LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122444.D
Acq On : 23 Nov 2020 13:07
Operator : JU/CG
Sample : PB133180BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB133180BL

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122444.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.646	259	265	274	rVB	154239	226285	2.80%	0.459%
2	4.481	403	407	414	rBV	343678	351866	4.35%	0.713%
3	5.098	505	512	519	rBV	1968532	2913719	36.01%	5.906%
4	5.498	575	580	583	rBV	4854214	5391828	66.63%	10.929%
5	5.881	641	645	649	rBV	374168	284235	3.51%	0.576%
6	6.498	744	750	753	rBV	4828863	5384688	66.54%	10.914%
7	6.863	808	812	815	rBV	1652454	1316973	16.28%	2.669%
8	7.428	902	908	911	rBV	3362694	3645453	45.05%	7.389%
9	8.151	1025	1031	1034	rBV	1682362	1706737	21.09%	3.459%
10	9.228	1208	1214	1217	rBV	6208114	6741798	83.32%	13.665%
11	9.910	1324	1330	1342	rBV	1966763	2037285	25.18%	4.129%
12	10.698	1458	1464	1484	rBV	4572794	4763348	58.87%	9.655%
13	11.398	1576	1583	1590	rBV	2048317	2153644	26.61%	4.365%
14	12.992	1847	1854	1857	rBV	7796186	8091922	100.00%	16.402%
15	14.039	2028	2032	2049	rVB	2290899	2275719	28.12%	4.613%
16	15.521	2278	2284	2301	rBV2	1333395	2050317	25.34%	4.156%

