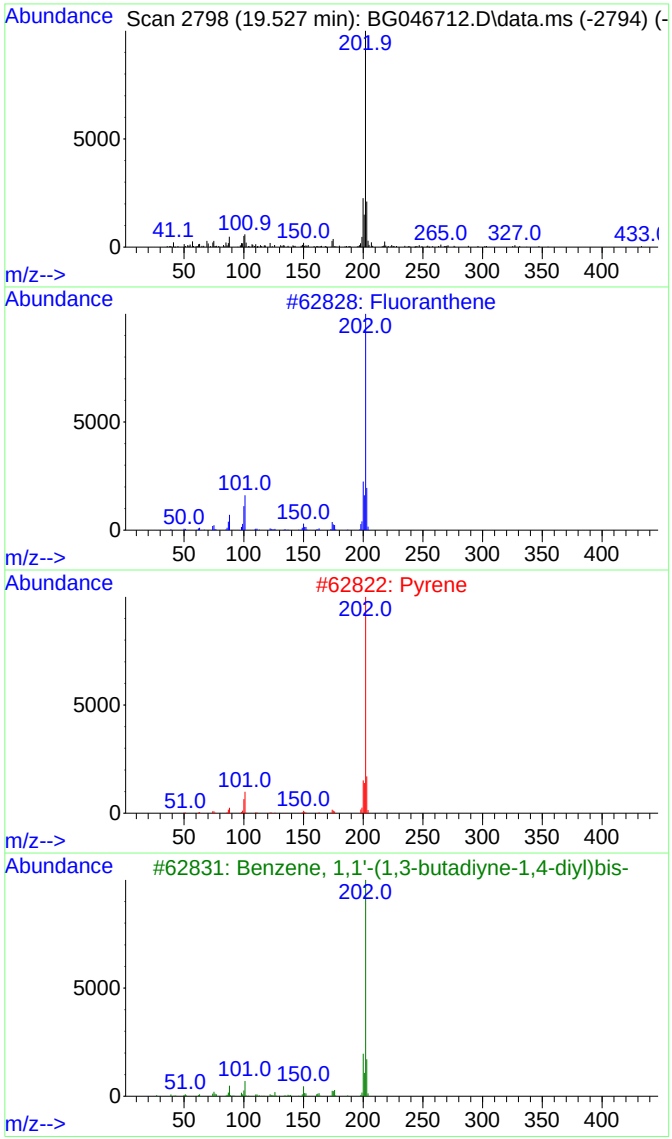
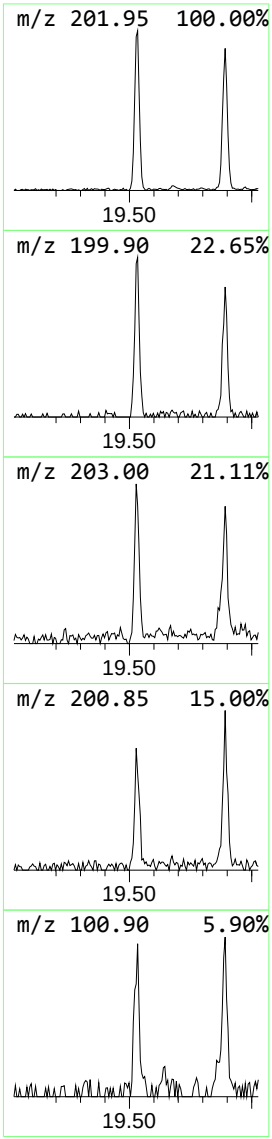
****

Peak Number 8 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.527	2.23 ng	123799	Phenanthrene-d10	17.489

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	81
2	Pyrene	202	C16H10	000129-00-0	76
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	72
4	2-Butenamide, 3-methyl-N-1H-puri...	217	C10H11N5O	021589-34-4	43
5	1H-Indole-3-propanoic acid, 1-(t...	275	C15H21NO2Si	056196-72-6	38





