LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062623\
Data File : BF133965.D
Acq On : 26 Jun 2023 22:09
Operator : CG\JU
Sample : 03365-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

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_F\Methods\8270-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133965.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	17	26	33	rBV	140406	217764	8.90%	1.693%
2	5.087	505	510	515	rBV	161535	222216	9.09%	1.727%
3	5.487	574	578	581	rBV	2398626	2199332	89.94%	17.095%
4	5.657	603	607	613	rVB	138471	140090	5.73%	1.089%
5	6.292	709	715	718	rBV	189237	210803	8.62%	1.639%
6	6.492	744	749	756	rVB	2152402	2263106	92.54%	17.591%
7	6.851	807	810	813	rBV	1594427	1364533	55.80%	10.606%
8	7.416	902	906	909	rBV	1494365	1301186	53.21%	10.114%
9	8.133	1024	1028	1031	rBV	1888067	1516704	62.02%	11.789%
10	8.910	1156	1160	1166	rBV2	197891	463698	18.96%	3.604%
11	9.122	1194	1196	1199	rBV3	113233	125370	5.13%	0.974%
12	9.210	1207	1211	1219	rBV	1850264	2445436	100.00%	19.008%
13	9.286	1221	1224	1227	rBV	291089	394829	16.15%	3.069%

Sum of corrected areas: 12865067

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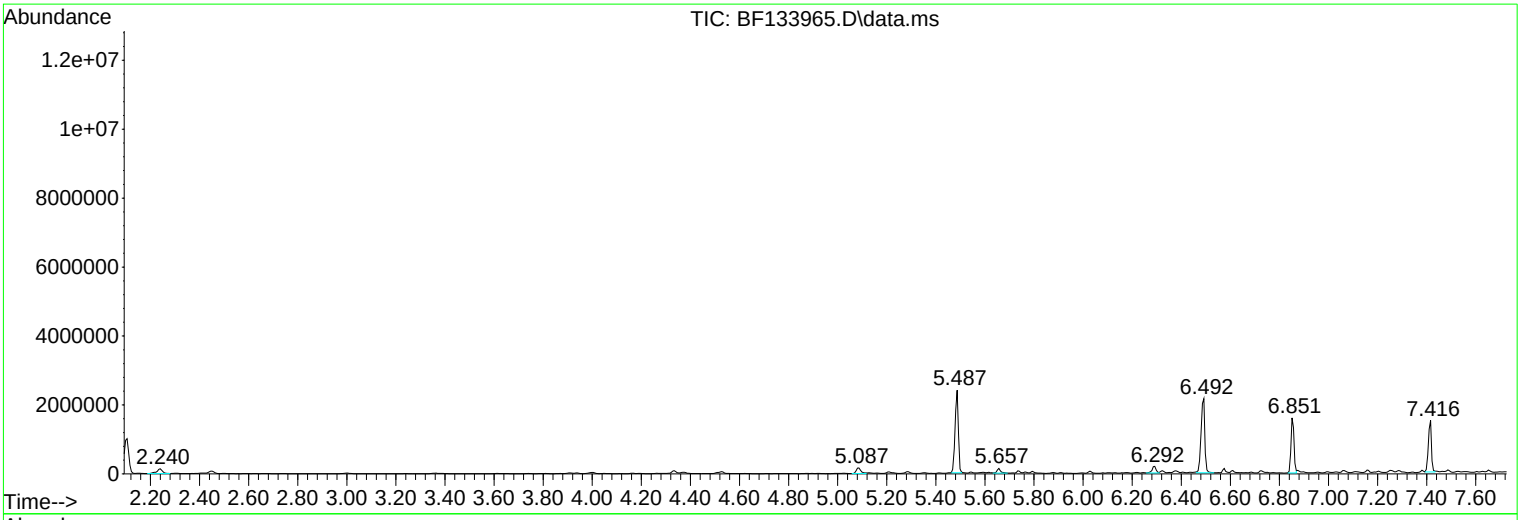
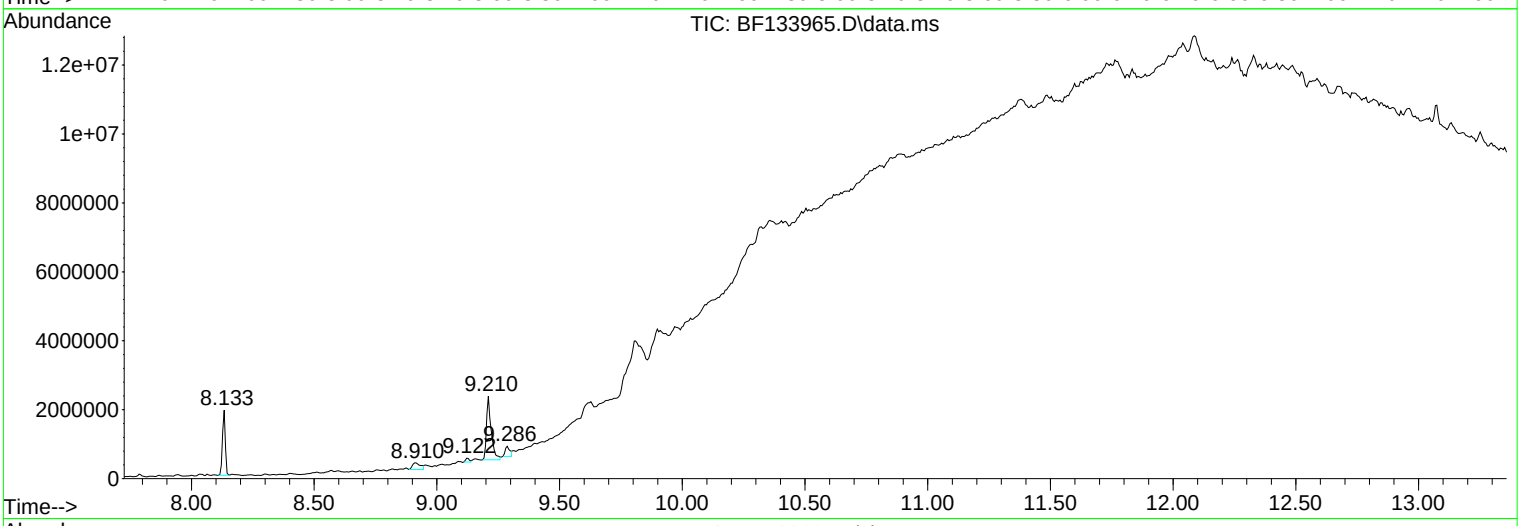
Misc :
ALS Vial : 13 Sample Multiplier: 1

