LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122405.D
Acq On : 20 Nov 2020 16:08
Operator : JU/CG
Sample : L4809-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-D

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: BF122405.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	20	rVB	561070	717035	1.90%	0.971%
2	3.569	244	252	261	rVB	754618	1224196	3.25%	1.659%
3	4.516	396	413	416	rBV	10565243	37721873	100.00%	51.106%
4	5.093	501	511	514	rBV	3891994	6857130	18.18%	9.290%
5	6.863	808	812	815	rBV	1563217	1224490	3.25%	1.659%
6	7.181	862	866	869	rBV	1089875	847285	2.25%	1.148%
7	7.422	903	907	910	rBV	2616520	2390641	6.34%	3.239%
8	7.551	925	929	939	rVB	472937	389202	1.03%	0.527%
9	7.681	947	951	954	rBV	545357	476277	1.26%	0.645%
10	8.151	1027	1031	1034	rBV	1820949	1603529	4.25%	2.172%
11	9.228	1209	1214	1217	rBV	5530846	4656294	12.34%	6.308%
12	9.910	1325	1330	1333	rBV	2091524	1940978	5.15%	2.630%
13	11.398	1578	1583	1586	rBV	2229787	2074010	5.50%	2.810%
14	12.986	1849	1853	1857	rBV	5951006	5824574	15.44%	7.891%
15	13.898	2004	2008	2024	rBV	574635	1132612	3.00%	1.534%
16	14.039	2027	2032	2036	rBV	2406039	2346441	6.22%	3.179%
17	15.521	2278	2284	2288	rBV2	1951666	2384103	6.32%	3.230%

