LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022021\
Data File : BF123250.D
Acq On : 20 Feb 2021 17:47
Operator : JU/CG
Sample : M1433-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FR-WEST

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-BF021921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	13	rVB	344441	383857	9.41%	1.597%
2	3.557	244	250	258	rBV	60300	93623	2.30%	0.389%
3	4.451	394	402	406	rBV	3147102	4078170	100.00%	16.962%
4	5.069	501	507	510	rBV	1381897	1538664	37.73%	6.400%
5	5.469	572	575	584	rVB	85566	87134	2.14%	0.362%
6	6.475	742	746	763	rBV	1568514	1386919	34.01%	5.768%
7	6.857	807	811	814	rBV	1025828	899234	22.05%	3.740%
8	7.175	862	865	874	rVB	62817	53439	1.31%	0.222%
9	7.416	901	906	909	rBV	2003222	1785287	43.78%	7.425%
10	8.139	1025	1029	1032	rBV	1167830	955159	23.42%	3.973%
11	9.216	1207	1212	1215	rBV	3563288	3161664	77.53%	13.150%
12	9.610	1275	1279	1283	rBV	210194	173481	4.25%	0.722%
13	9.898	1324	1328	1331	rBV	1341377	1099247	26.95%	4.572%
14	11.386	1577	1581	1585	rBV	1386605	1176463	28.85%	4.893%
15	11.915	1667	1671	1686	rBV3	167093	313369	7.68%	1.303%
16	12.704	1801	1805	1819	rBV	263056	478365	11.73%	1.990%
17	12.980	1847	1852	1855	rBV	4014770	3749858	91.95%	15.596%
18	13.921	2007	2012	2027	rBV7	71076	286450	7.02%	1.191%
19	14.033	2027	2031	2035	rVB	1162417	1097451	26.91%	4.564%
20	14.509	2107	2112	2117	rBV	49943	55665	1.36%	0.232%
21	14.892	2174	2177	2182	rBV	69400	70599	1.73%	0.294%
22	15.156	2218	2222	2227	rBV	62796	74420	1.82%	0.310%
23	15.509	2277	2282	2286	rBV	770195	895394	21.96%	3.724%
24	15.980	2358	2362	2366	rVB	39699	53567	1.31%	0.223%
25	16.256	2404	2409	2419	rVB2	45399	95998	2.35%	0.399%