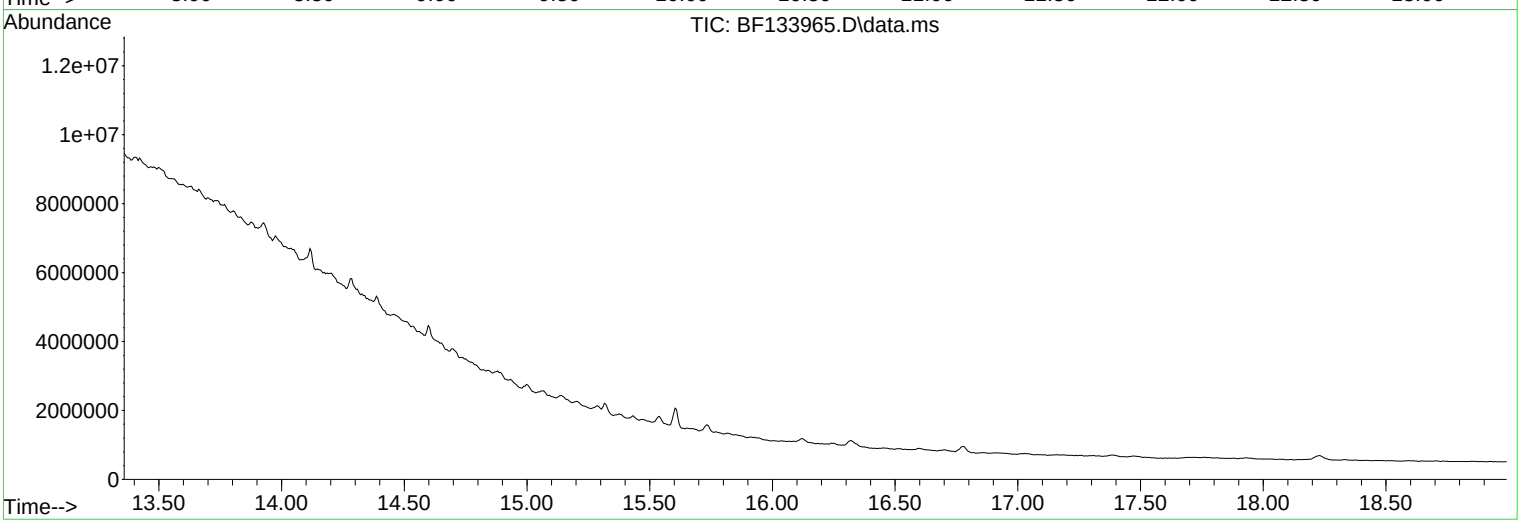
Instrument :
BNA_F
ClientSampleId :
TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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_F\Data\BF062623\
Data File : BF133965.D
Acq On : 26 Jun 2023 22:09
Operator : CG\JU
Sample : 03365-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

