LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122406.D
Acq On : 20 Nov 2020 16:40
Operator : JU/CG
Sample : L4809-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-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_F\METHODS\8270-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122406.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	13	rVB	507999	671432	3.83%	1.349%
2	3.569	245	252	259	rVB	288343	459654	2.62%	0.924%
3	4.487	396	408	411	rBV	8206389	17532625	100.00%	35.234%
4	5.075	500	508	511	rBV	2367129	2932723	16.73%	5.894%
5	5.481	573	577	590	rBV	765946	693468	3.96%	1.394%
6	6.492	745	749	761	rBV	2208822	1941907	11.08%	3.902%
7	6.863	808	812	815	rBV	1561598	1207865	6.89%	2.427%
8	7.181	862	866	869	rBV	598480	454944	2.59%	0.914%
9	7.422	902	907	910	rBV	2645936	2451045	13.98%	4.926%
10	7.681	947	951	960	rBV	254603	240447	1.37%	0.483%
11	8.151	1027	1031	1034	rBV	1745873	1572682	8.97%	3.160%
12	9.228	1209	1214	1217	rBV	5547691	4793623	27.34%	9.633%
13	9.910	1325	1330	1333	rBV	2046958	1894734	10.81%	3.808%
14	11.392	1578	1582	1586	rBV	2122766	2010688	11.47%	4.041%
15	12.986	1849	1853	1857	rBV	5744273	5858090	33.41%	11.773%
16	13.904	2004	2009	2024	rBV2	234993	581721	3.32%	1.169%
17	14.039	2028	2032	2036	rBV	2418610	2218979	12.66%	4.459%
18	15.521	2278	2284	2288	rBV	1845061	2243975	12.80%	4.510%