Sum of corrected areas: 24043477

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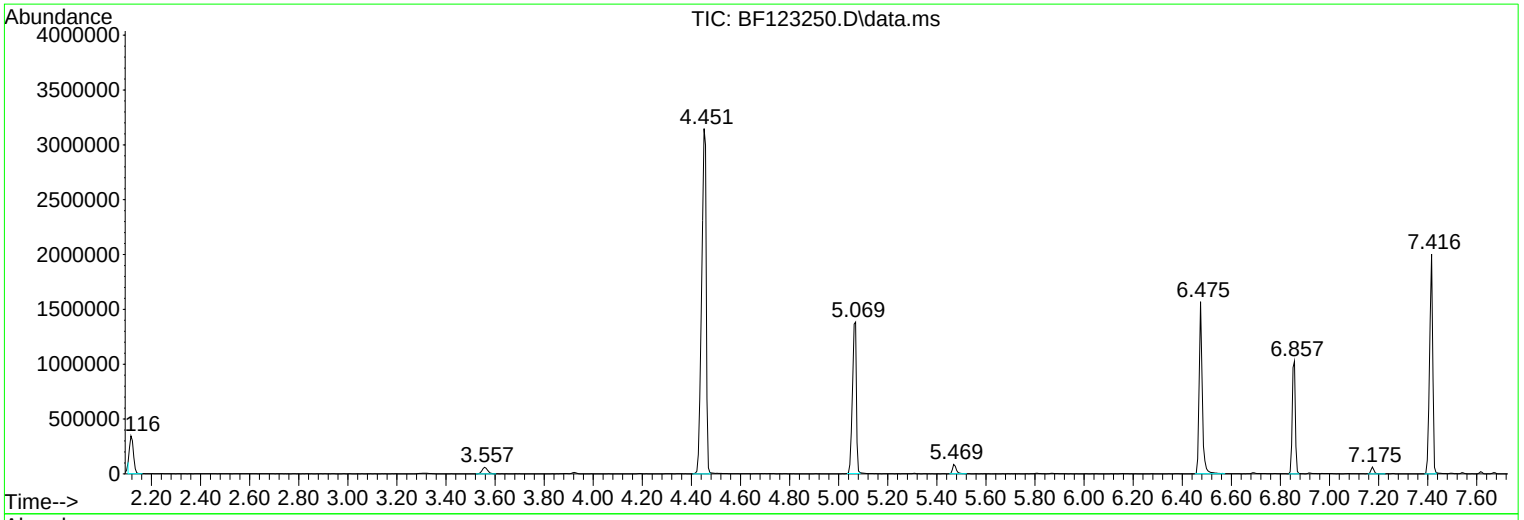
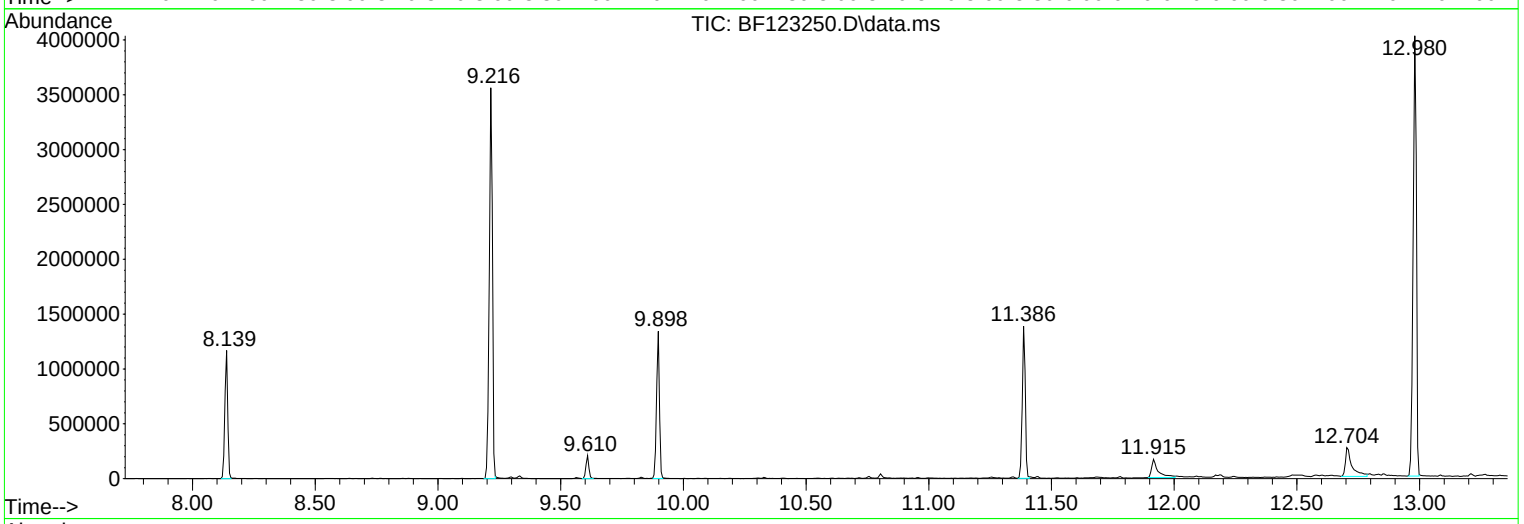
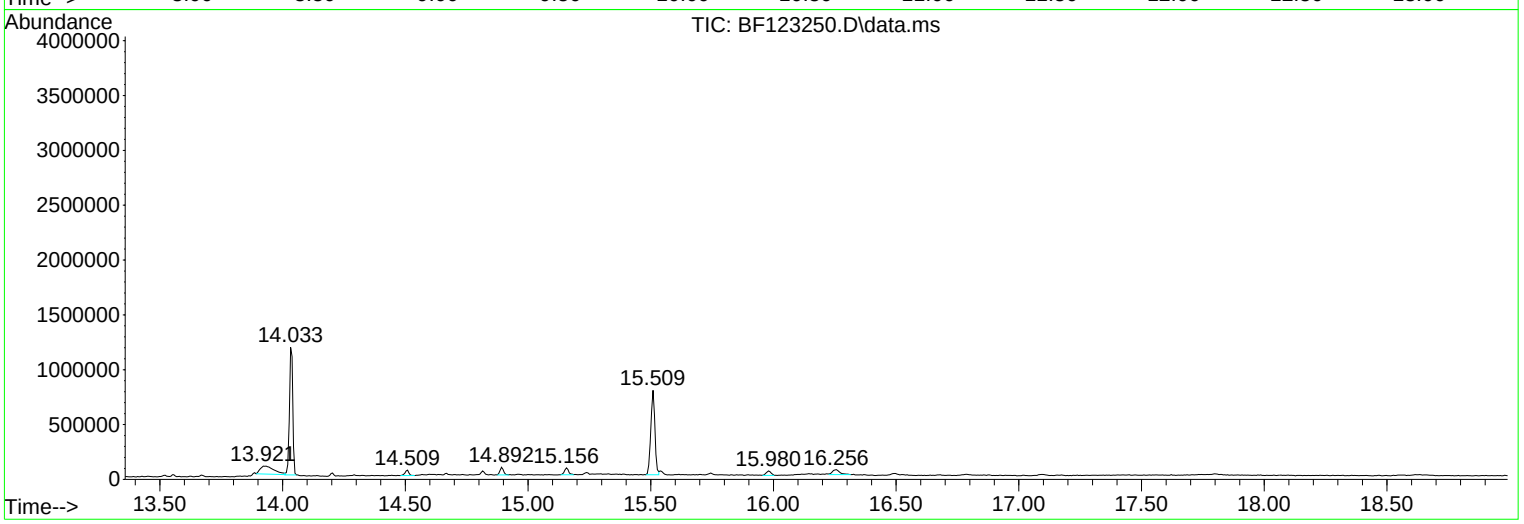
Instrument :
BNA_F
ClientSampleId :
FR-WEST