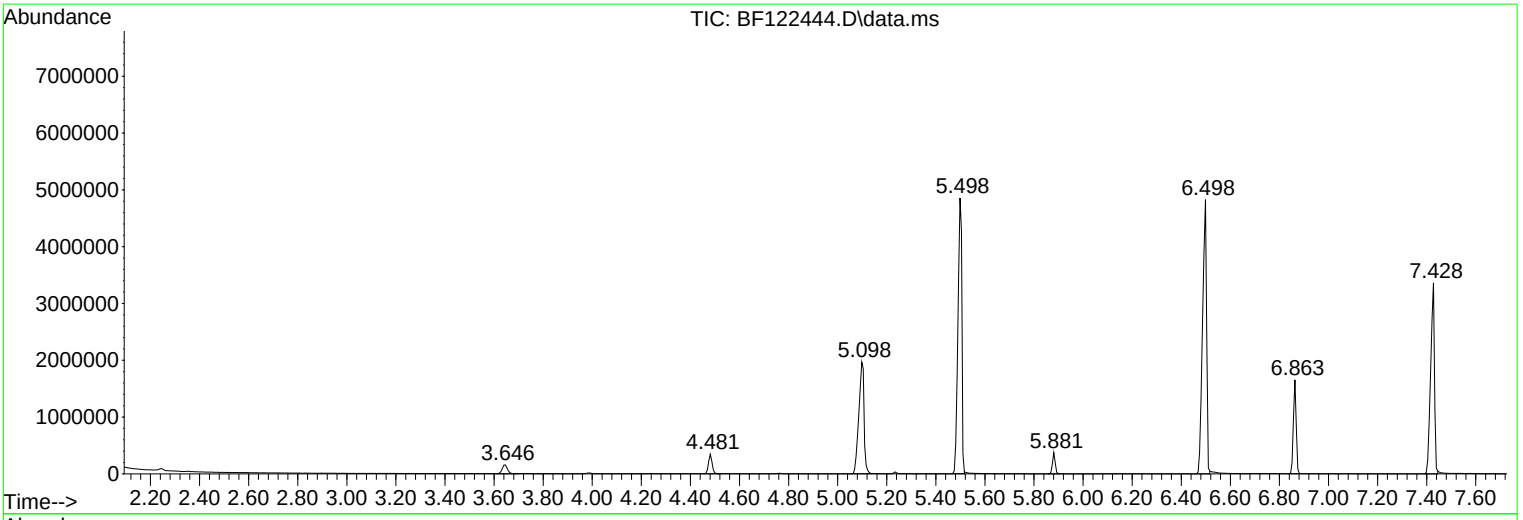
Sum of corrected areas: 49335817

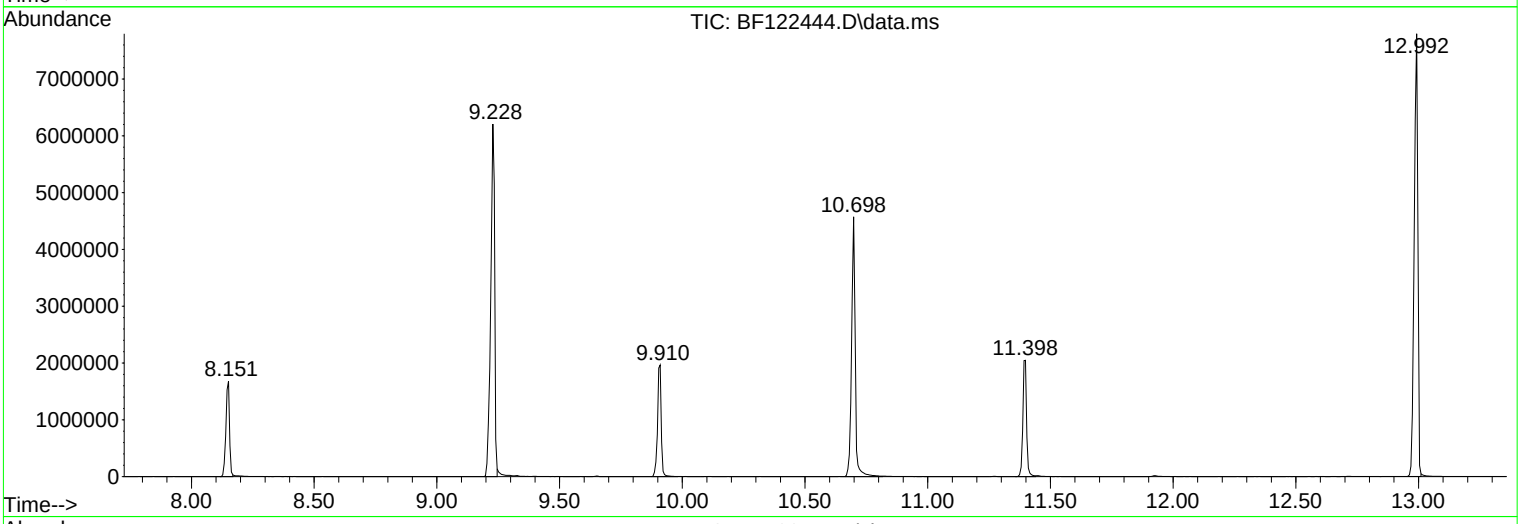
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122444.D
Acq On : 23 Nov 2020 13:07
Operator : JU/CG
Sample : PB133180BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

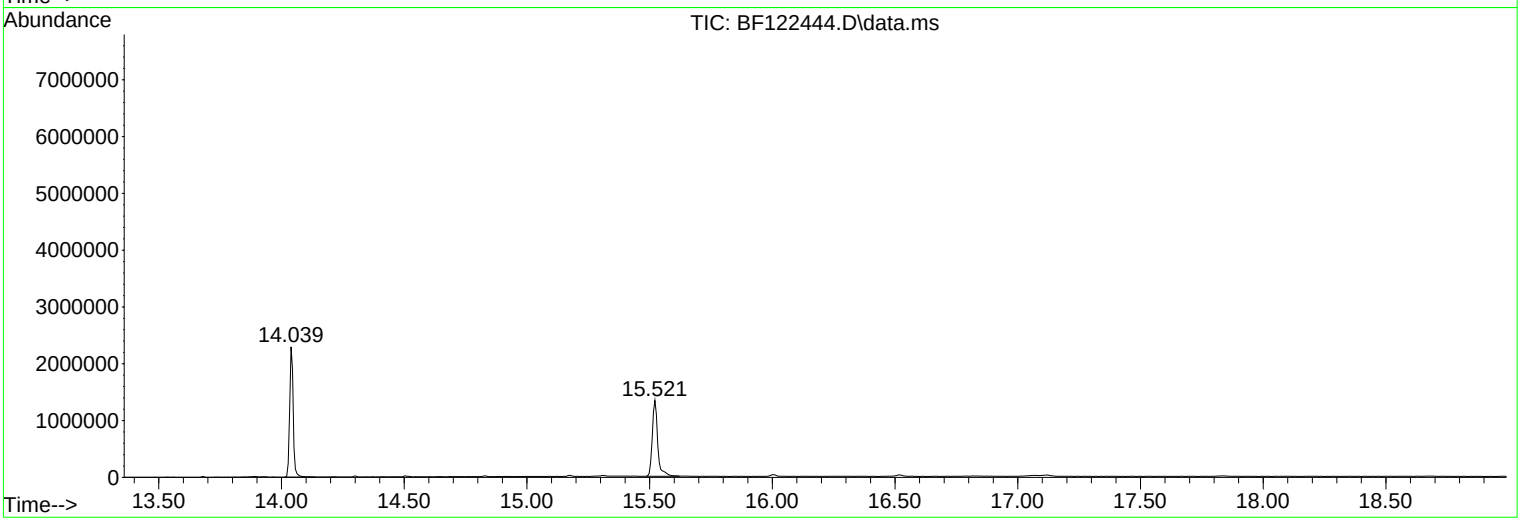
Instrument :
BNA_F
ClientSampleId :
PB133180BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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_F\Data\BF112320\
Data File : BF122444.D
Acq On : 23 Nov 2020 13:07
Operator : JU/CG
Sample : PB133180BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB133180BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