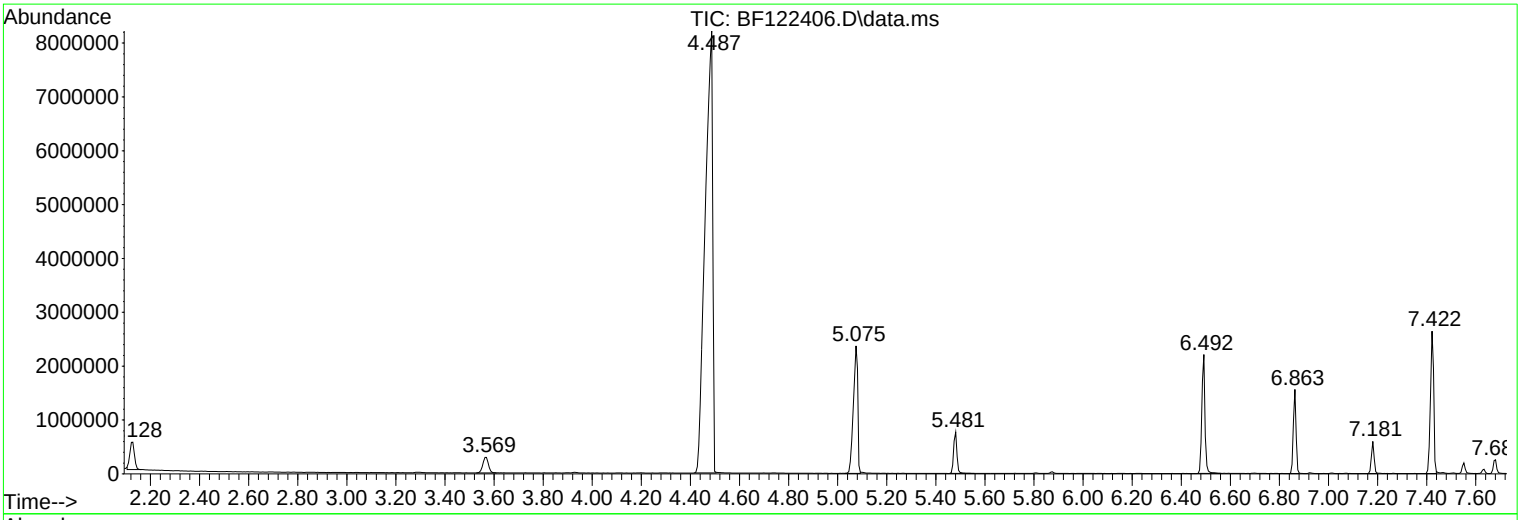
Sum of corrected areas: 49760602

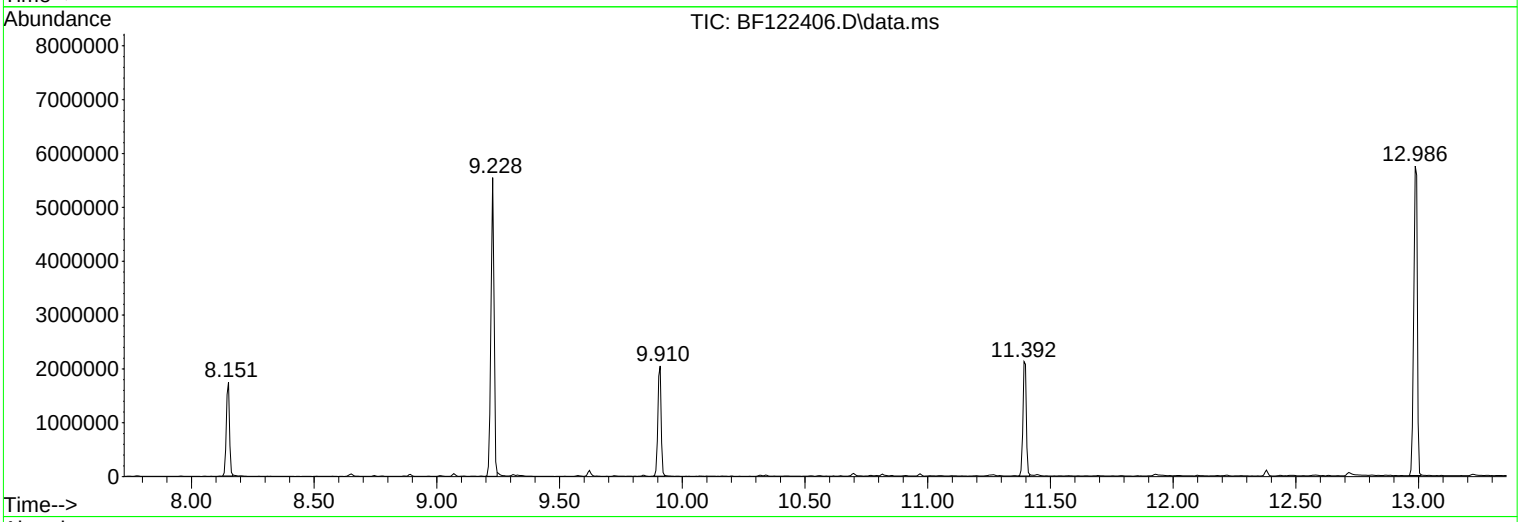
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122406.D
Acq On : 20 Nov 2020 16:40
Operator : JU/CG
Sample : L4809-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