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Data File : BG046712.D
Acq On : 25 Sep 2020 21:51
Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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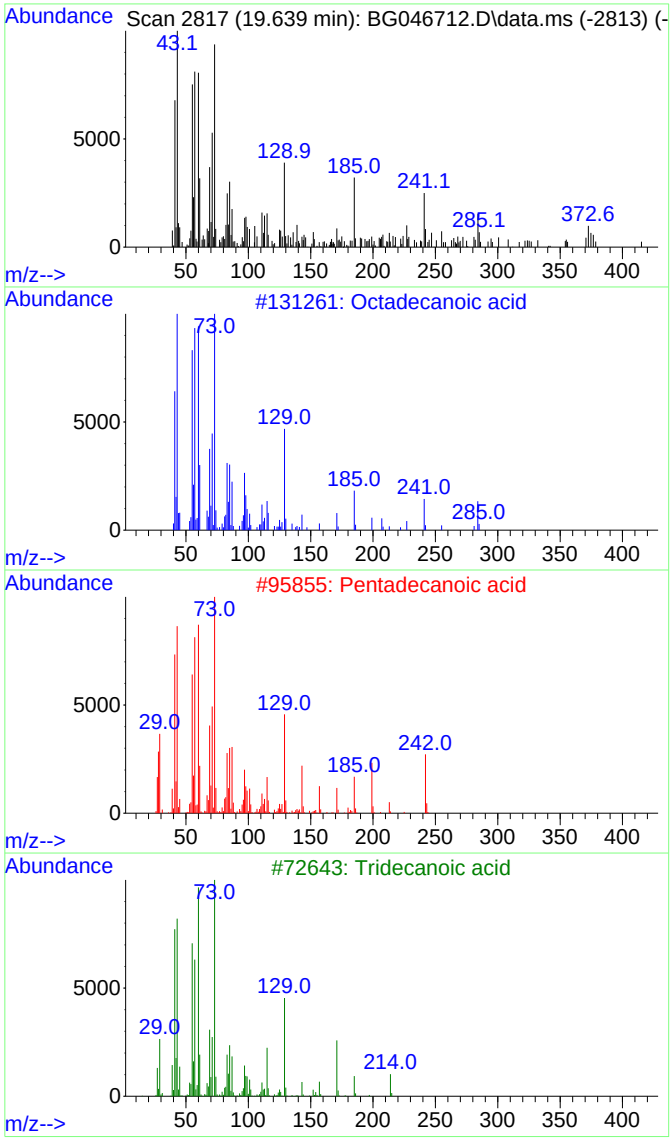
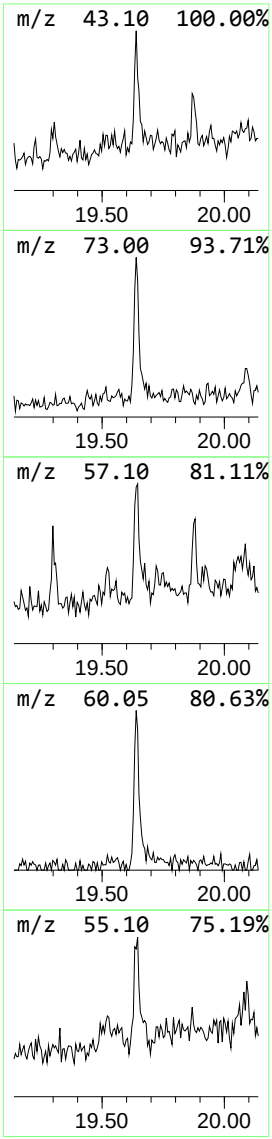
****

Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.639	2.11 ng	116414	Chrysene-d12	21.766

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tridecanoic acid	214	C13H26O2	000638-53-9	60
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





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Data File : BG046712.D
Acq On : 25 Sep 2020 21:51
Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