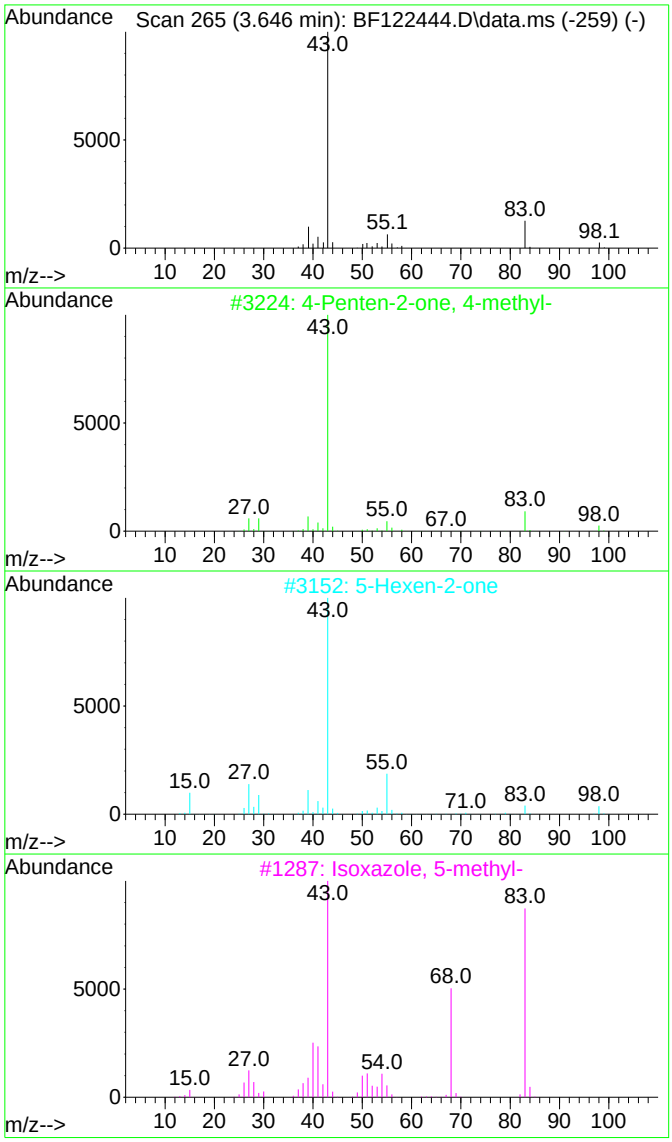
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