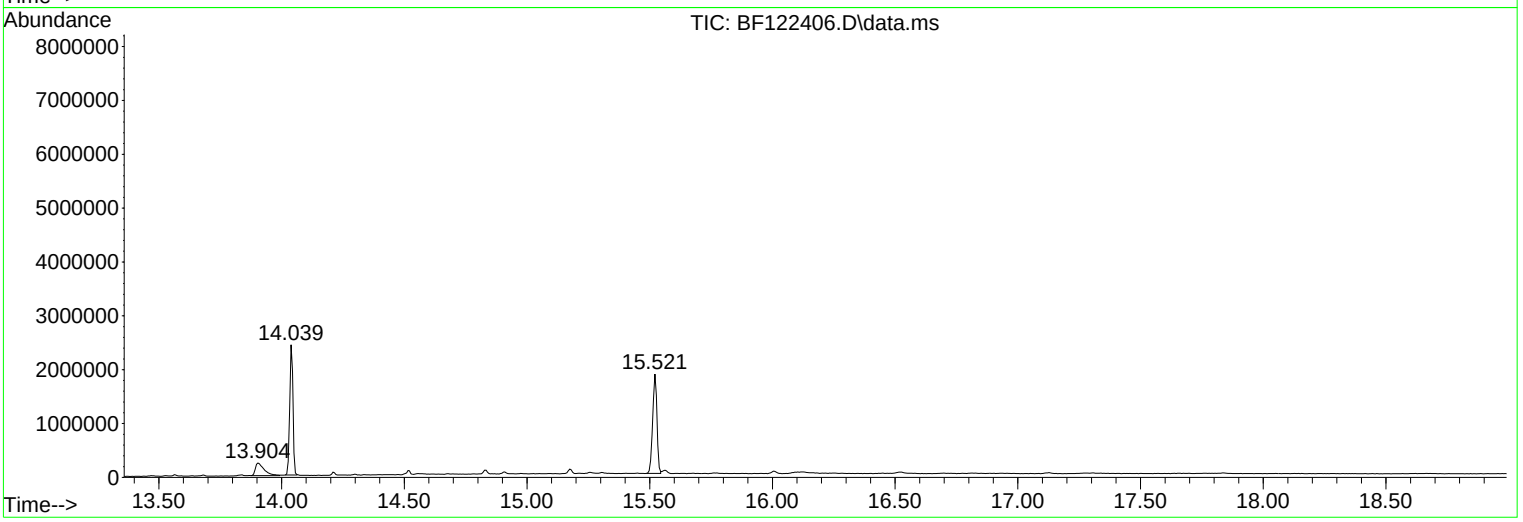
Instrument :
BNA_F
ClientSampleId :
MS-CON-E

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\BF112020\
Data File : BF122406.D
Acq On : 20 Nov 2020 16:40
Operator : JU/CG
Sample : L4809-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-E

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

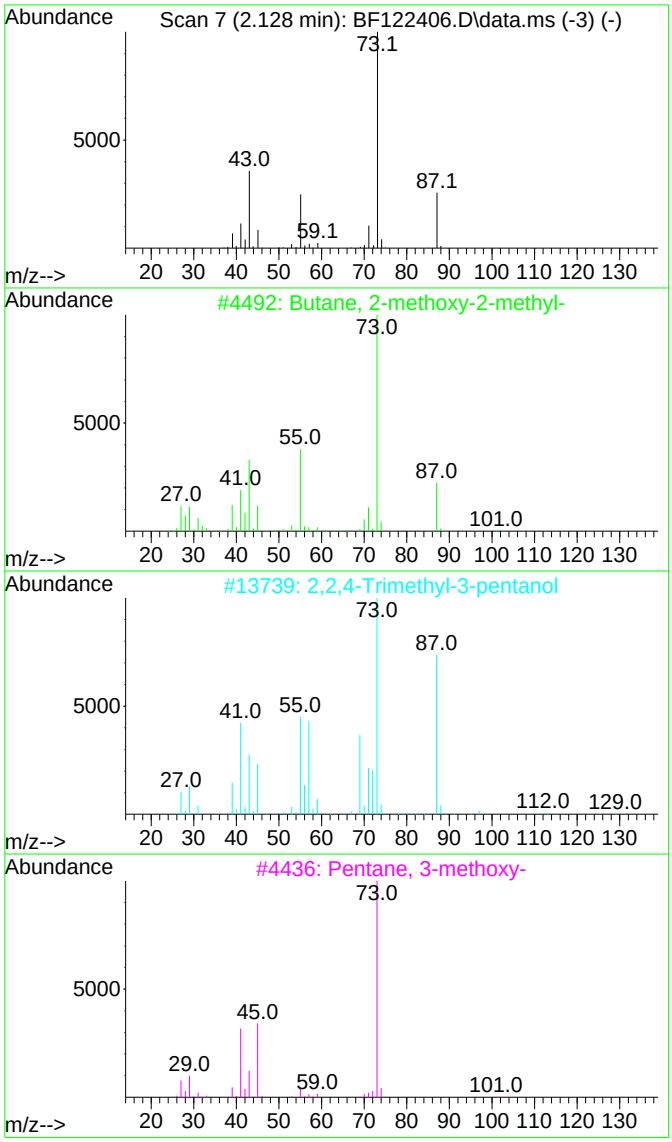
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

