LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122404.D
Acq On : 20 Nov 2020 15:37
Operator : JU/CG
Sample : L4809-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-C

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: BF122404.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	24	rVB	603416	846683	6.77%	1.754%
2	3.569	246	252	260	rVB	206107	314246	2.51%	0.651%
3	4.475	394	406	409	rBV	6790446	12504721	100.00%	25.909%
4	5.075	497	508	511	rBV	2287958	2804213	22.43%	5.810%
5	5.481	573	577	590	rBV	1409283	1207633	9.66%	2.502%
6	6.493	745	749	762	rBV	2941375	2777849	22.21%	5.756%
7	6.863	808	812	815	rBV	1597109	1226646	9.81%	2.542%
8	7.181	862	866	869	rBV	307511	235112	1.88%	0.487%
9	7.422	902	907	911	rBV	2756362	2704923	21.63%	5.604%
10	7.681	947	951	958	rBV	141370	130922	1.05%	0.271%
11	8.151	1026	1031	1034	rBV	1803481	1627501	13.02%	3.372%
12	9.228	1209	1214	1217	rBV	5798639	5191897	41.52%	10.757%
13	9.622	1277	1281	1289	rVB	154845	143794	1.15%	0.298%
14	9.910	1325	1330	1333	rBV	2117960	1945753	15.56%	4.031%
15	10.698	1458	1464	1472	rBV	160050	183264	1.47%	0.380%
16	11.398	1578	1583	1586	rBV	2295778	2080143	16.63%	4.310%
17	12.716	1803	1807	1817	rBV	135708	246450	1.97%	0.511%
18	12.992	1848	1854	1857	rBV	6194269	6474050	51.77%	13.414%
19	13.898	2004	2008	2026	rBV	427022	941763	7.53%	1.951%
20	14.039	2028	2032	2036	rBV	2453610	2307829	18.46%	4.782%
21	15.521	2279	2284	2289	rBV	1950281	2368542	18.94%	4.907%