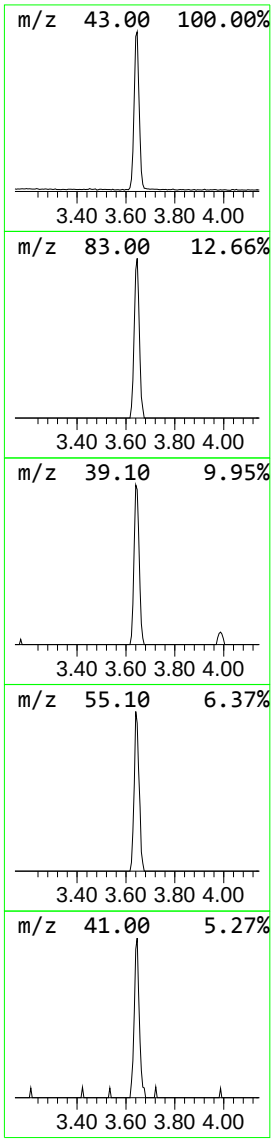
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.646	3.44 ng	226285	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	90
2	5-Hexen-2-one	98	C6H10O	000109-49-9	46
3	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9
4	2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	9
5	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122444.D
Acq On : 23 Nov 2020 13:07
Operator : JU/CG
Sample : PB133180BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB133180BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

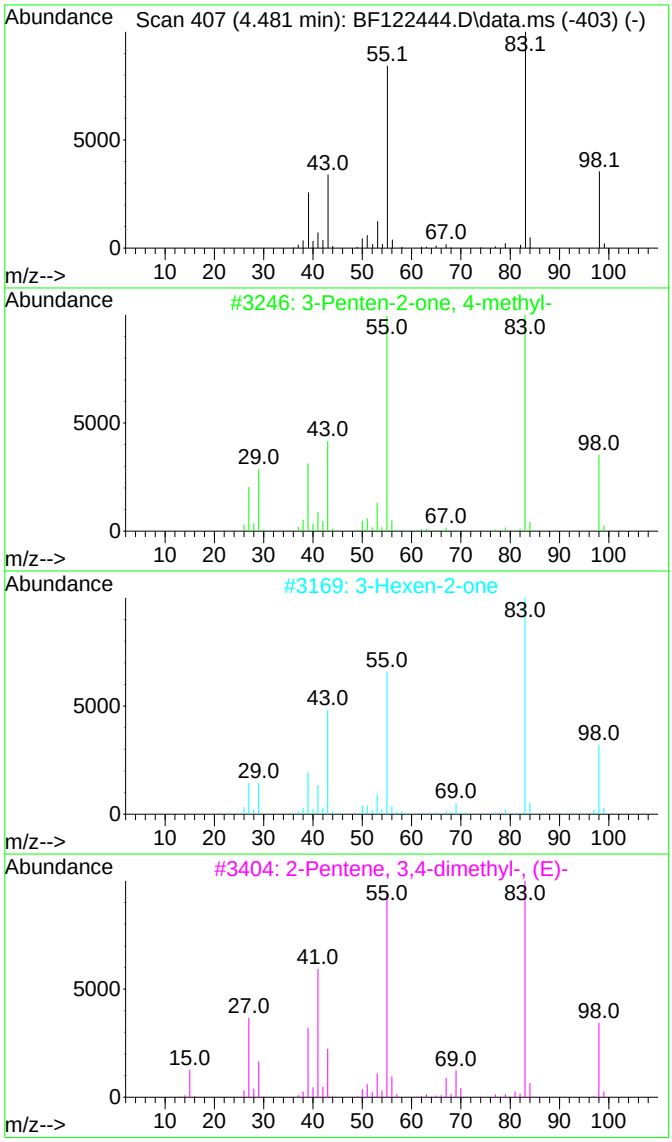
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

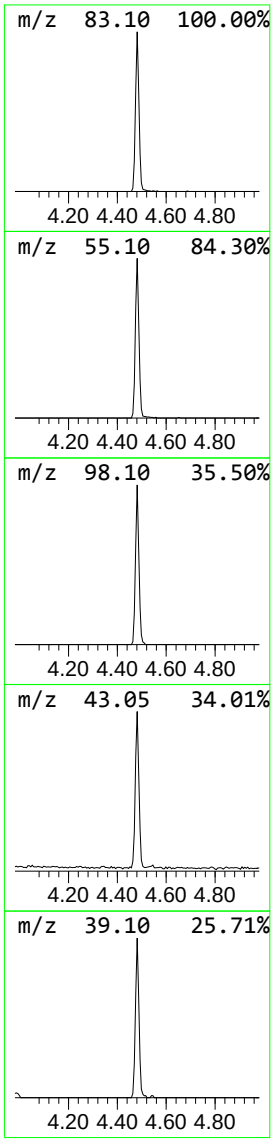
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	5.34 ng	351866	1,4-Dichlorobenzene-d4	6.863