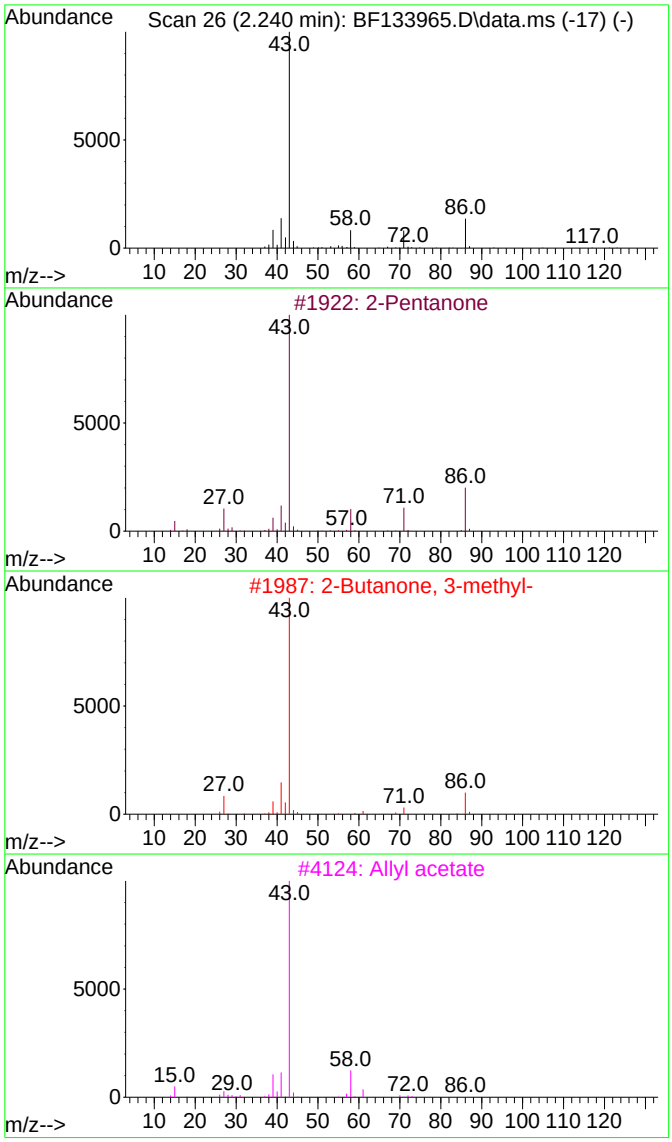
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

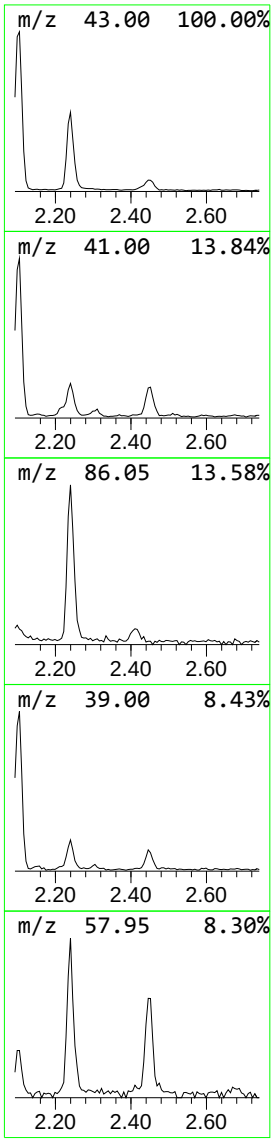
****

Peak Number 1 2-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	3.19 ng	217764	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	86
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
3	Allyl acetate	100	C5H8O2	000591-87-7	25
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	12
5	3-Aminopyrrolidine	86	C4H10N2	079286-79-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062623\
Data File : BF133965.D
Acq On : 26 Jun 2023 22:09
Operator : CG\JU
Sample : 03365-13
Misc :
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Instrument :
BNA_F
ClientSampleId :
TP4