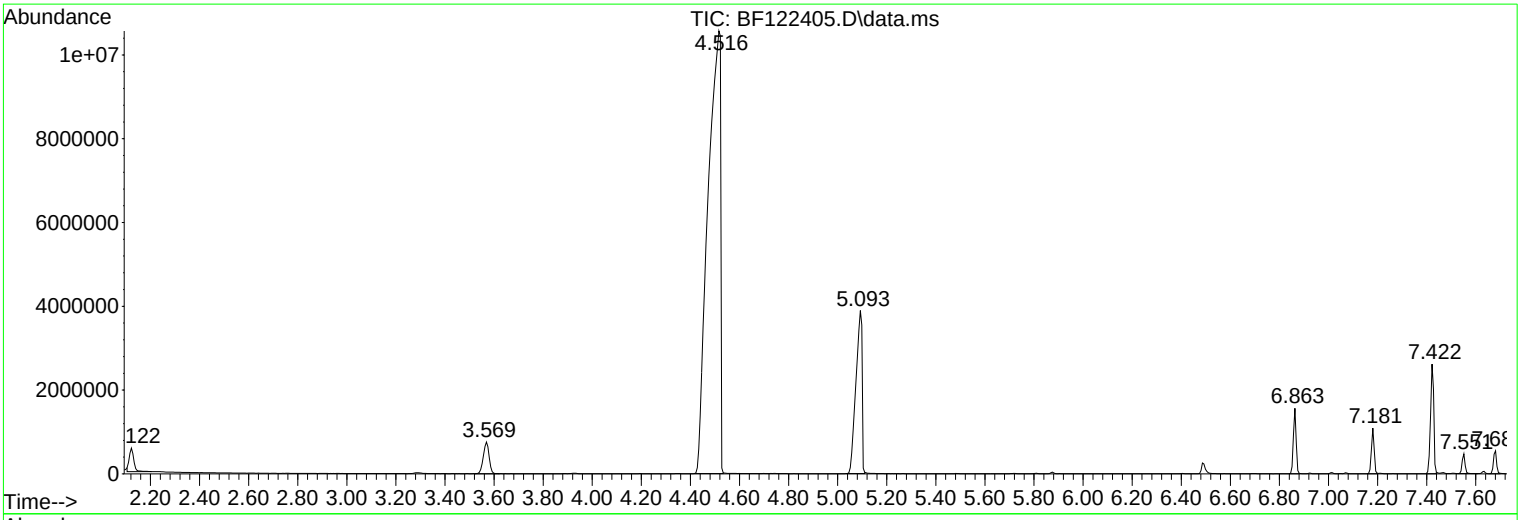
Sum of corrected areas: 73810670

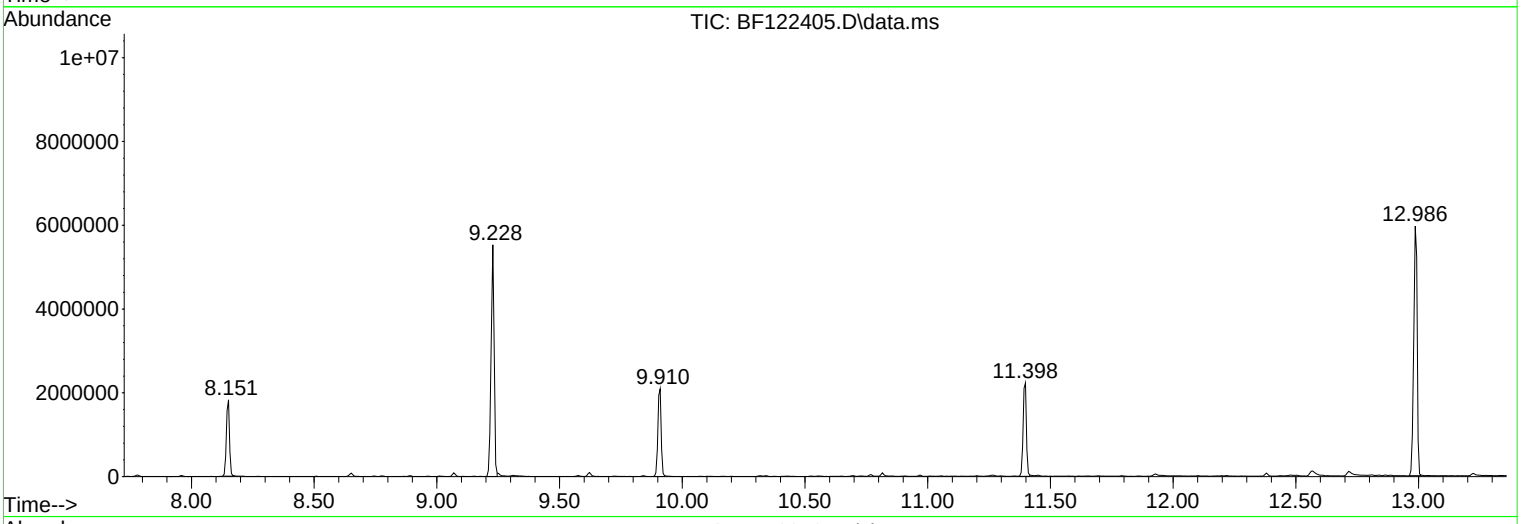
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122405.D
Acq On : 20 Nov 2020 16:08
Operator : JU/CG
Sample : L4809-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

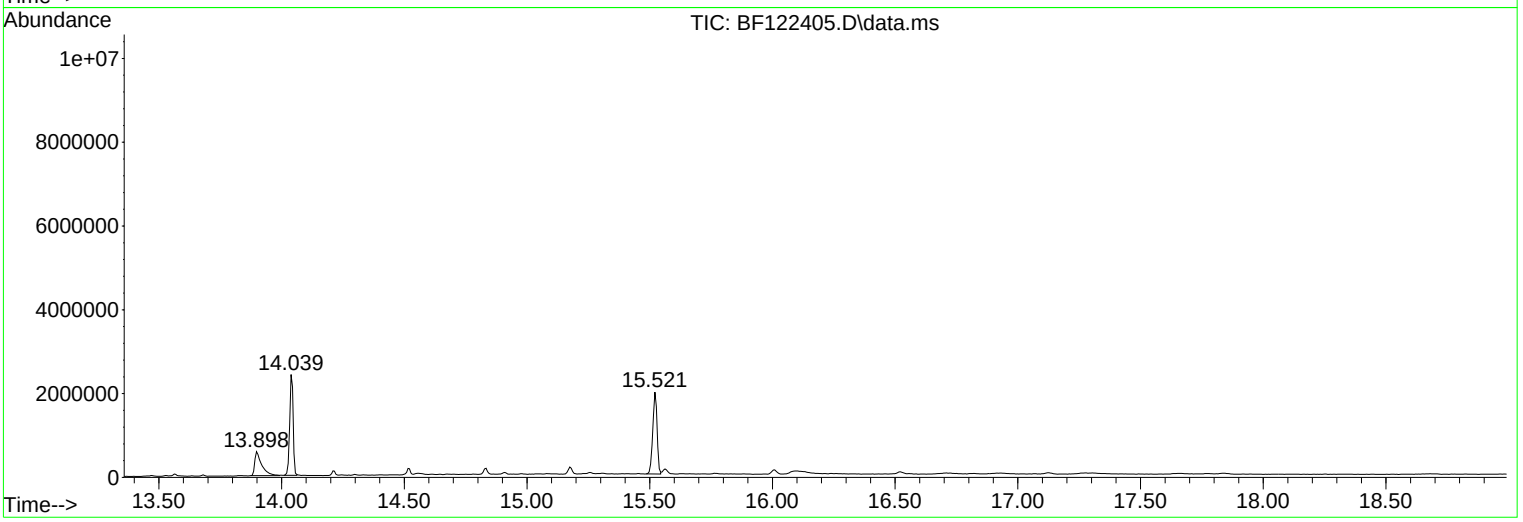
Instrument :
BNA_F
ClientSampleId :
MS-CON-D