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	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122444.D
Acq On : 23 Nov 2020 13:07
Operator : JU/CG
Sample : PB133180BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB133180BL

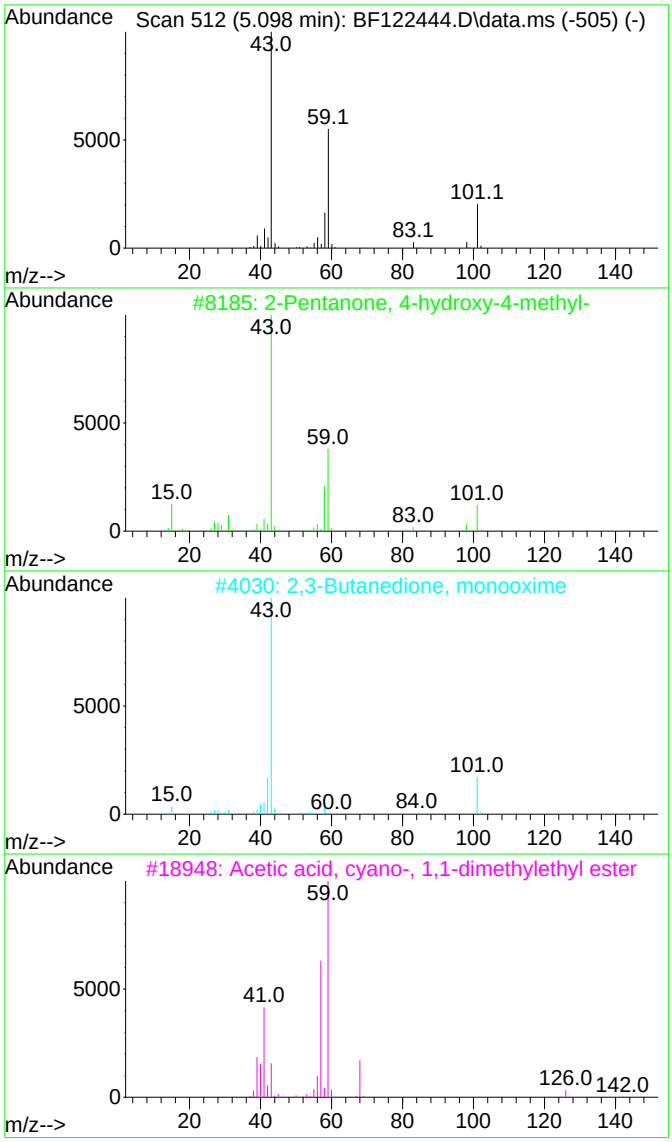
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

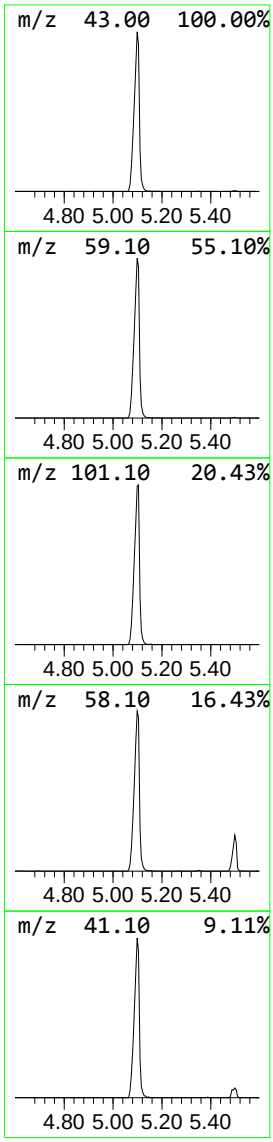
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	44.25 ng	2913720	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122444.D
Acq On : 23 Nov 2020 13:07
Operator : JU/CG
Sample : PB133180BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB133180BL