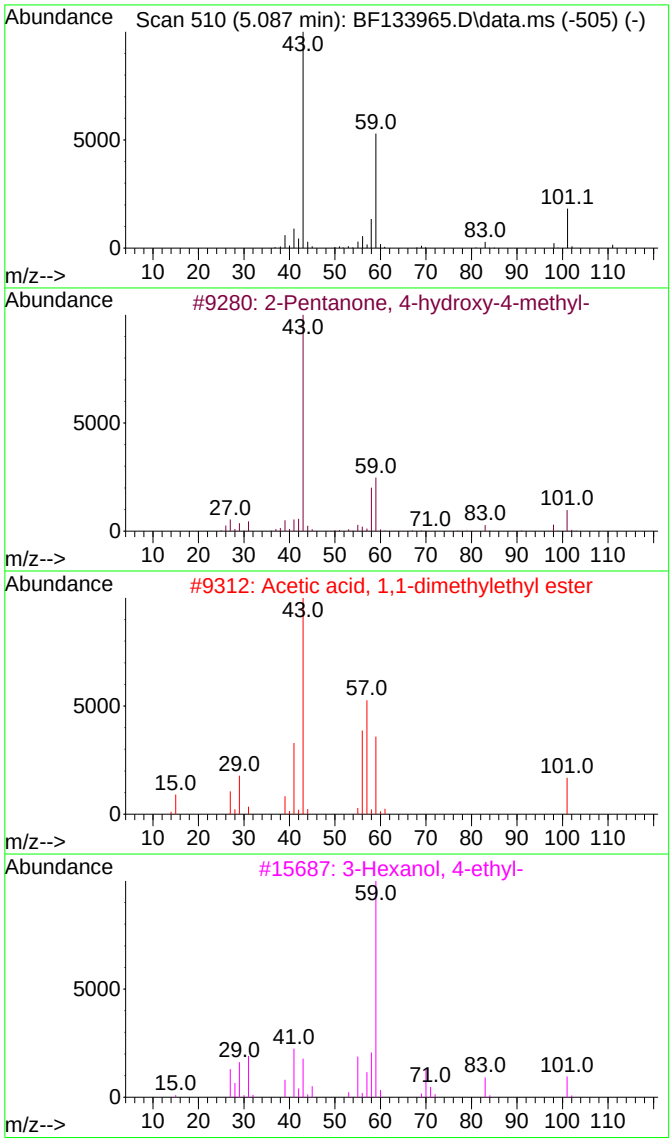
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

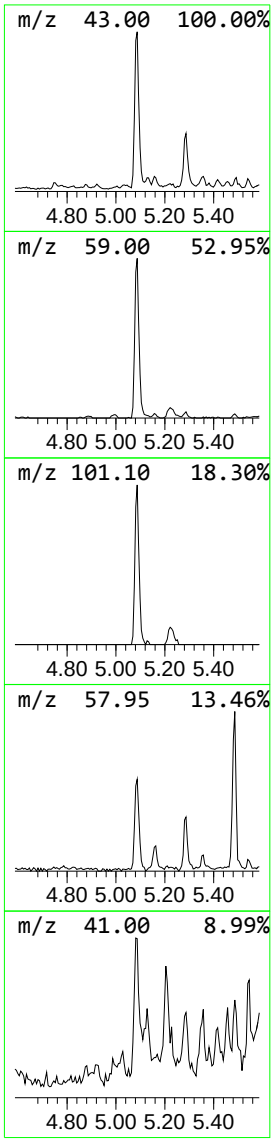
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	3.26 ng	222216	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062623\
Data File : BF133965.D
Acq On : 26 Jun 2023 22:09
Operator : CG\JU
Sample : 03365-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

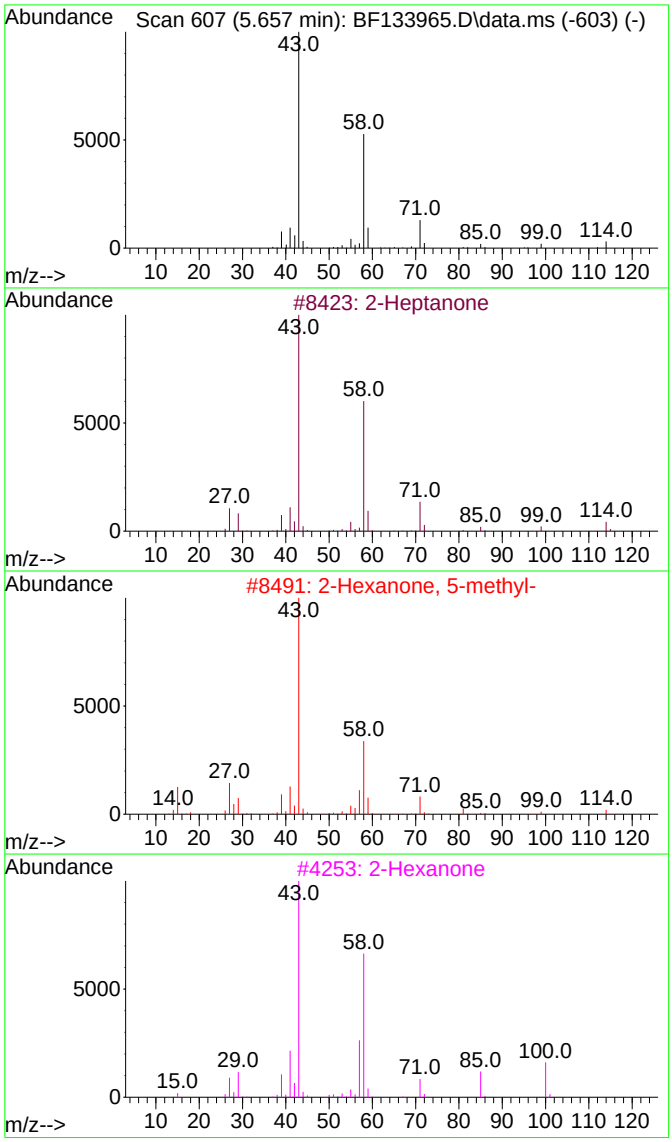
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