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 : BF122405.D
Acq On : 20 Nov 2020 16:08
Operator : JU/CG
Sample : L4809-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-D

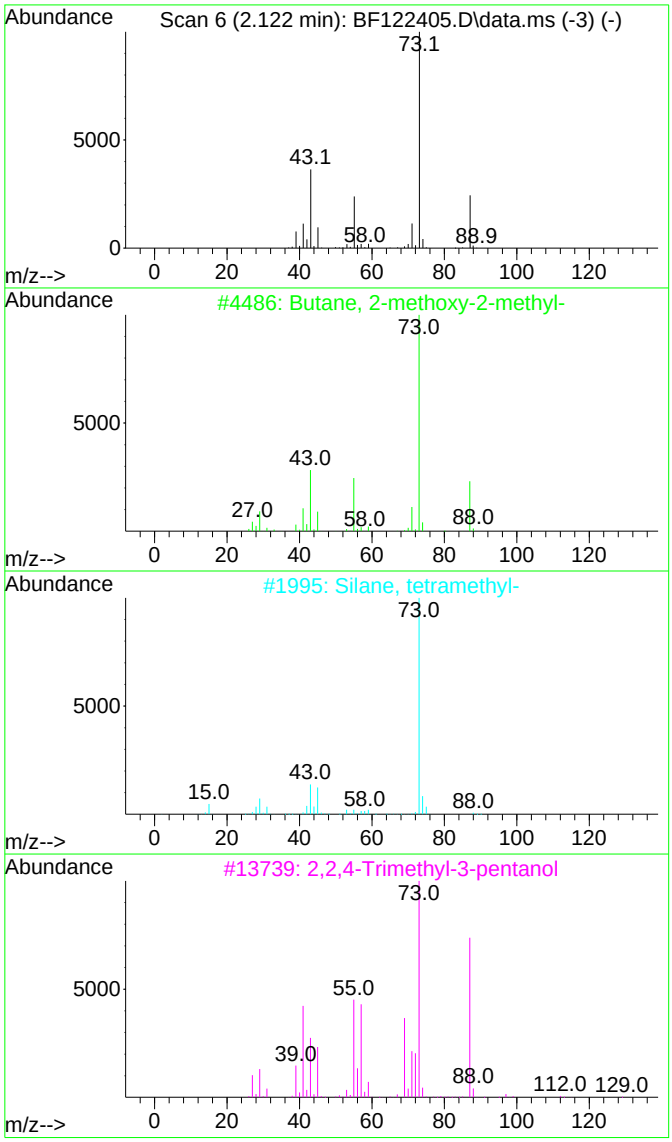
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

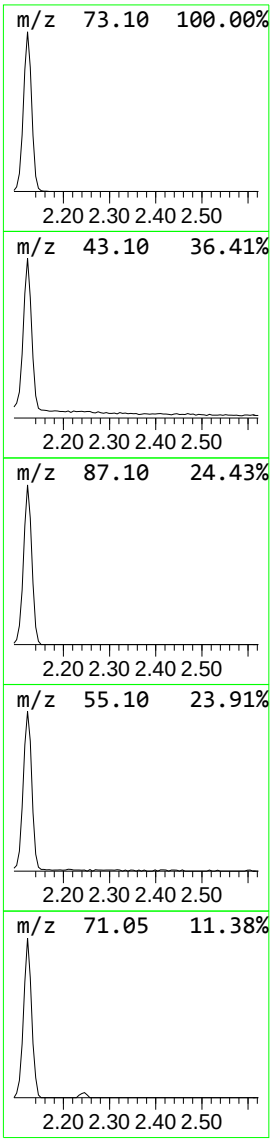
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	11.71 ng	717035	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	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122405.D
Acq On : 20 Nov 2020 16:08
Operator : JU/CG
Sample : L4809-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-D