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

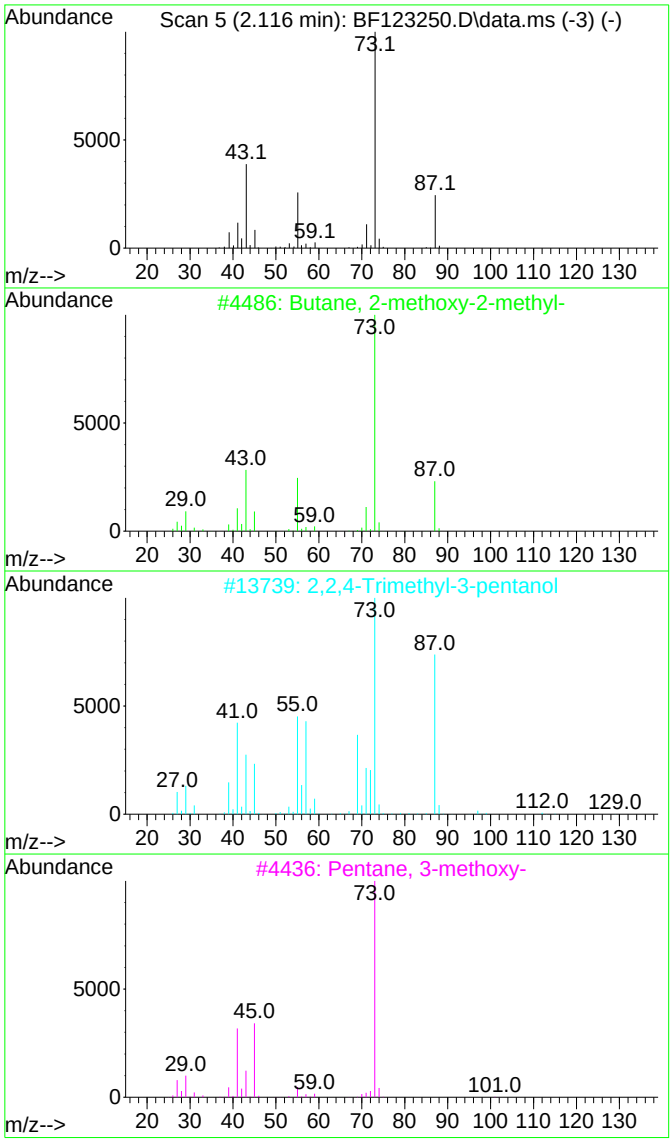
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