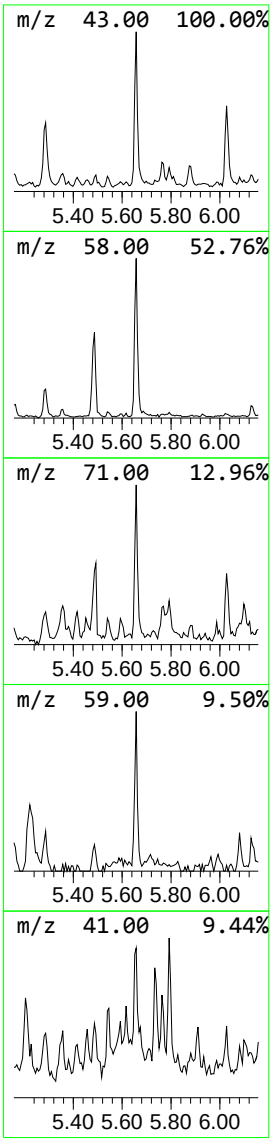
****

Peak Number 3 2-Heptanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.657	2.05 ng	140090	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	90
3	2-Hexanone	100	C6H12O	000591-78-6	56
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	56
5	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062623\
Data File : BF133965.D
Acq On : 26 Jun 2023 22:09
Operator : CG\JU
Sample : 03365-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

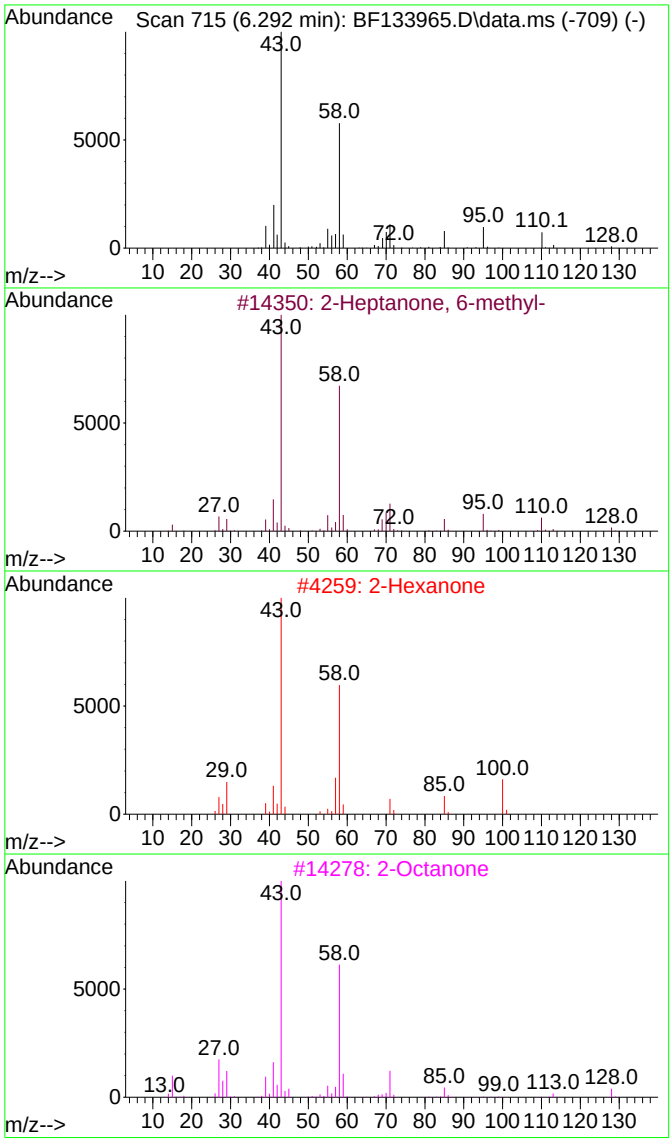
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