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

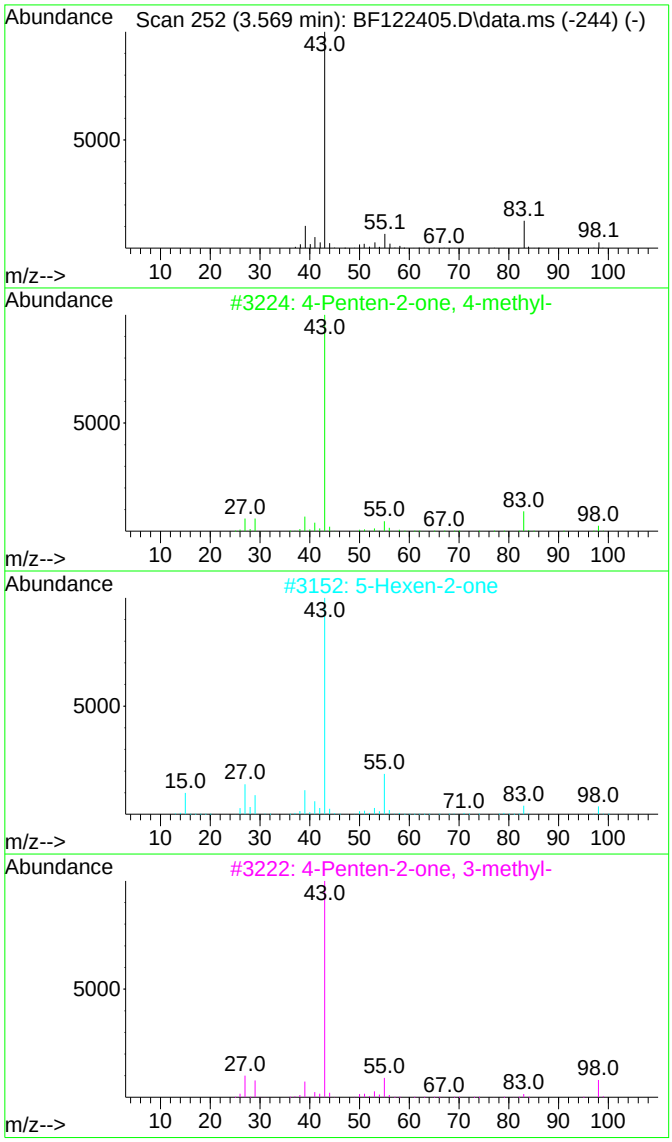
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

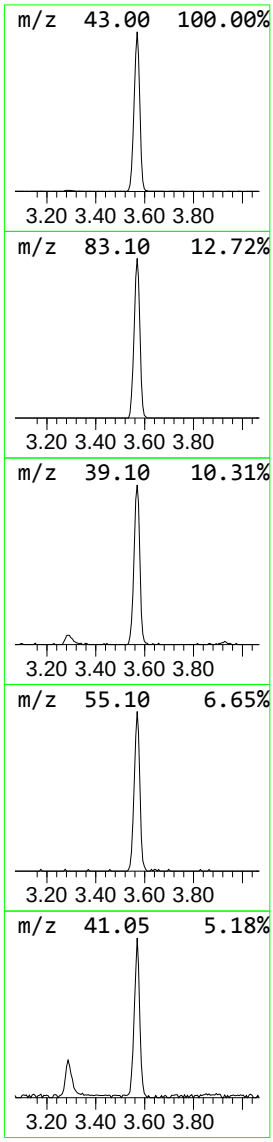
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.569	20.00 ng	1224200	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	50
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	33
4	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	23
5	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122405.D
Acq On : 20 Nov 2020 16:08
Operator : JU/CG
Sample : L4809-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-D