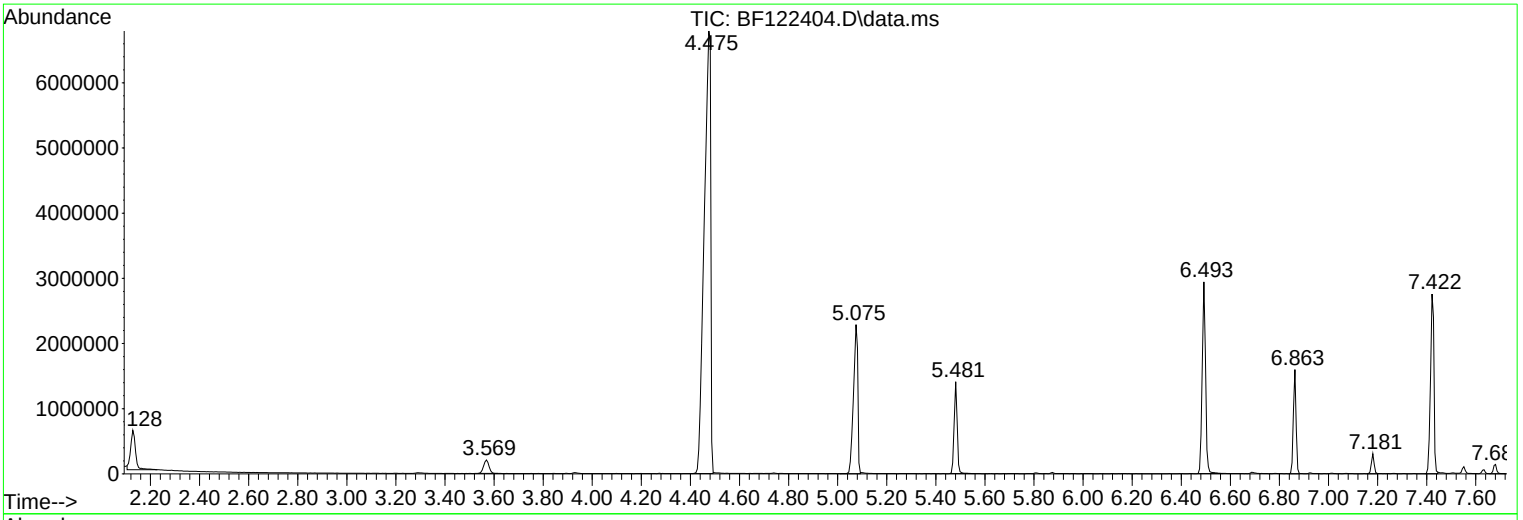
Sum of corrected areas: 48263934

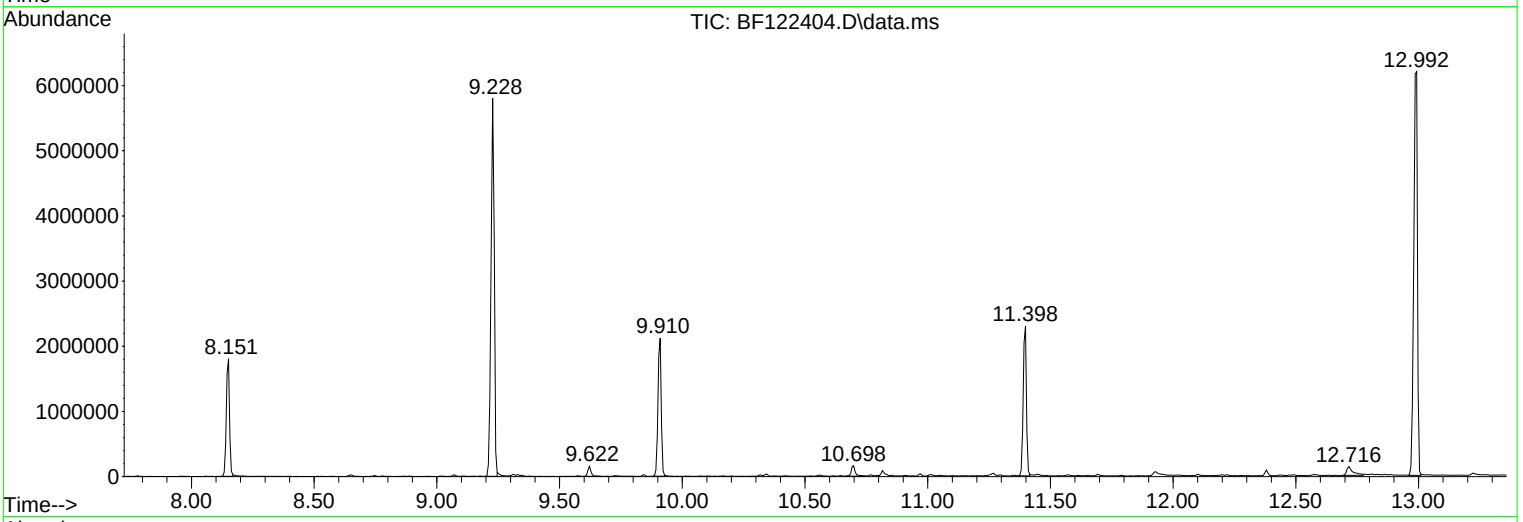
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122404.D
Acq On : 20 Nov 2020 15:37
Operator : JU/CG
Sample : L4809-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

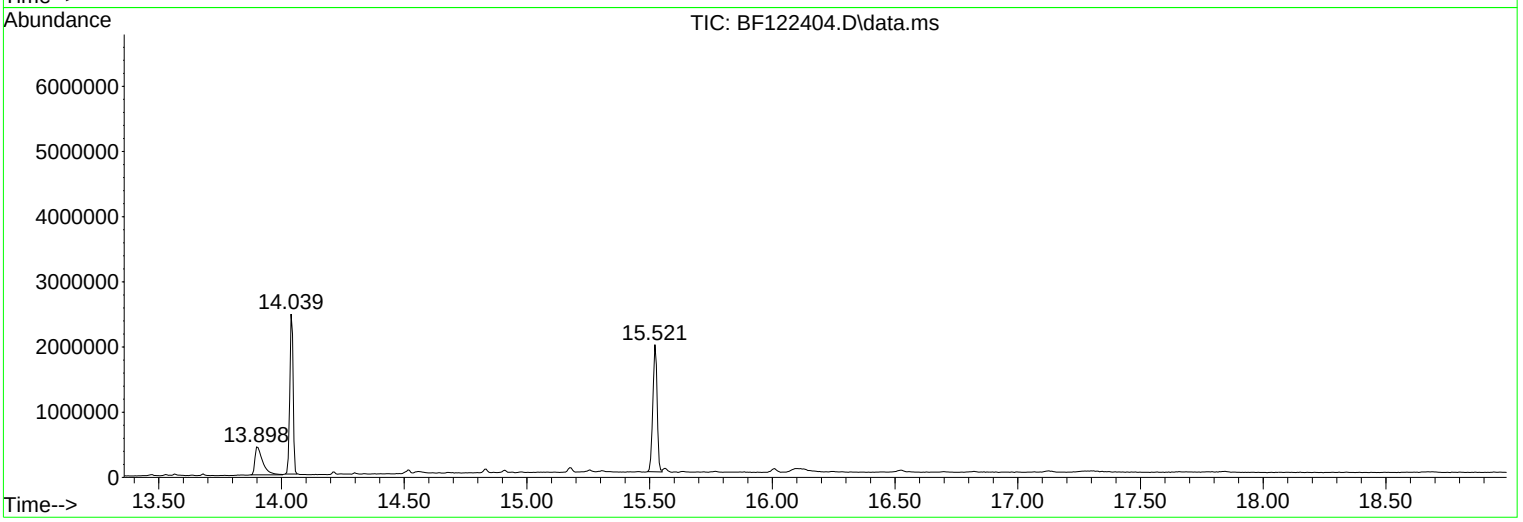
Instrument :
BNA_F
ClientSampleId :
MS-CON-C