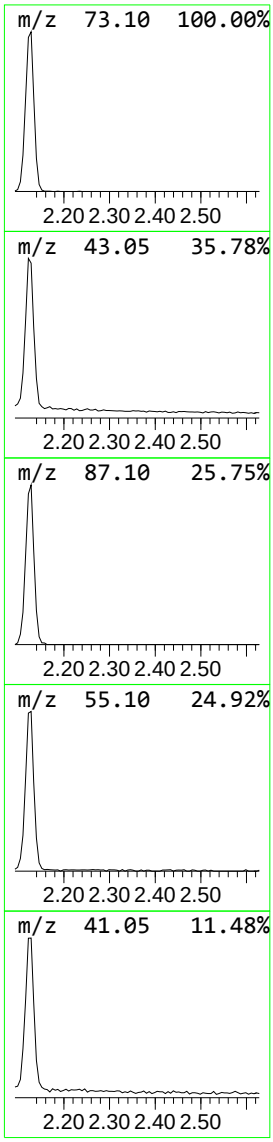
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	11.12 ng	671432	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122406.D
Acq On : 20 Nov 2020 16:40
Operator : JU/CG
Sample : L4809-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-E

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

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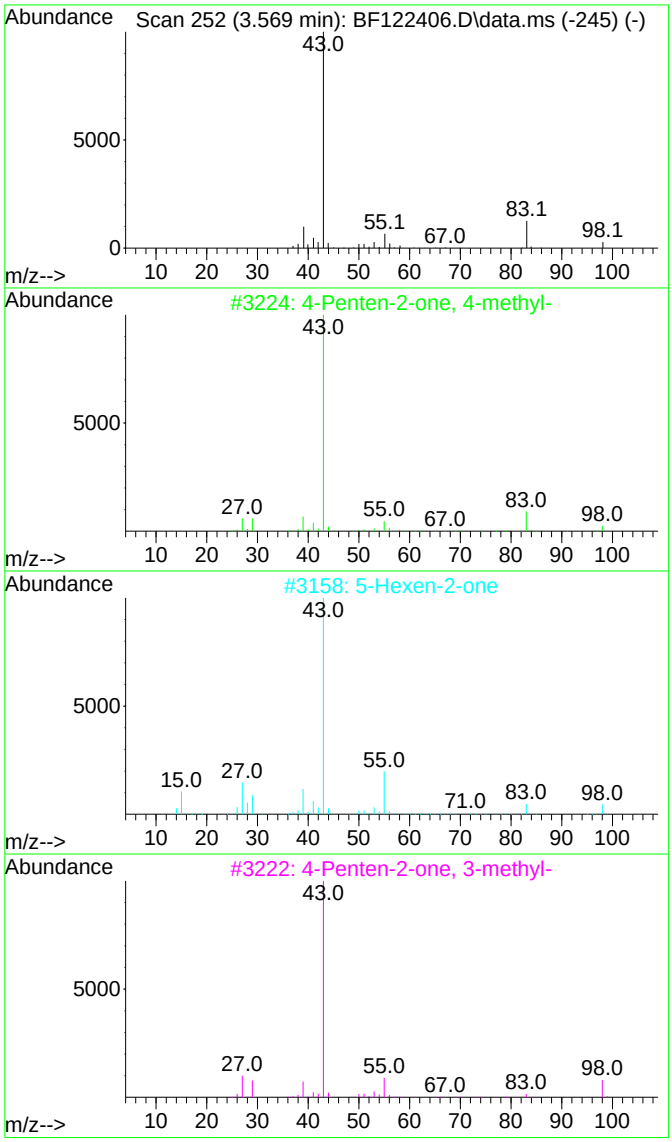
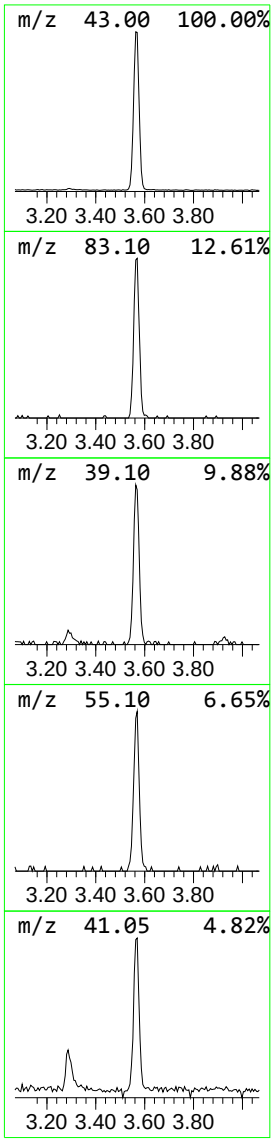
Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.569	7.61 ng	459654	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	86
2	5-Hexen-2-one	98	C6H10O	000109-49-9	47
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	32
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	22
5	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122406.D
Acq On : 20 Nov 2020 16:40
Operator : JU/CG
Sample : L4809-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-E