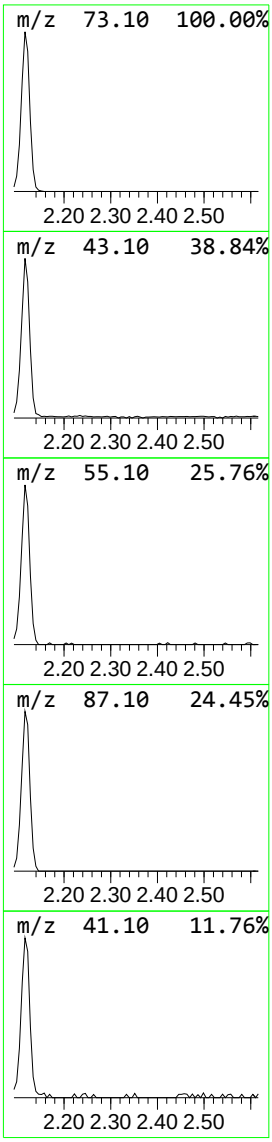
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	8.54 ng	383857	1,4-Dichlorobenzene-d4	6.857

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	40
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





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Data File : BF123250.D
Acq On : 20 Feb 2021 17:47
Operator : JU/CG
Sample : M1433-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FR-WEST

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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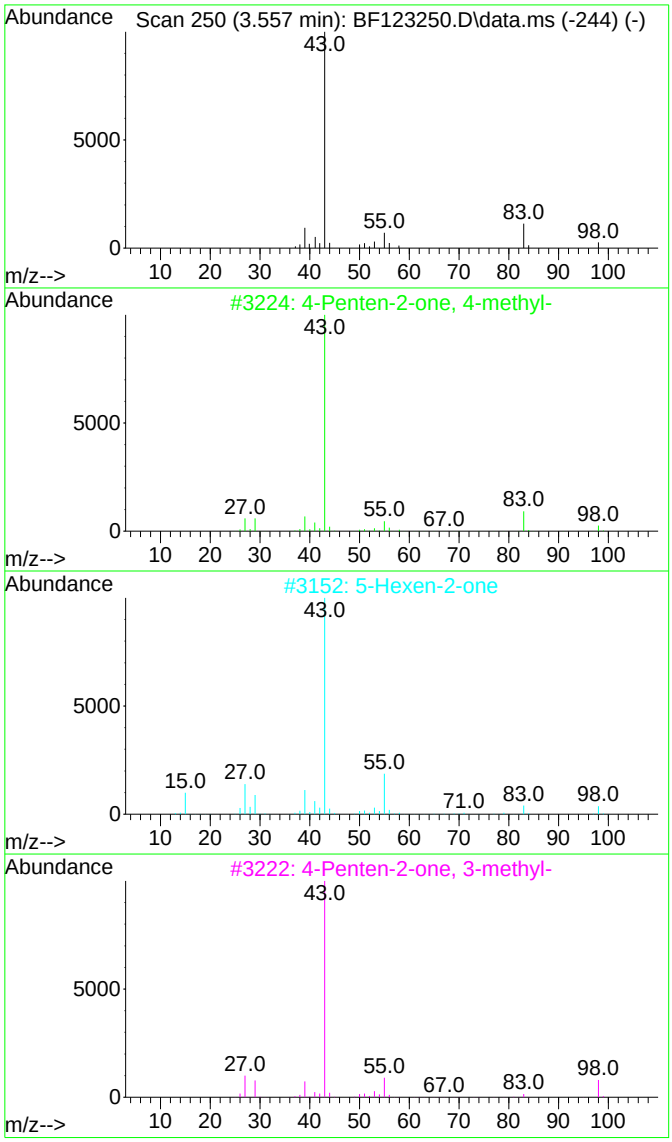
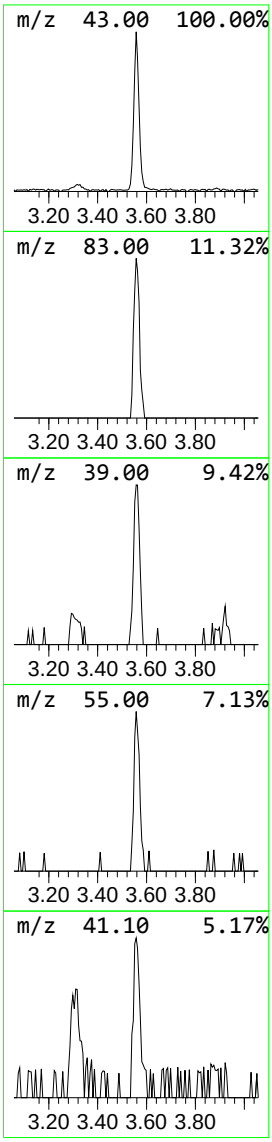
Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.557	2.08 ng	93623	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	50
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	28
4	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	23
5	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9