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

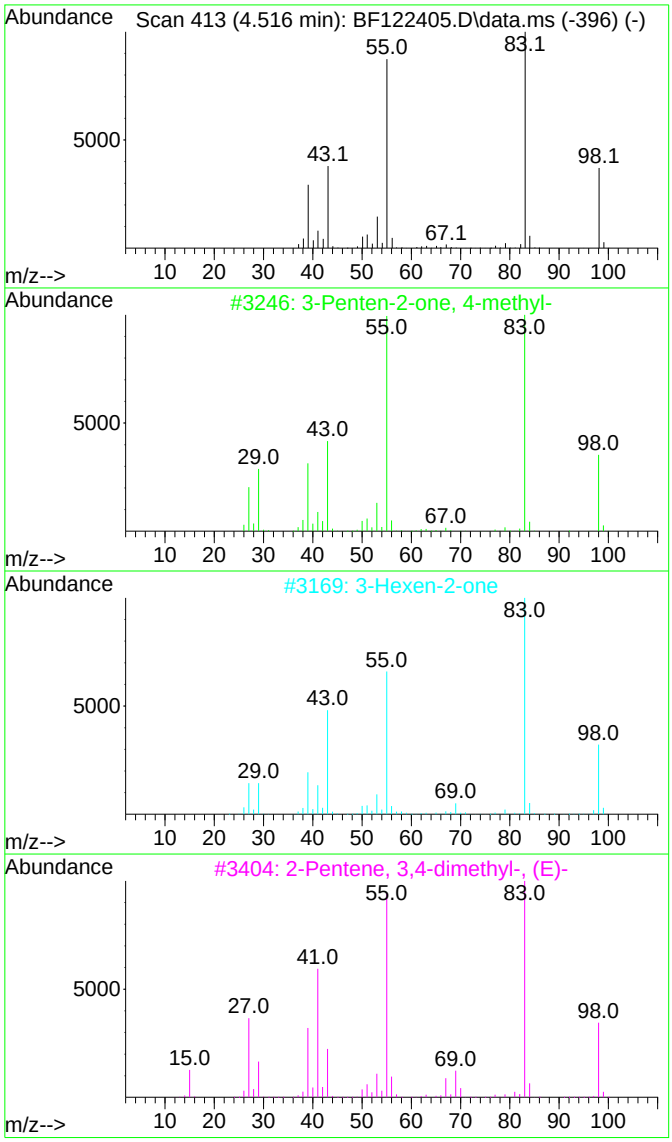
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

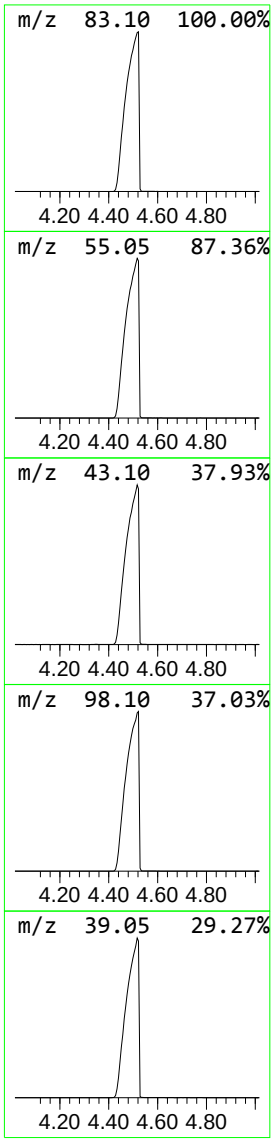
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.516	616.12 ng	37721900	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	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	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122405.D
Acq On : 20 Nov 2020 16:08
Operator : JU/CG
Sample : L4809-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-D

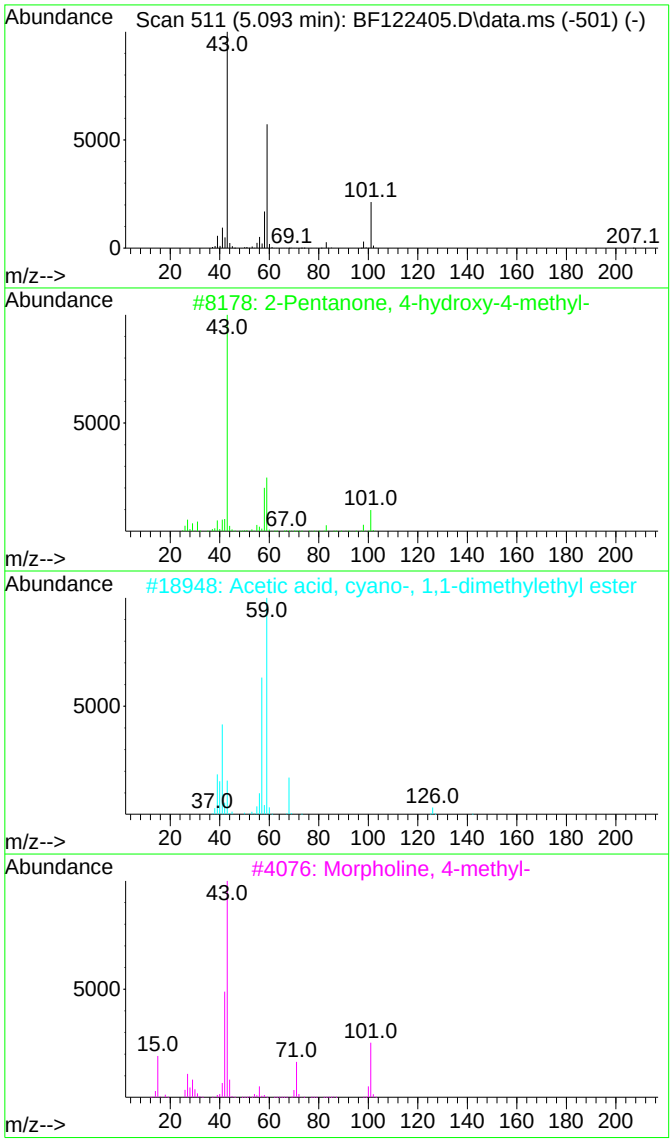
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