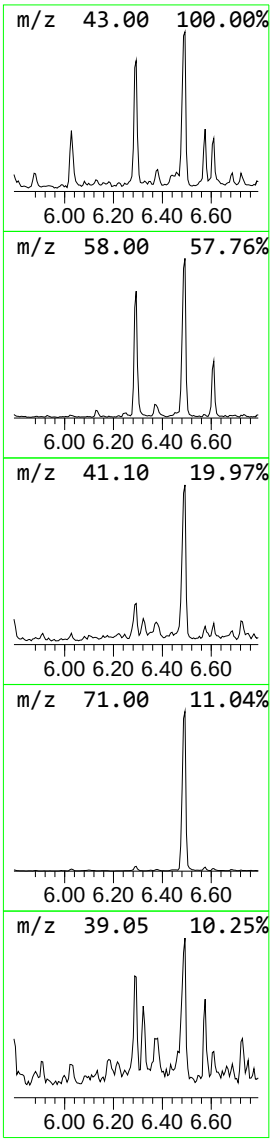
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Heptanone, 6-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.292	3.09 ng	210803	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	78
2	2-Hexanone	100	C6H12O	000591-78-6	64
3	2-Octanone	128	C8H16O	000111-13-7	45
4	2-Heptanone	114	C7H14O	000110-43-0	45
5	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062623\
Data File : BF133965.D
Acq On : 26 Jun 2023 22:09
Operator : CG\JU
Sample : 03365-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

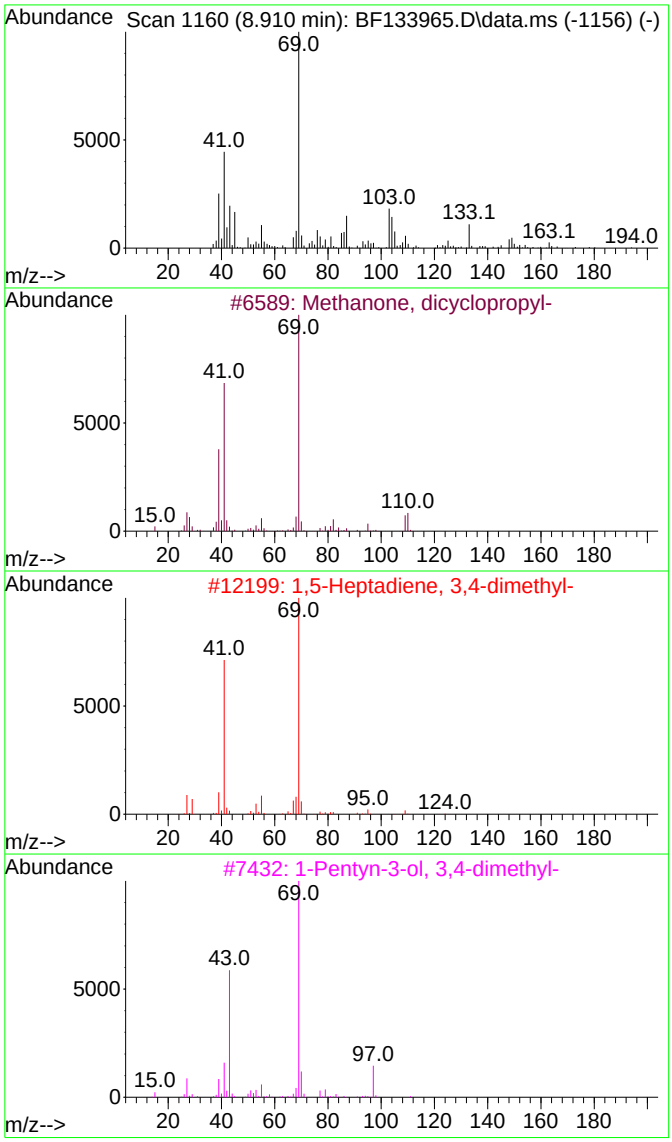
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