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 : BF122404.D
Acq On : 20 Nov 2020 15:37
Operator : JU/CG
Sample : L4809-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-C

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

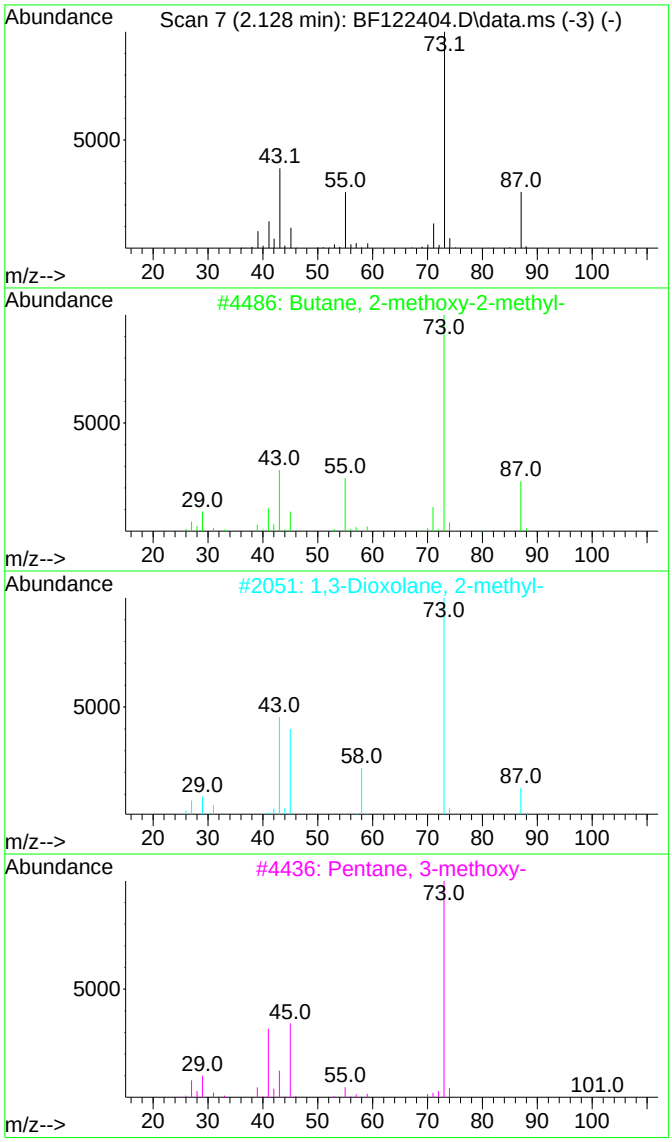
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

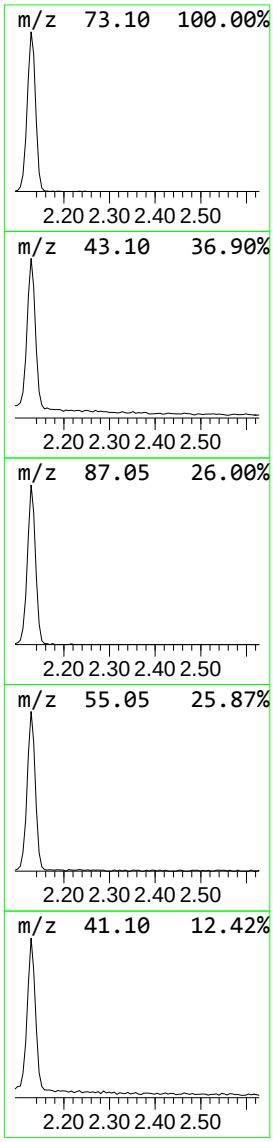
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	13.80 ng	846683	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122404.D
Acq On : 20 Nov 2020 15:37
Operator : JU/CG
Sample : L4809-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-C