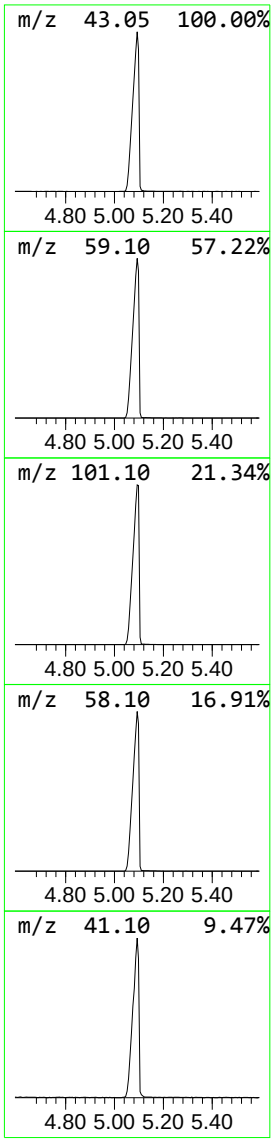
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	112.00 ng	6857130	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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122405.D
Acq On : 20 Nov 2020 16:08
Operator : JU/CG
Sample : L4809-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-D

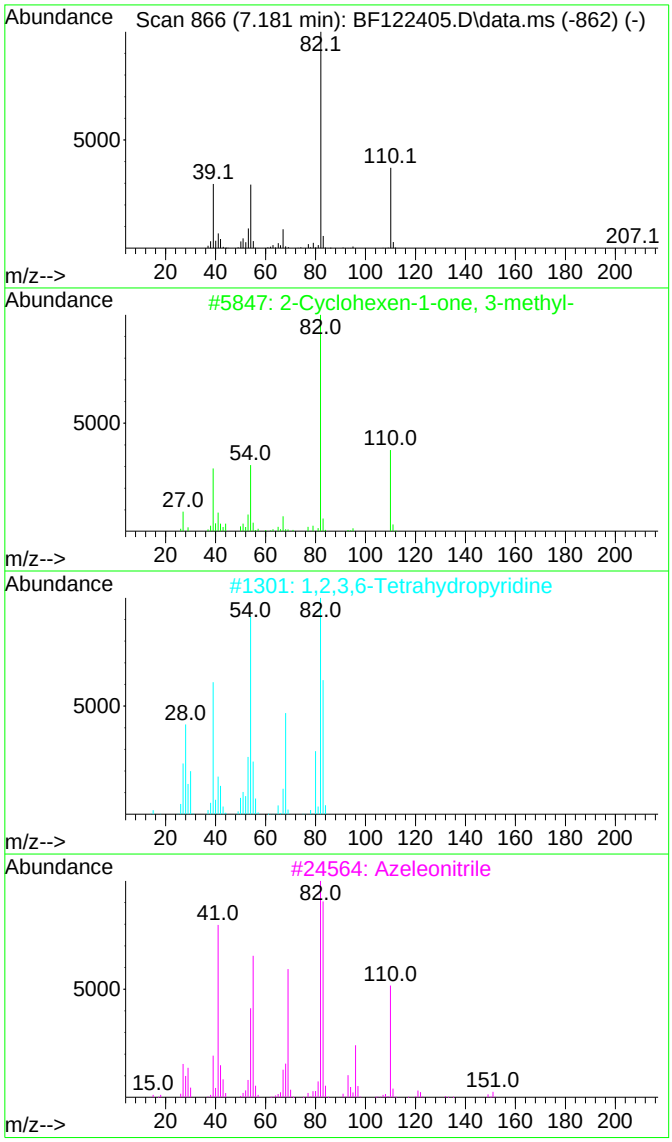
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