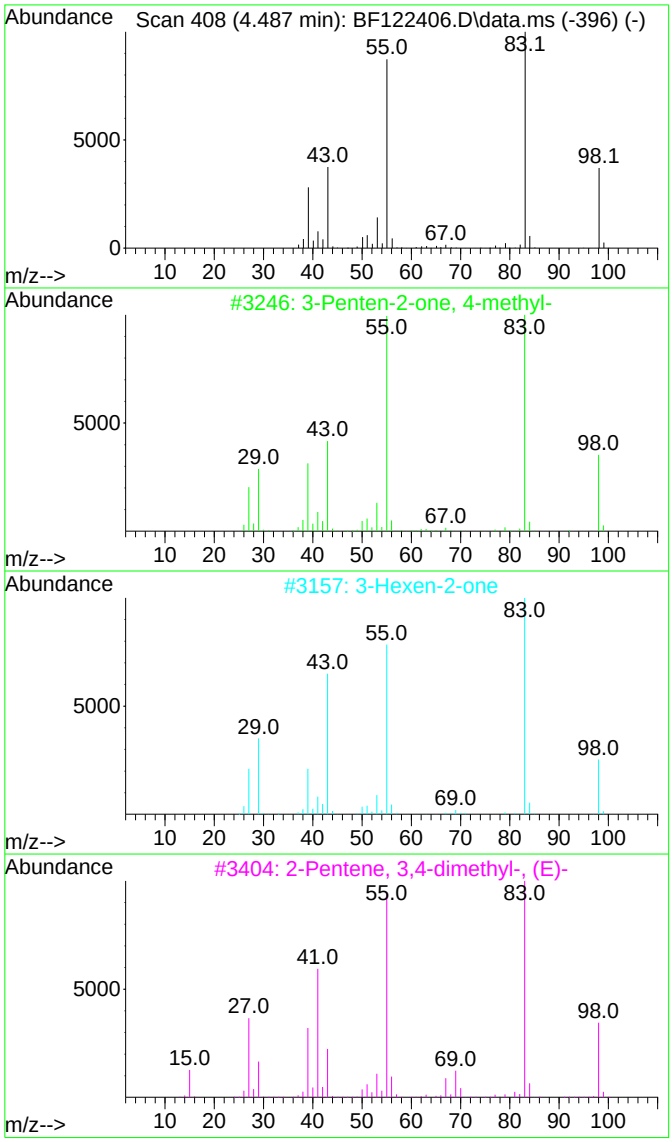
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

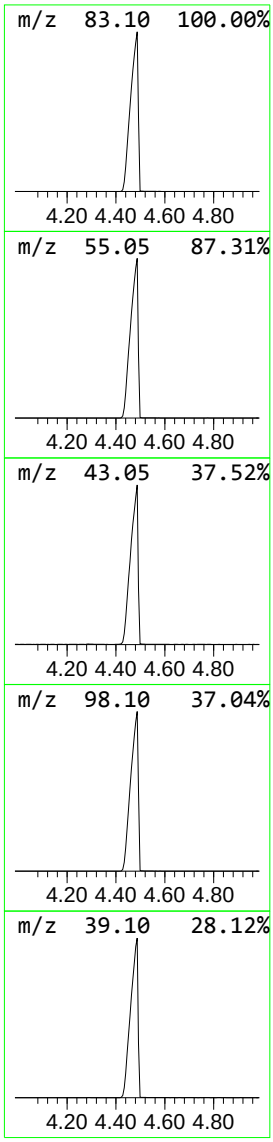
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.487	290.31 ng	17532600	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	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
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	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122406.D
Acq On : 20 Nov 2020 16:40
Operator : JU/CG
Sample : L4809-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-E