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Data File : BF123250.D
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Operator : JU/CG
Sample : M1433-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FR-WEST

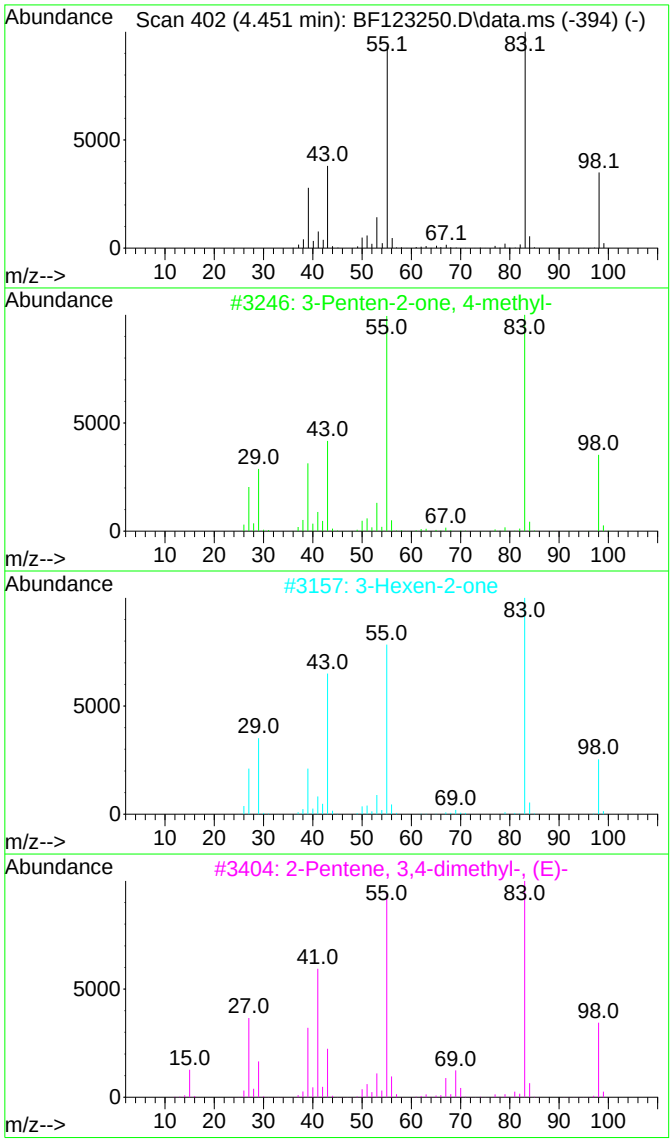
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

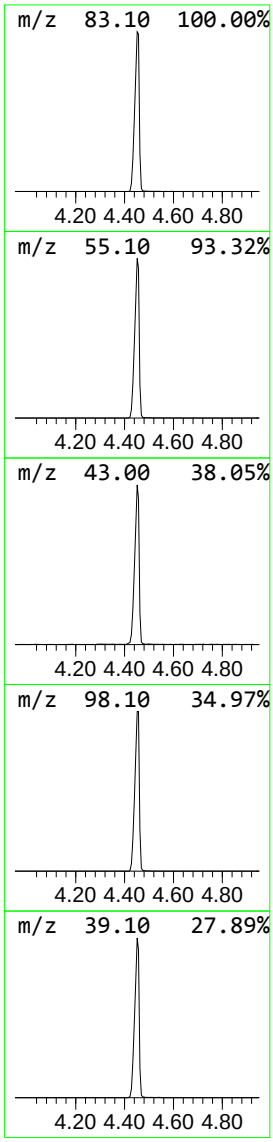
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.451	90.70 ng	4078170	1,4-Dichlorobenzene-d4	6.857

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-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Sample : M1433-05
Misc :
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Instrument :
BNA_F
ClientSampleId :
FR-WEST