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

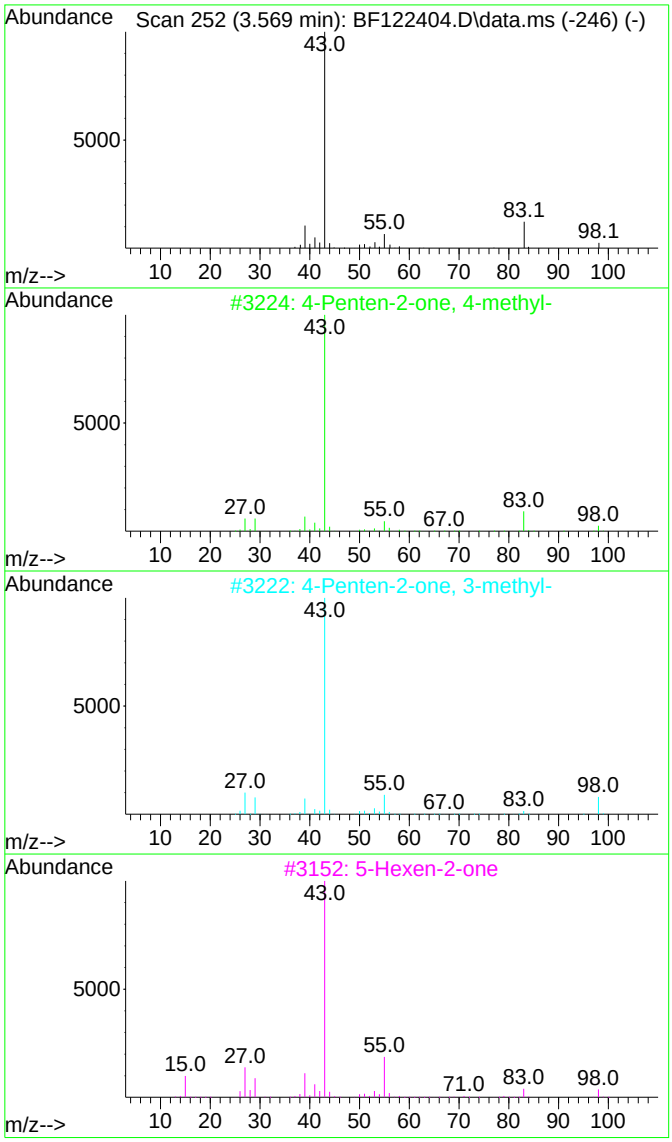
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

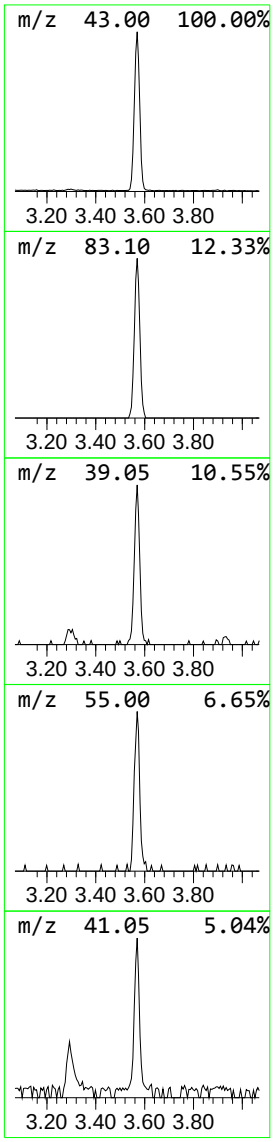
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.569	5.12 ng	314246	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	80
2	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	50
3	5-Hexen-2-one	98	C6H10O	000109-49-9	50
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 : BF122404.D
Acq On : 20 Nov 2020 15:37
Operator : JU/CG
Sample : L4809-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-C