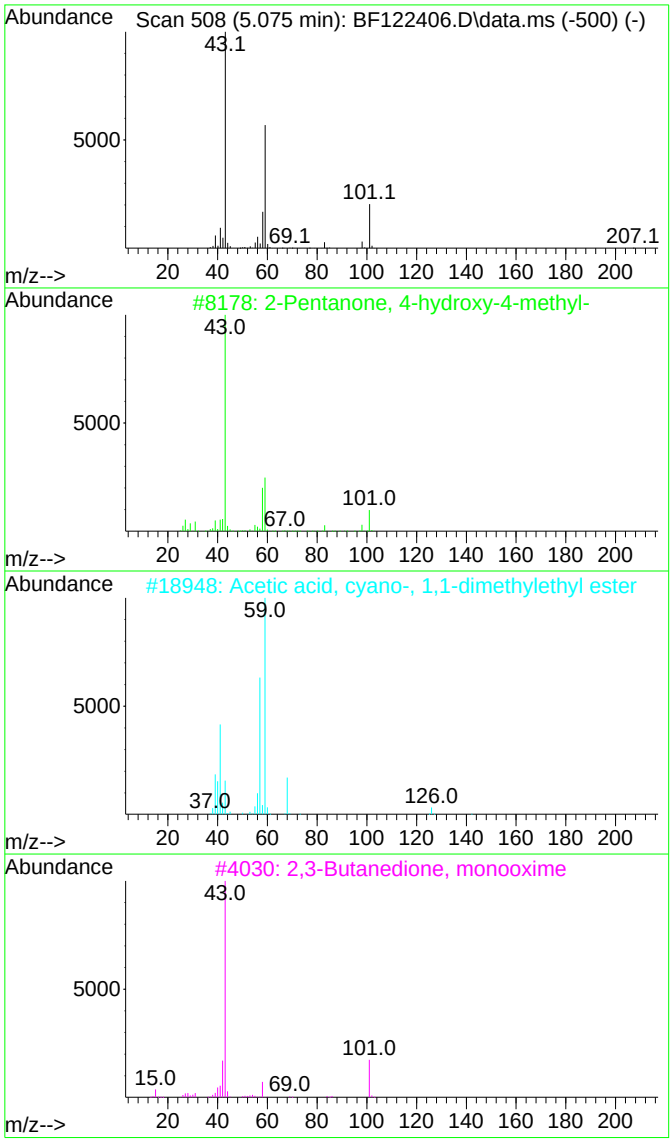
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

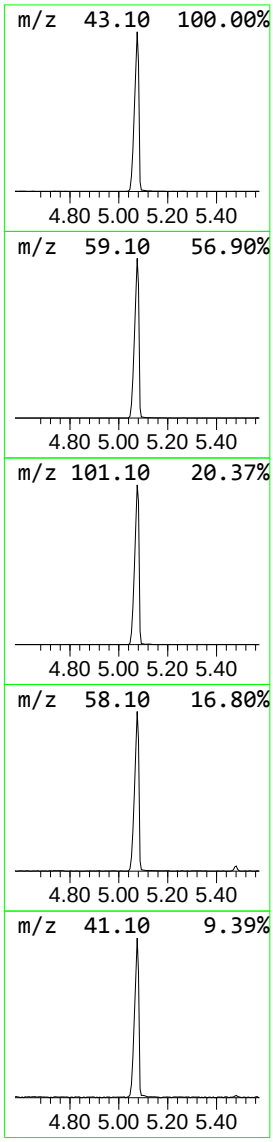
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	48.56 ng	2932720	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	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
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\BF112020\
Data File : BF122406.D
Acq On : 20 Nov 2020 16:40
Operator : JU/CG
Sample : L4809-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-E