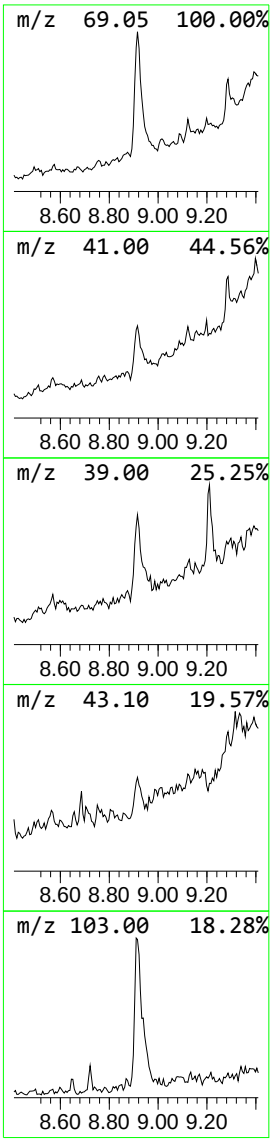
****

Peak Number 5 unknown8.910 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.910	6.11 ng	463698	Naphthalene-d8	8.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	47
2	1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	47
3	1-Pentyn-3-ol, 3,4-dimethyl-	112	C7H12O	001482-15-1	43
4	Cyclopropanecarboxyllic acid, tr...	264	C17H28O2	1000299-38-2	43
5	Cyclopropanecarboxylic acid,isop...	128	C7H12O2	006887-83-8	43





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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

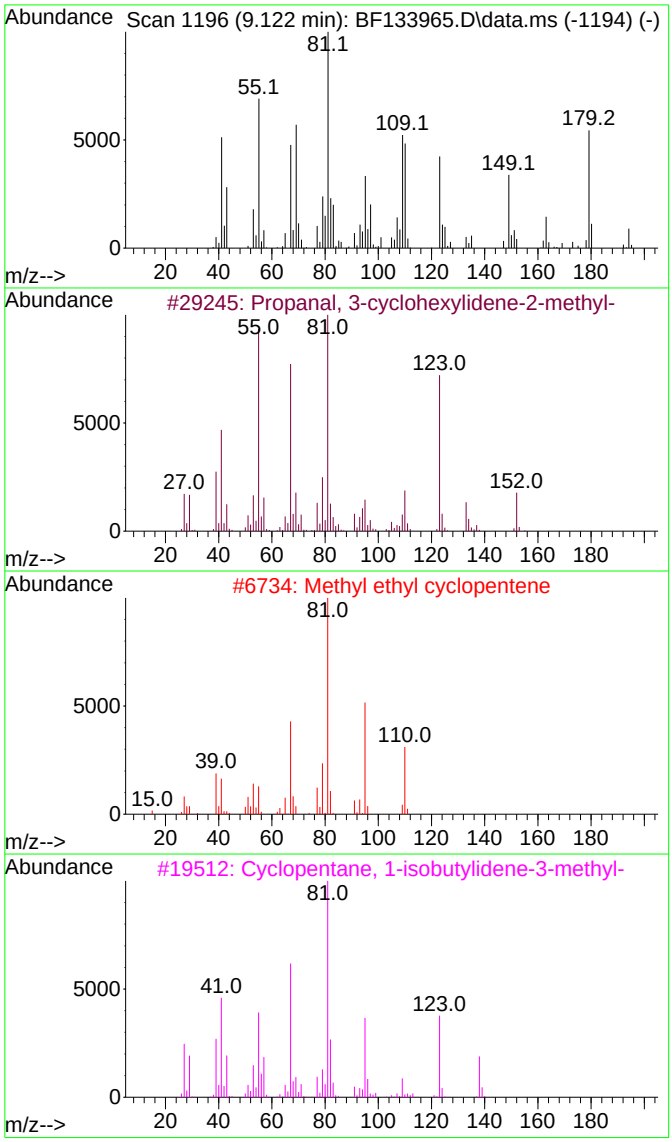
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

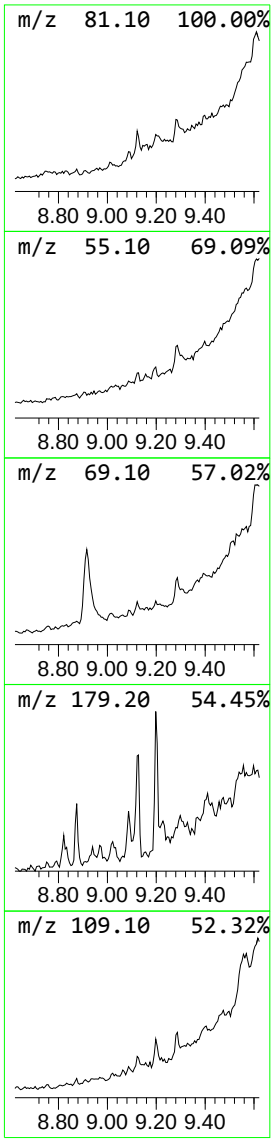
****

Peak Number 6 unknown9.122 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.122	6.35 ng	125370	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 3-cyclohexylidene-2-me...	152	C10H16O	053155-83-2	43
2	Methyl ethyl cyclopentene	110	C8H14	019780-56-4	38
3	Cyclopentane, 1-isobutylidene-3-...	138	C10H18	1000150-62-1	38
4	Cyclohexanol, 4-sec-butyl-	156	C10H20O	006292-20-2	35
5	Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	27