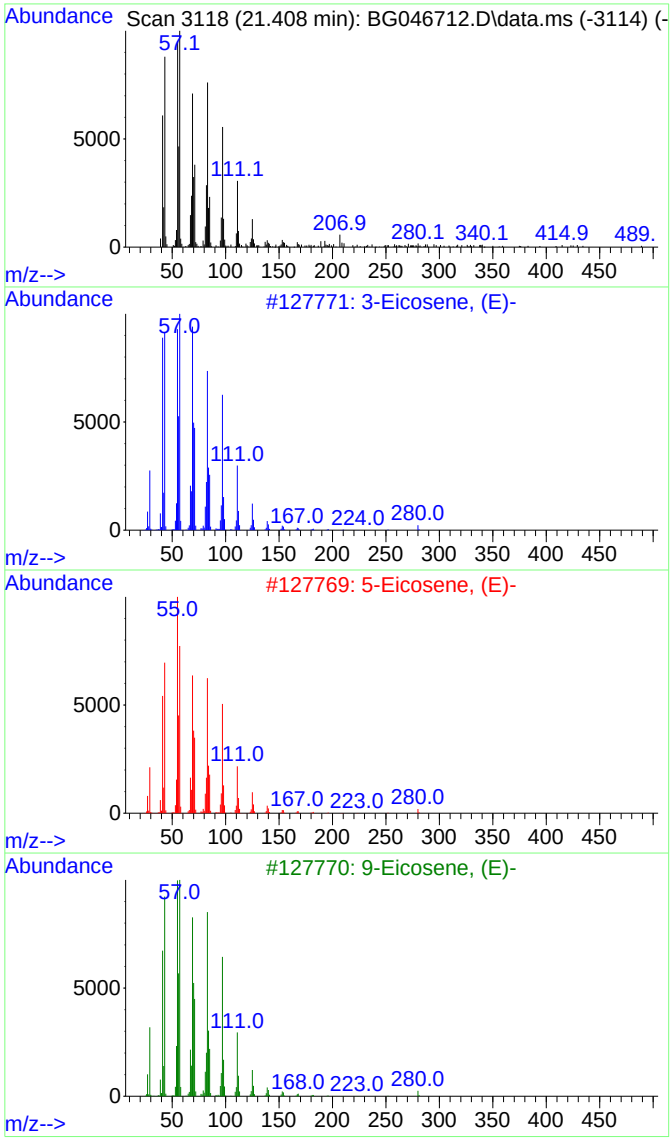
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

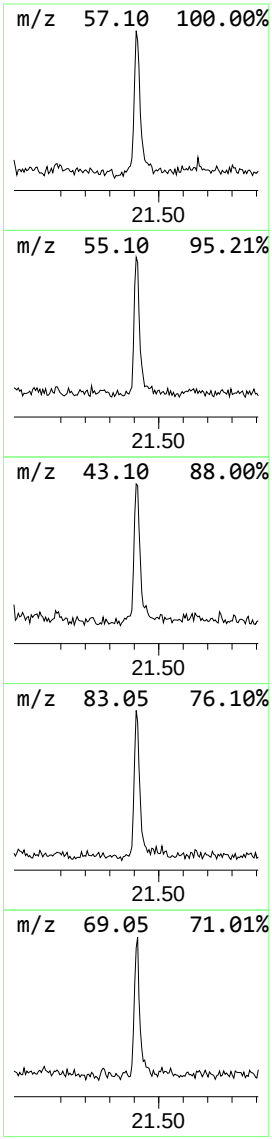
****

Peak Number 10 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.408	8.81 ng	485826	Chrysene-d12	21.766

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	Cycloeicosane	280	C20H40	000296-56-0	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	94





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Data File : BG046712.D
Acq On : 25 Sep 2020 21:51
Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