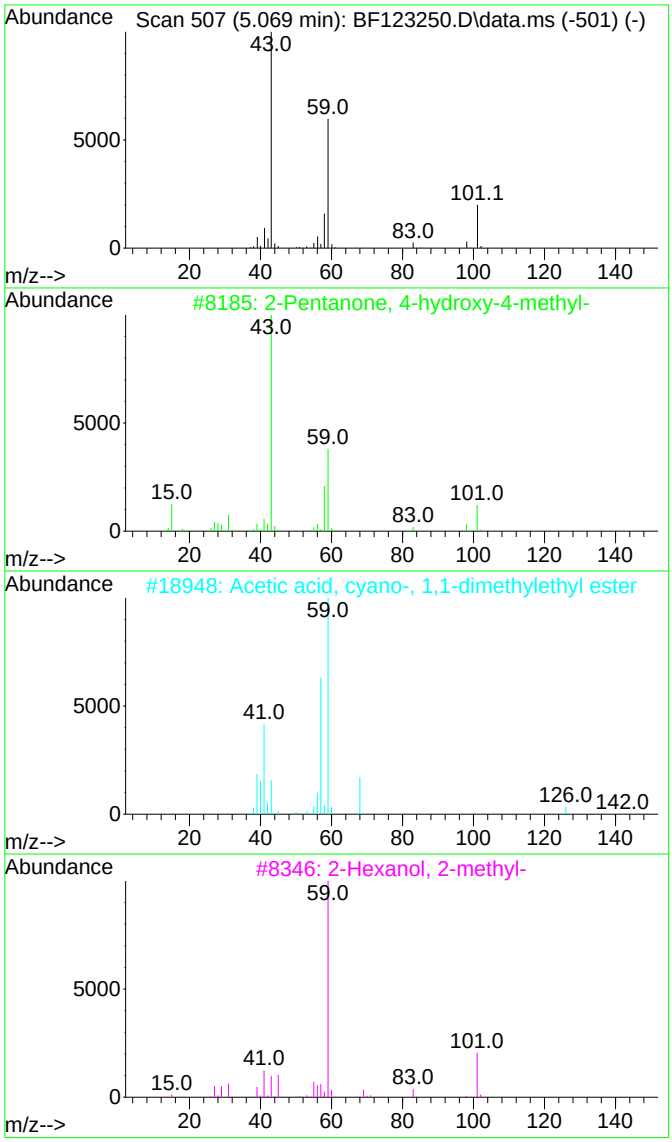
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

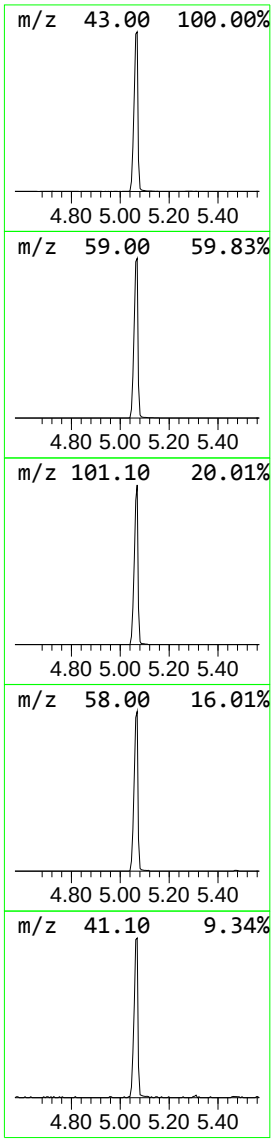
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	34.22 ng	1538660	1,4-Dichlorobenzene-d4	6.857

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	23
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022021\
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Operator : JU/CG
Sample : M1433-05
Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