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ClientSampleId :
TP4

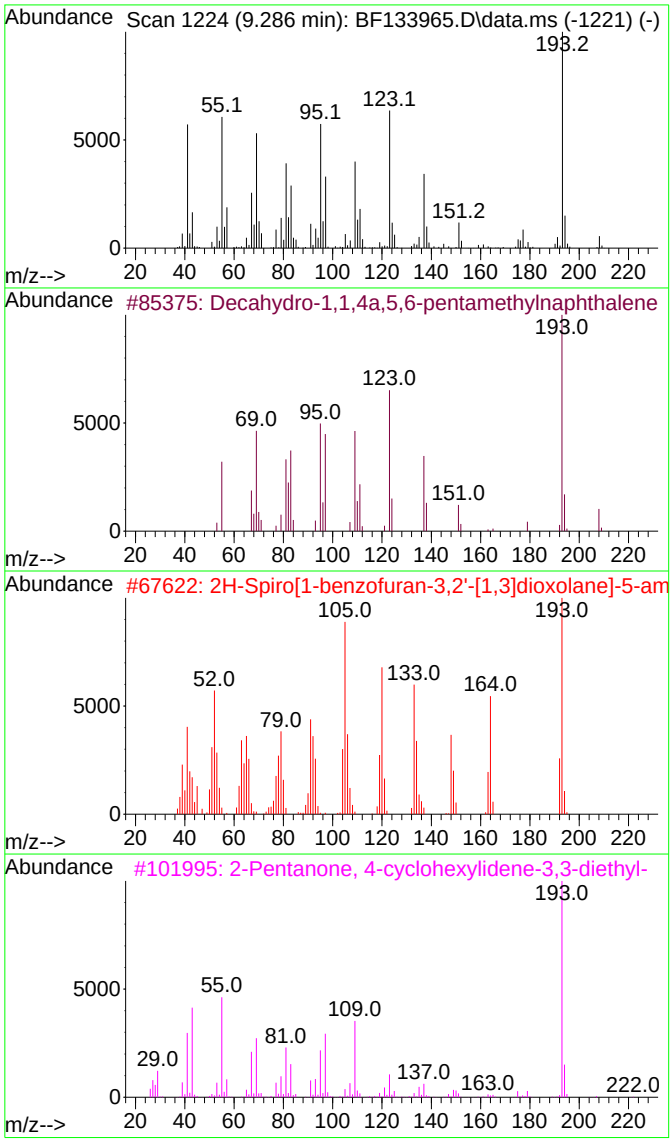
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

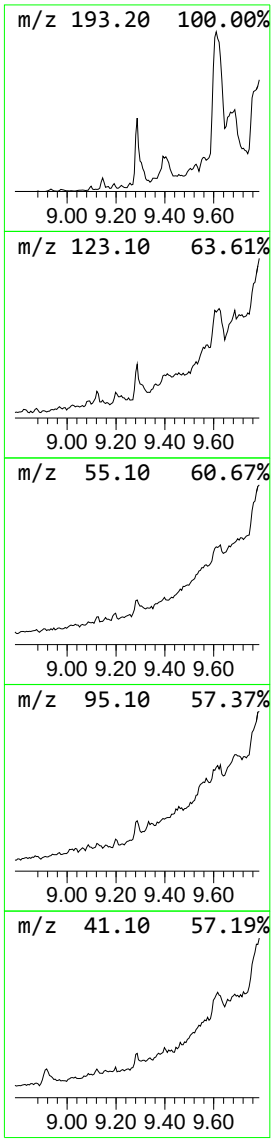
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.286	20.00 ng	394829	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	86
2	2H-Spiro[1-benzofuran-3,2'-[1,3]...	193	C10H11NO3	1000387-33-4	64
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	52
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	46
5	Toxoflavin	193	C7H7N5O2	000084-82-2	30





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone	2.240	3.2	ng	217764	1	6.851	1364530	20.0
2-Pentanone, 4-...	5.087	3.3	ng	222216	1	6.851	1364530	20.0
2-Heptanone	5.657	2.0	ng	140090	1	6.851	1364530	20.0
2-Heptanone, 6-...	6.292	3.1	ng	210803	1	6.851	1364530	20.0
unknown8.910	8.910	6.1	ng	463698	2	8.133	1516700	20.0
unknown9.122	9.122	6.3	ng	125370	3	9.922	394829	20.0
Decahydro-1,1,4...	9.286	20.0	ng	394829	3	9.922	394829	20.0