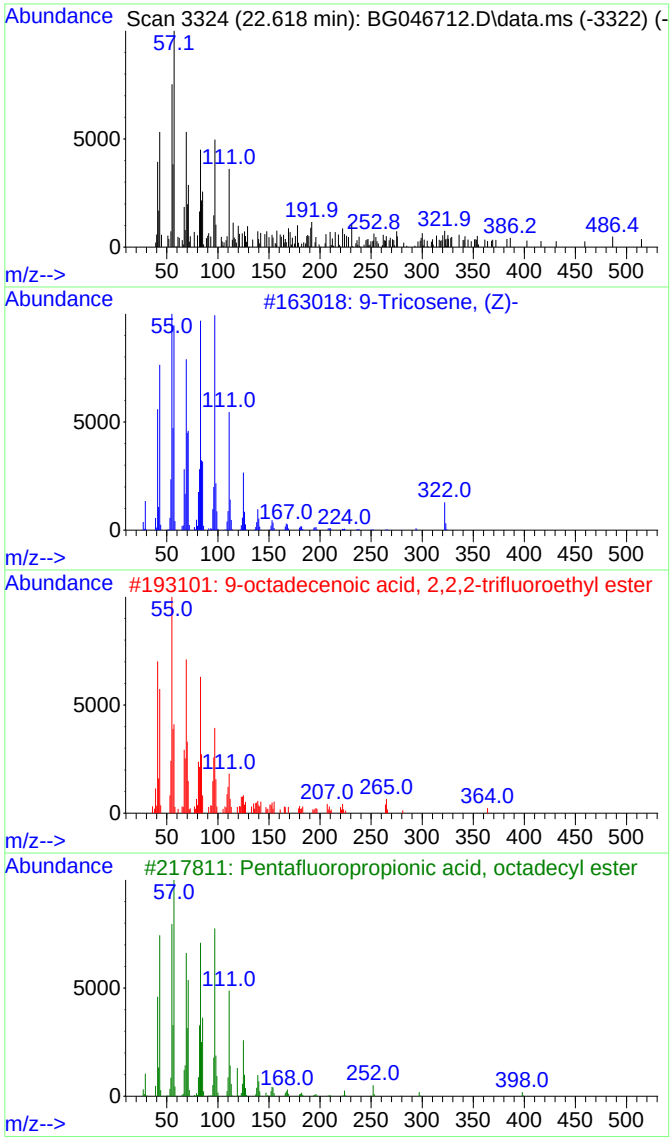
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

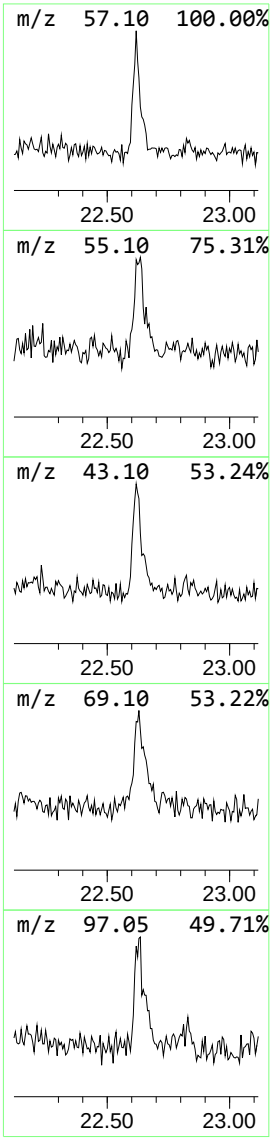
****

Peak Number 11 9-Tricosene, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.618	4.65 ng	256590	Chrysene-d12	21.766

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	86
2	9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	64
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	62
4	2-Methyl-E-7-hexadecene	238	C17H34	064183-52-4	58
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092520\
Data File : BG046712.D
Acq On : 25 Sep 2020 21:51
Operator : CG/JU
Sample : L4155-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FK-GF-02-061-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.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
Cyclohexane	3.211	14.2	ng	359493	1	8.123	508216	20.0
Butane, 2-metho...	3.293	5.1	ng	129724	1	8.123	508216	20.0
unknown3.816	3.816	2.1	ng	53419	1	8.123	508216	20.0
2-Pentanone, 4-...	5.221	2.9	ng	74303	1	8.123	508216	20.0
Ethanol, 2-(2-e...	7.706	5.7	ng	144681	1	8.123	508216	20.0
2,4,7,9-Tetrame...	13.640	5.2	ng	248713	3	14.745	952254	20.0
n-Hexadecanoic ...	18.376	7.7	ng	425402	4	17.489	1109070	20.0
Benzene, 1,1'-(...	19.527	2.2	ng	123799	4	17.489	1109070	20.0
Octadecanoic acid	19.639	2.1	ng	116414	5	21.766	1102800	20.0
3-Eicosene, (E)-	21.408	8.8	ng	485826	5	21.766	1102800	20.0
9-Tricosene, (Z)-	22.618	4.7	ng	256590	5	21.766	1102800	20.0