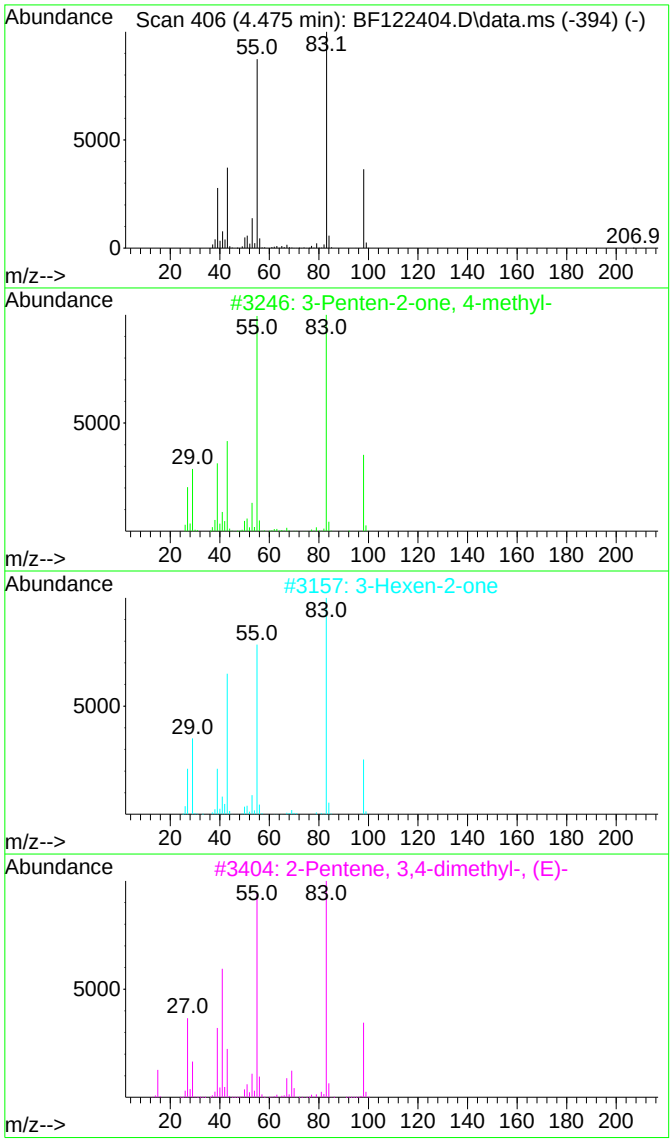
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

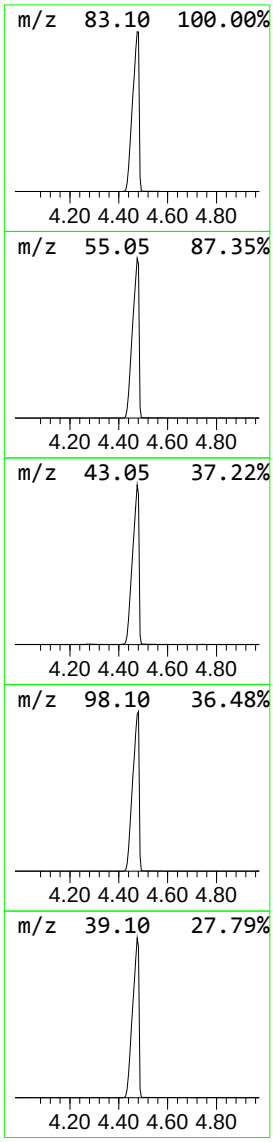
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.475	203.88 ng	12504700	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, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122404.D
Acq On : 20 Nov 2020 15:37
Operator : JU/CG
Sample : L4809-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-C

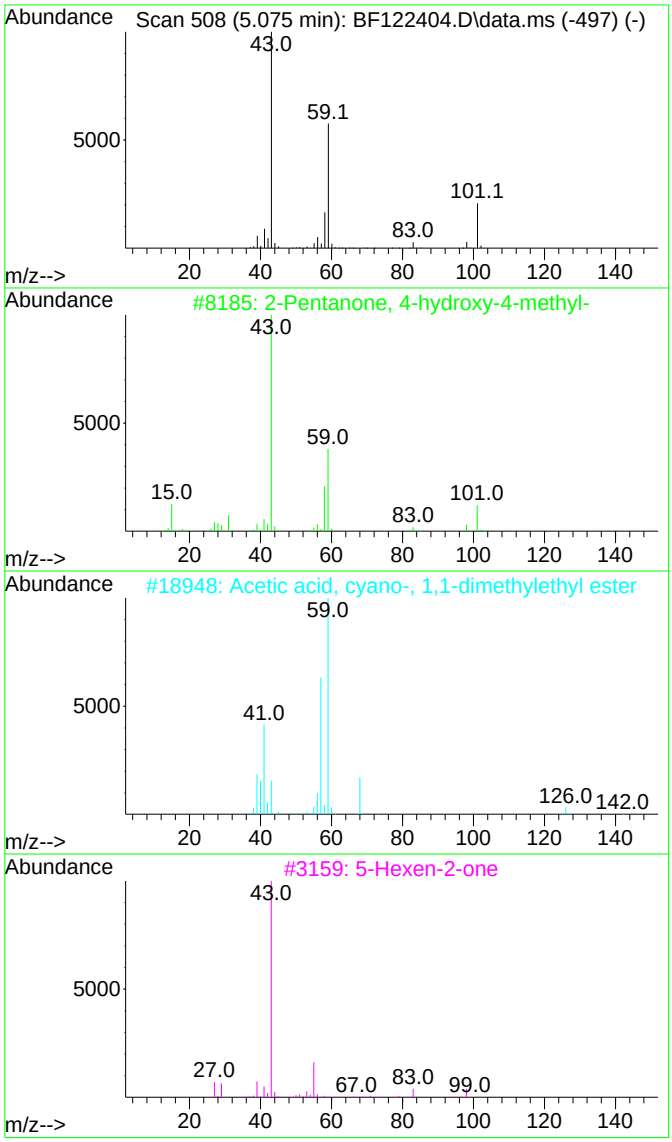
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