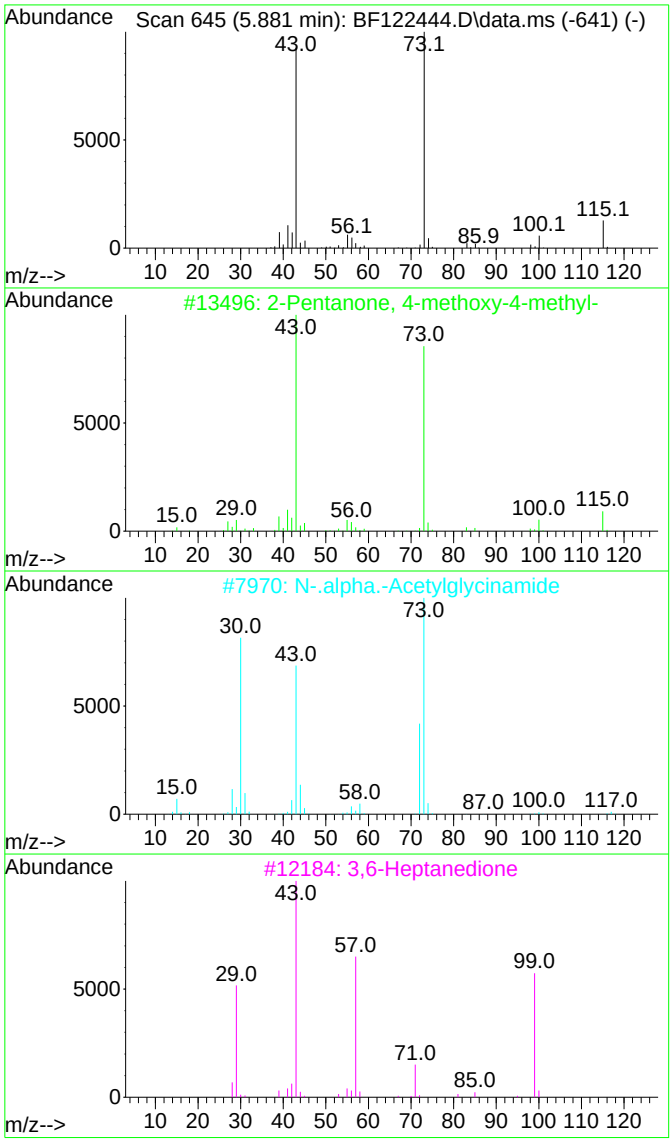
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

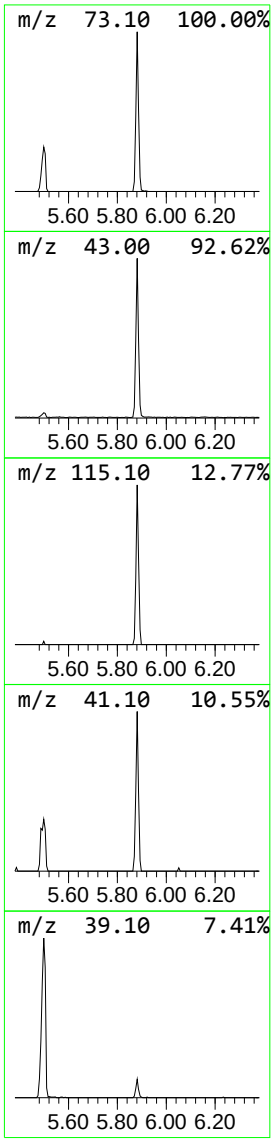
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.881	4.32 ng	284235	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	40
3	3,6-Heptanedione	128	C7H12O2	001703-51-1	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122444.D
Acq On : 23 Nov 2020 13:07
Operator : JU/CG
Sample : PB133180BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB133180BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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
4-Penten-2-one,...	3.646	3.4	ng	226285	1	6.863	1316970	20.0
3-Penten-2-one,...	4.481	5.3	ng	351866	1	6.863	1316970	20.0
2-Pentanone, 4-...	5.098	44.3	ng	2913720	1	6.863	1316970	20.0
2-Pentanone, 4-...	5.881	4.3	ng	284235	1	6.863	1316970	20.0