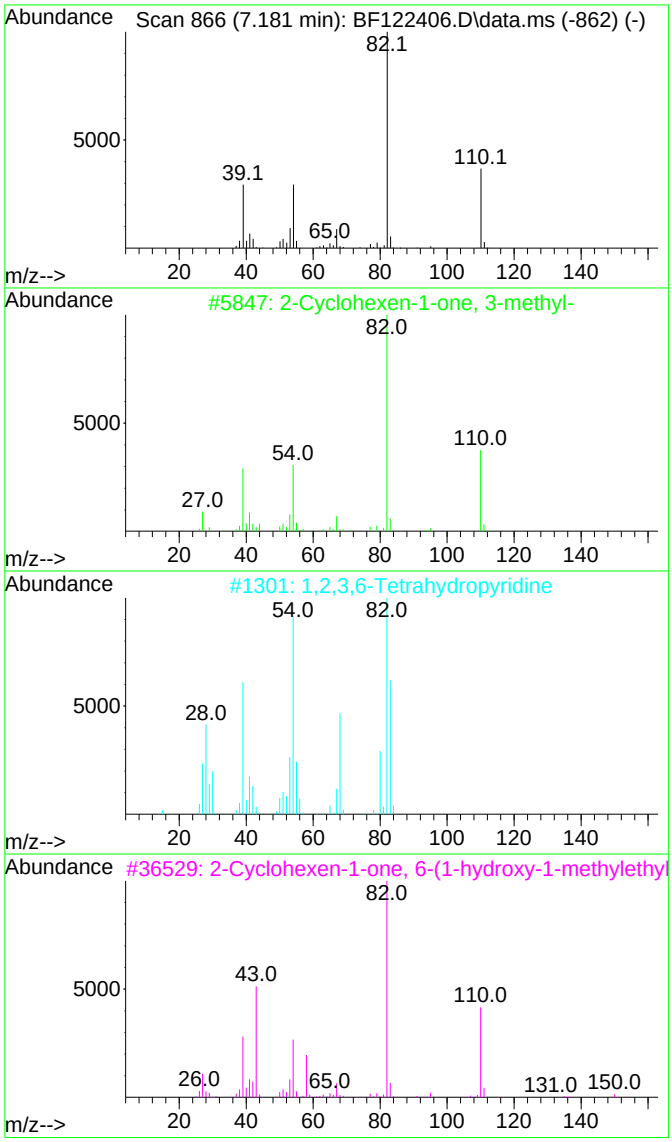
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

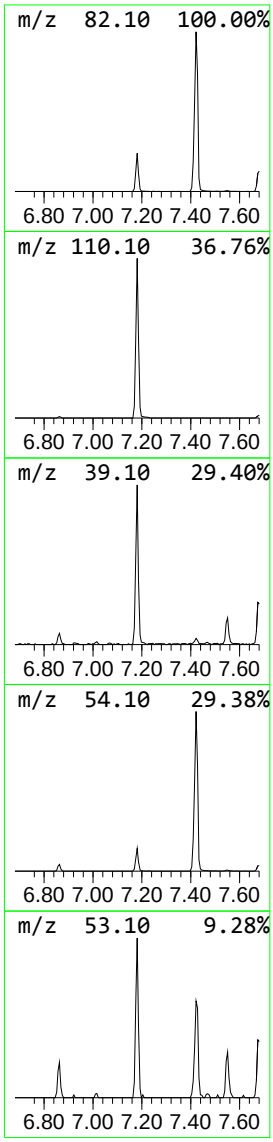
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.181	7.53 ng	454944	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	1,2,3,6-Tetrahydropyridine	83	C5H9N	000694-05-3	64
3	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	56
4	Azeleonitrile	150	C9H14N2	001675-69-0	50
5	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122406.D
Acq On : 20 Nov 2020 16:40
Operator : JU/CG
Sample : L4809-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-E