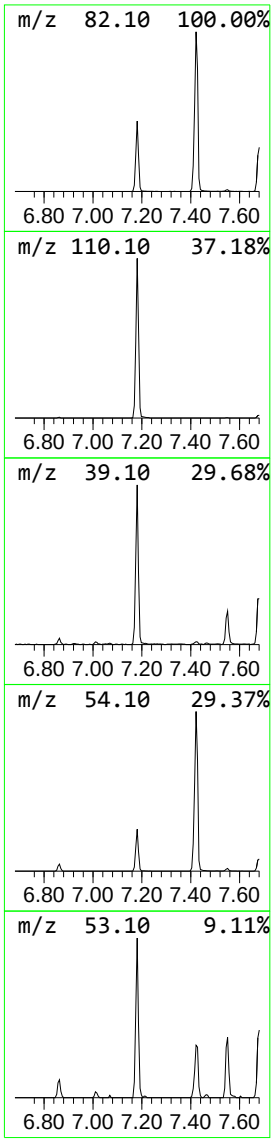
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.181	13.84 ng	847285	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	Azeleonitrile	150	C9H14N2	001675-69-0	50
4	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	42
5	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122405.D
Acq On : 20 Nov 2020 16:08
Operator : JU/CG
Sample : L4809-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-D

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

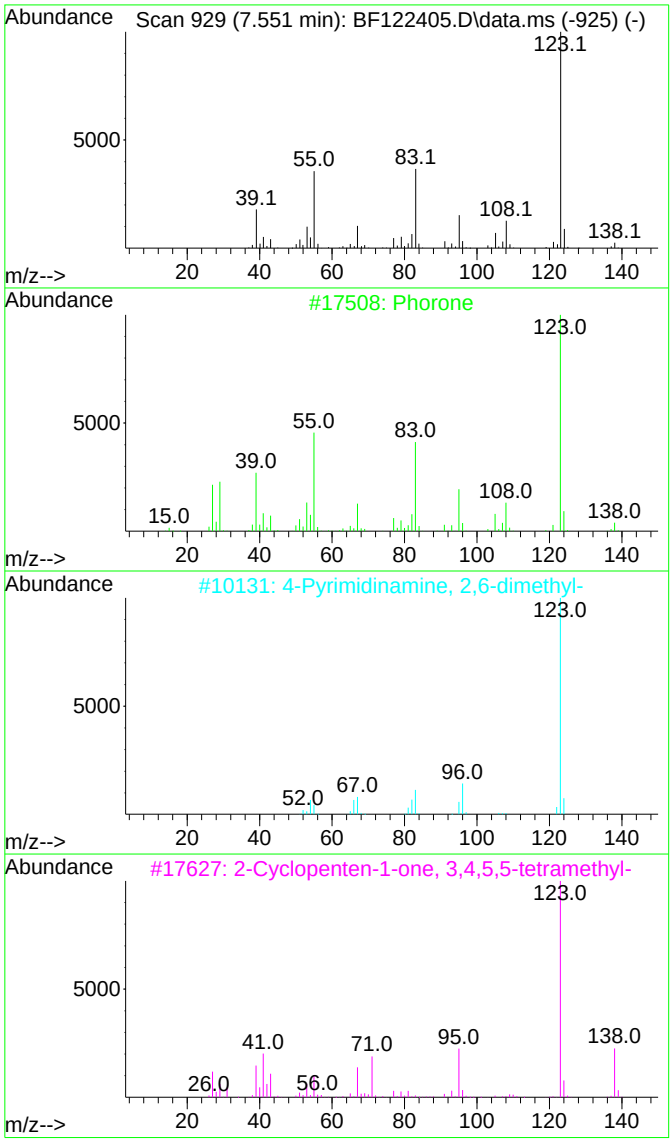
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

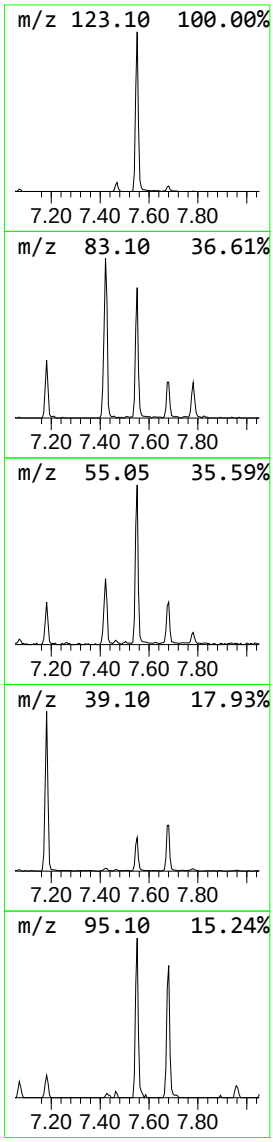
****

Peak Number 6 Phorone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.551	4.85 ng	389202	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phorone	138	C9H14O	000504-20-1	92
2	4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	53
3	2-Cyclopenten-1-one, 3,4,5,5-tet...	138	C9H14O	090611-02-2	53
4	3-Pyridinol, 2,6-dimethyl-	123	C7H9NO	001122-43-6	52
5	1-(1-Ethyl-2,3-dimethyl-cyclopen...	166	C11H18O	1000185-18-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122405.D
Acq On : 20 Nov 2020 16:08
Operator : JU/CG
Sample : L4809-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-D