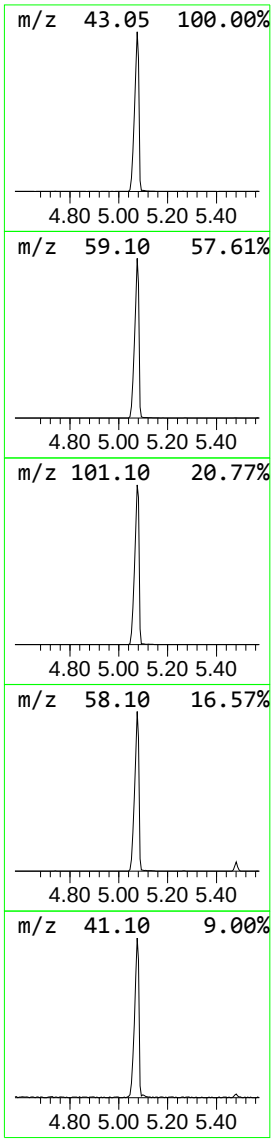
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	45.72 ng	2804210	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	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122404.D
Acq On : 20 Nov 2020 15:37
Operator : JU/CG
Sample : L4809-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-C

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

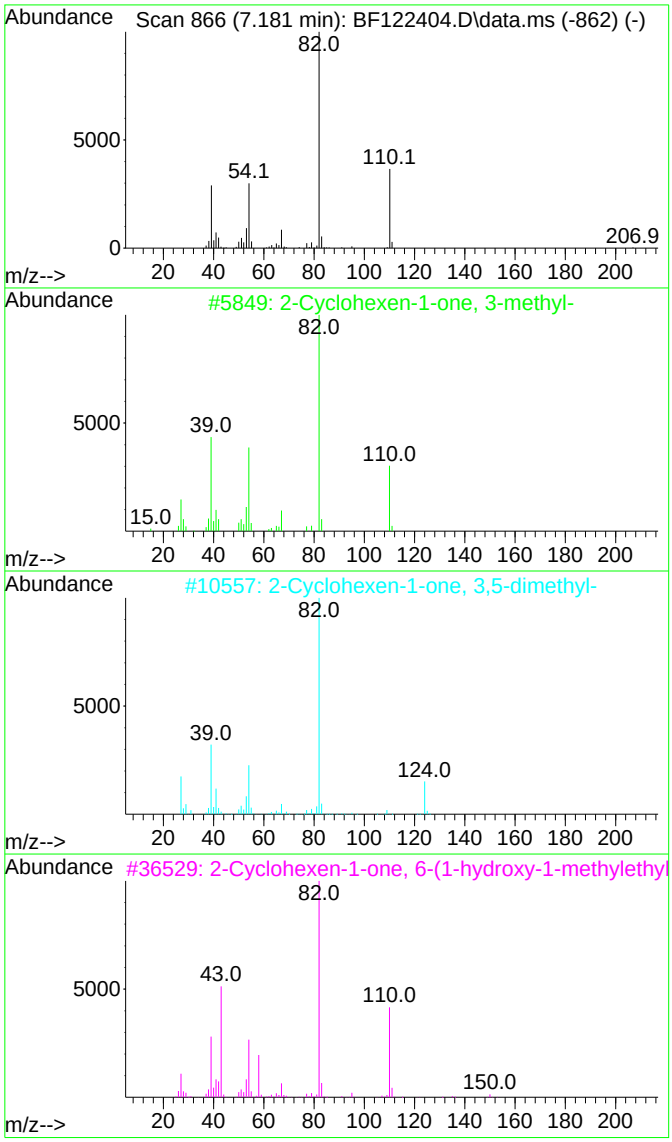
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