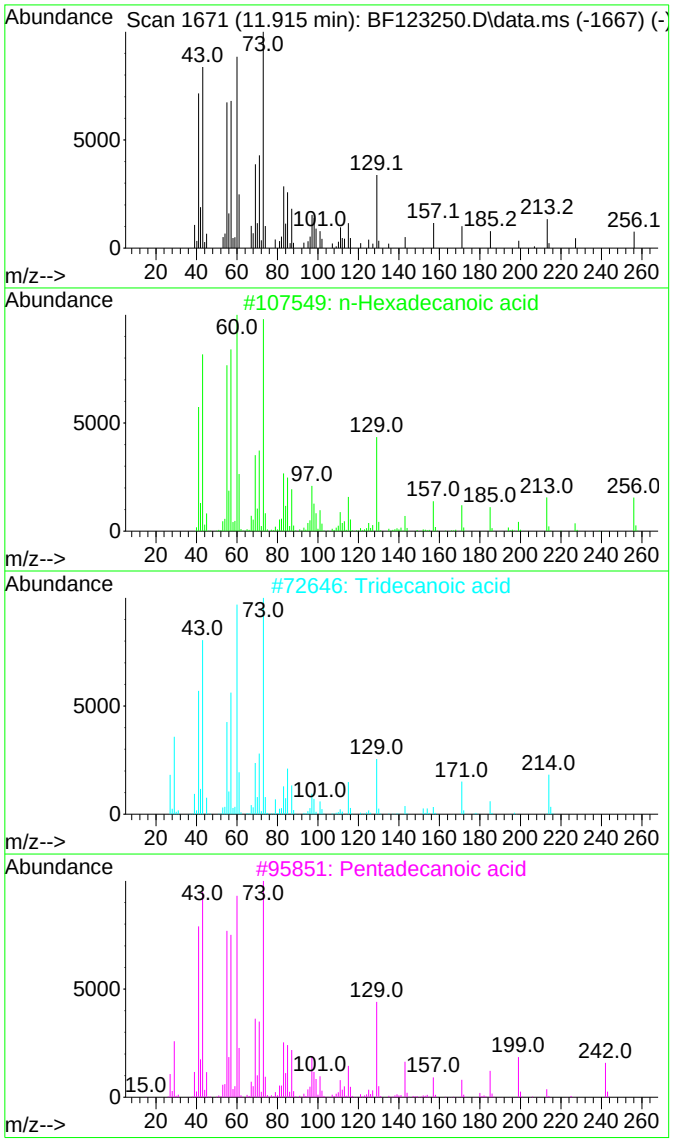
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

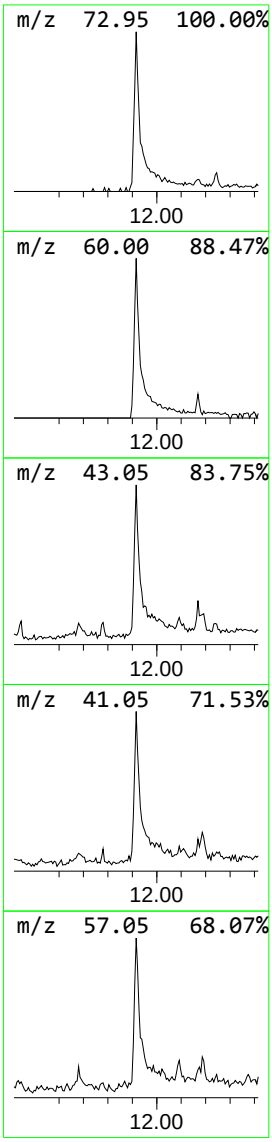
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	5.33 ng	313369	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	18





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BNA_F
ClientSampleId :
FR-WEST

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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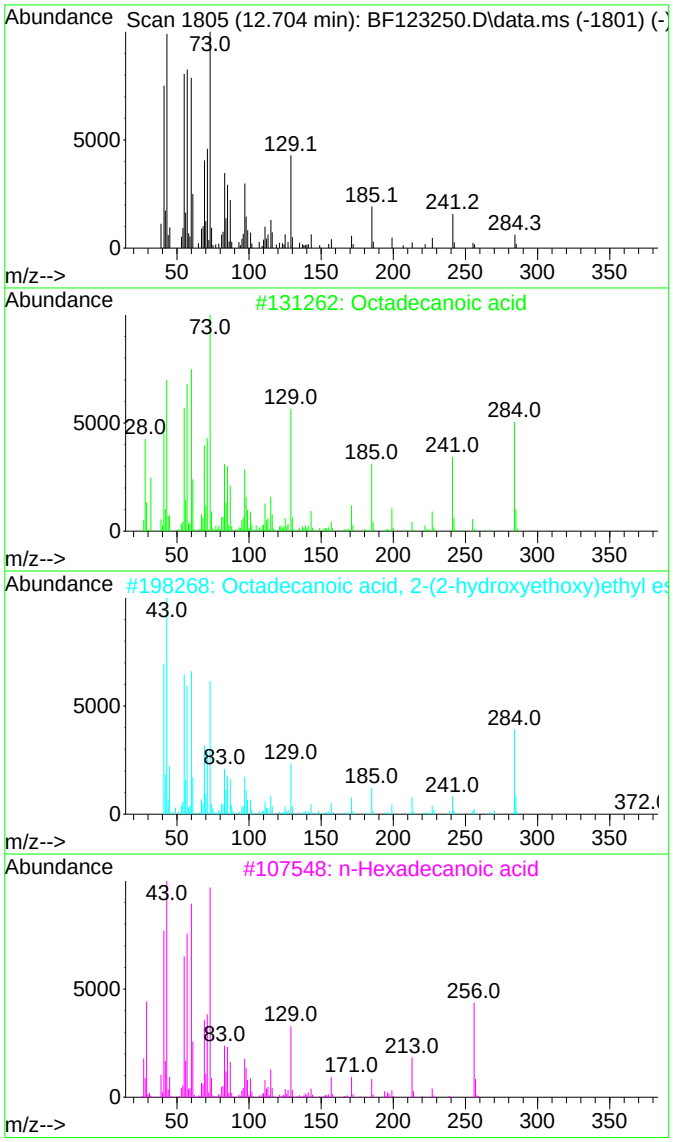
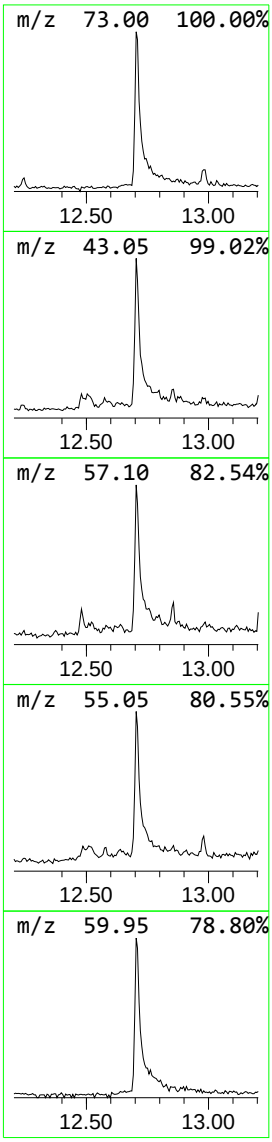
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	8.13 ng	478365	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Sample : M1433-05
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Instrument :
BNA_F
ClientSampleId :
FR-WEST