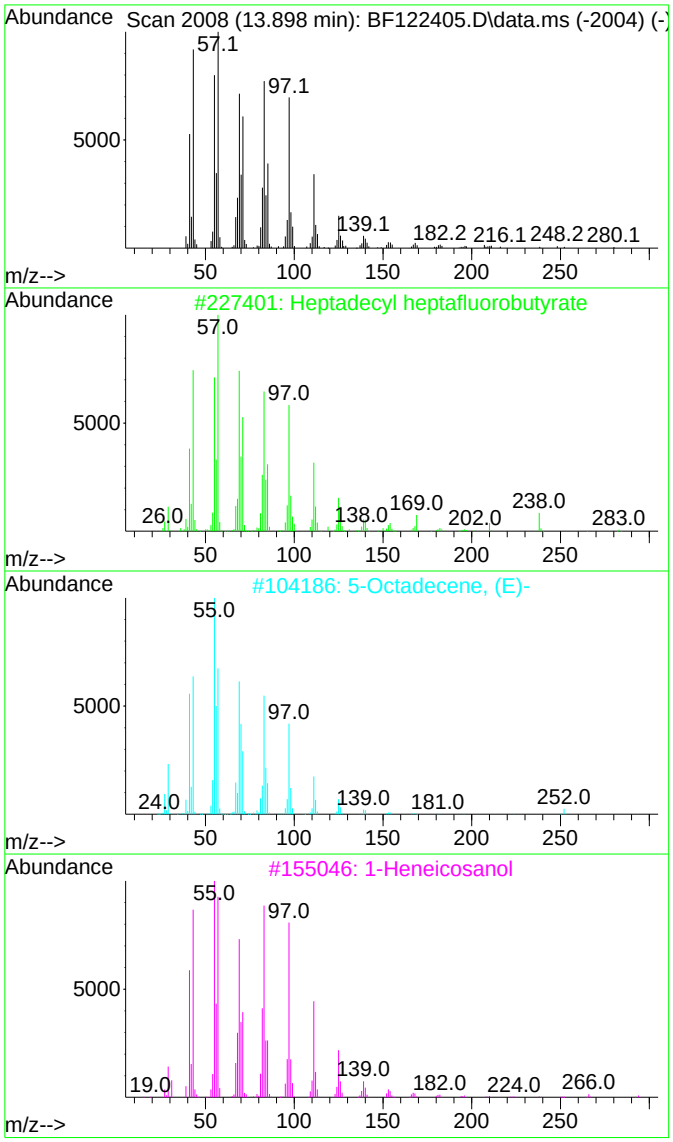
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

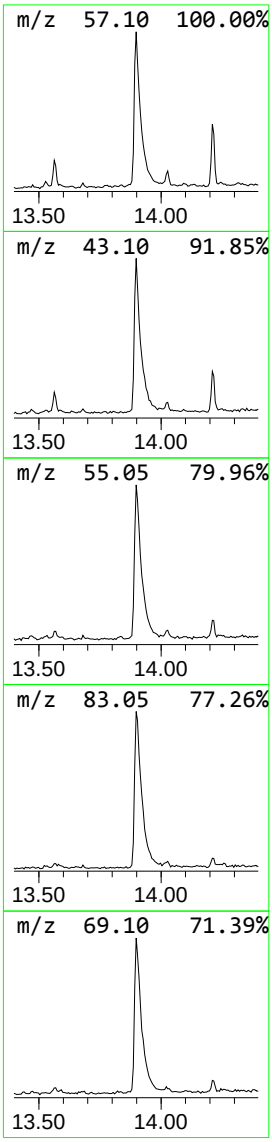
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	9.65 ng	1132610	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122405.D
Acq On : 20 Nov 2020 16:08
Operator : JU/CG
Sample : L4809-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-D

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...	2.122	11.7	ng	717035	1	6.863	1224490	20.0
4-Penten-2-one,...	3.569	20.0	ng	1224200	1	6.863	1224490	20.0
3-Penten-2-one,...	4.516	616.1	ng	37721900	1	6.863	1224490	20.0
2-Pentanone, 4-...	5.093	112.0	ng	6857130	1	6.863	1224490	20.0
2-Cyclohexen-1-...	7.181	13.8	ng	847285	1	6.863	1224490	20.0
Phorone	7.551	4.8	ng	389202	2	8.151	1603530	20.0
Heptadecyl hept...	13.898	9.7	ng	1132610	5	14.039	2346440	20.0