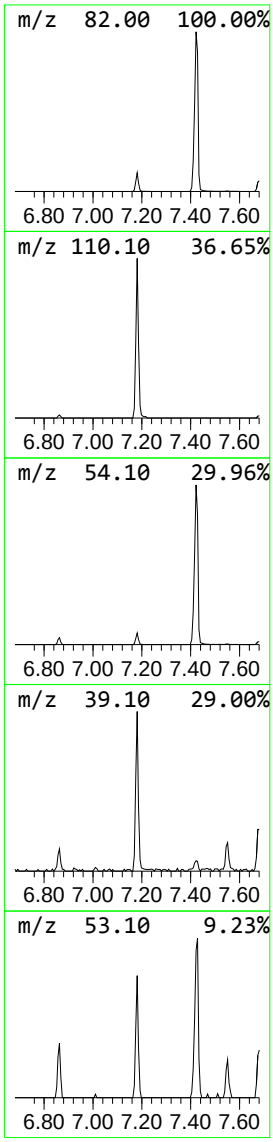
****

Peak Number 5 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.181	3.83 ng	235112	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	2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	64
3	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	64
4	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	53
5	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122404.D
Acq On : 20 Nov 2020 15:37
Operator : JU/CG
Sample : L4809-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-C

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

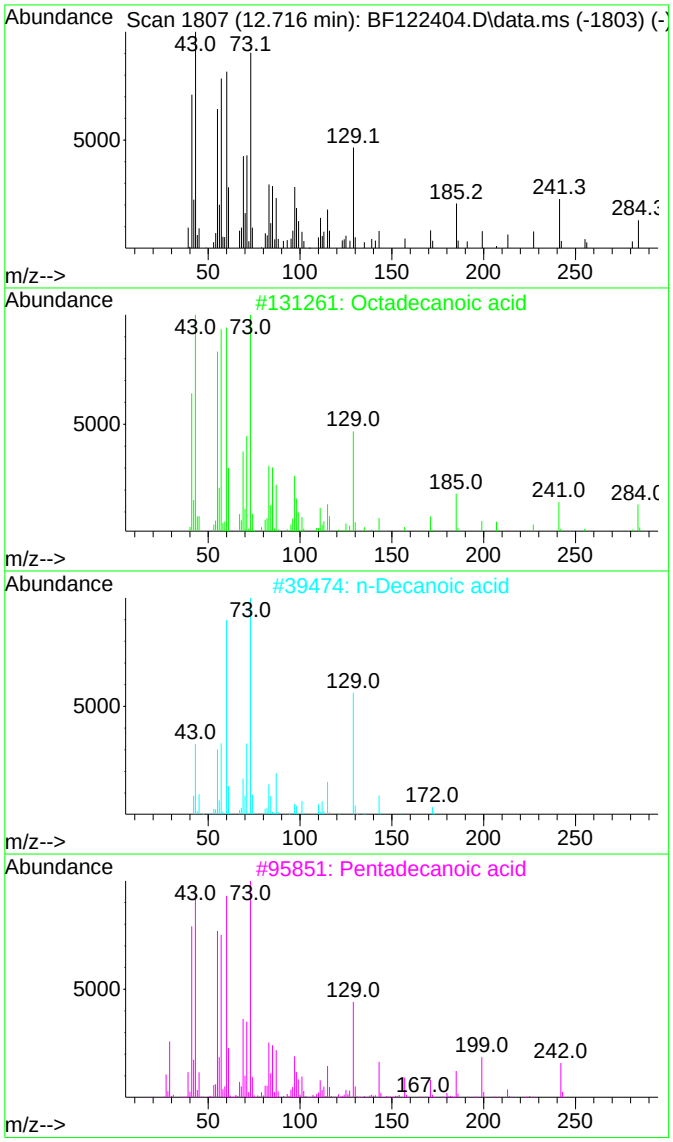
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

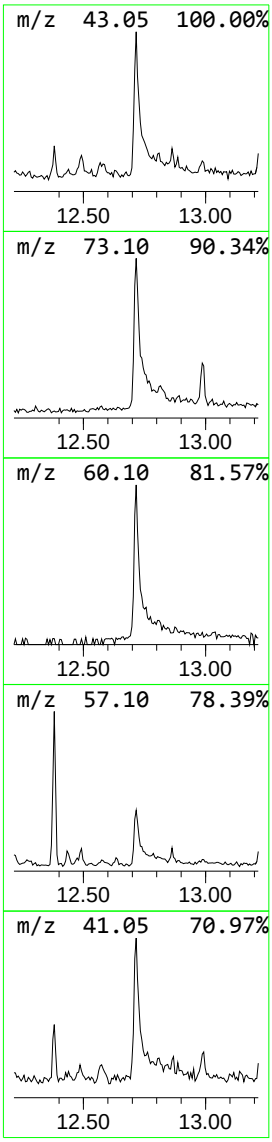
****

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.37 ng	246450	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122404.D
Acq On : 20 Nov 2020 15:37
Operator : JU/CG
Sample : L4809-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-C