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

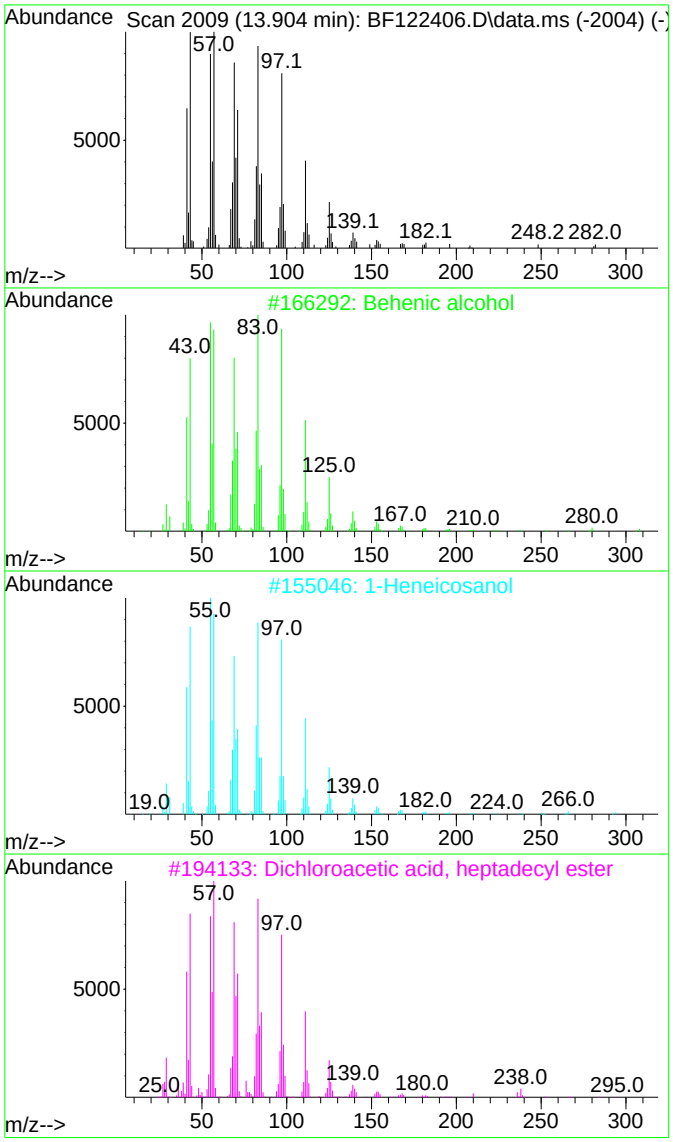
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

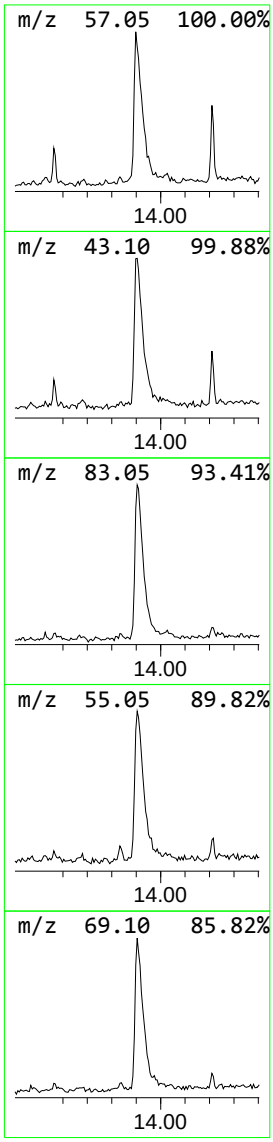
****

Peak Number 6 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	5.24 ng	581721	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122406.D
Acq On : 20 Nov 2020 16:40
Operator : JU/CG
Sample : L4809-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-E

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
Butane, 2-metho...	2.128	11.1	ng	671432	1	6.863	1207870	20.0
4-Penten-2-one,...	3.569	7.6	ng	459654	1	6.863	1207870	20.0
3-Penten-2-one,...	4.487	290.3	ng	17532600	1	6.863	1207870	20.0
2-Pentanone, 4-...	5.075	48.6	ng	2932720	1	6.863	1207870	20.0
2-Cyclohexen-1-...	7.181	7.5	ng	454944	1	6.863	1207870	20.0
Behenic alcohol	13.904	5.2	ng	581721	5	14.039	2218980	20.0