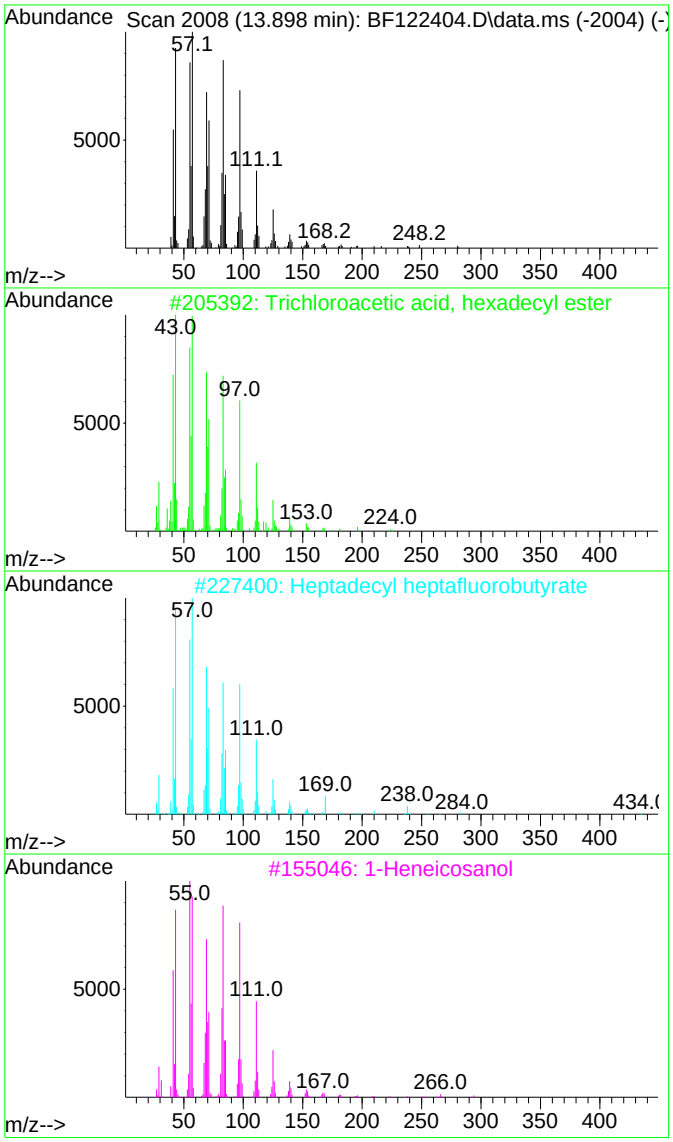
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

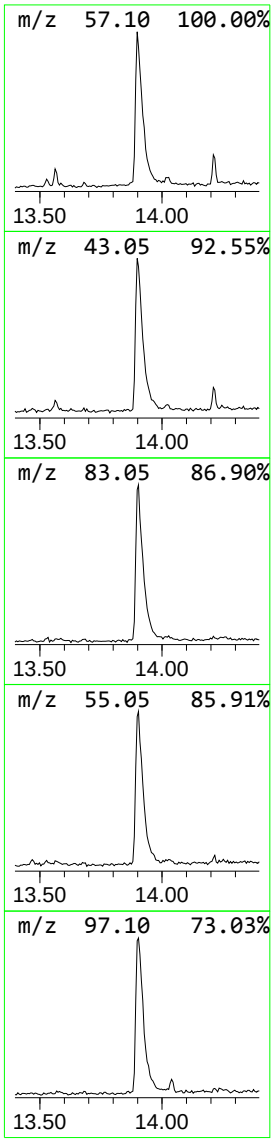
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	8.16 ng	941763	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122404.D
Acq On : 20 Nov 2020 15:37
Operator : JU/CG
Sample : L4809-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-C

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	13.8	ng	846683	1	6.863	1226650	20.0
4-Penten-2-one,...	3.569	5.1	ng	314246	1	6.863	1226650	20.0
3-Penten-2-one,...	4.475	203.9	ng	12504700	1	6.863	1226650	20.0
2-Pentanone, 4-...	5.075	45.7	ng	2804210	1	6.863	1226650	20.0
2-Cyclohexen-1-...	7.181	3.8	ng	235112	1	6.863	1226650	20.0
Octadecanoic acid	12.716	2.4	ng	246450	4	11.398	2080140	20.0
Trichloroacetic...	13.898	8.2	ng	941763	5	14.039	2307830	20.0