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

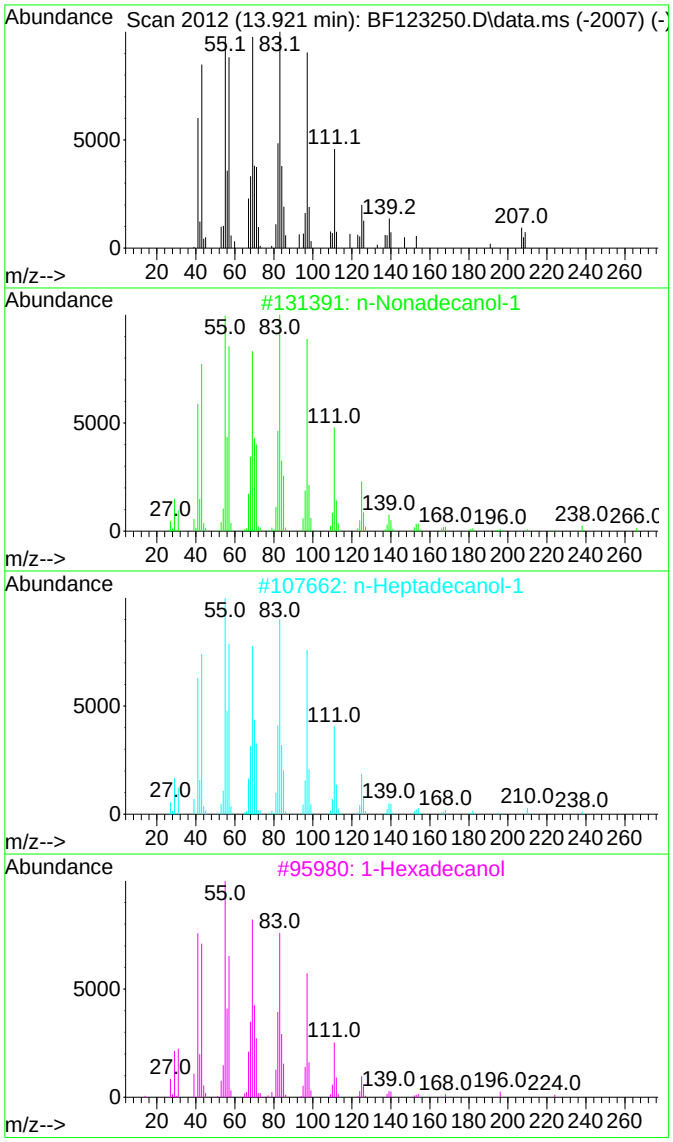
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

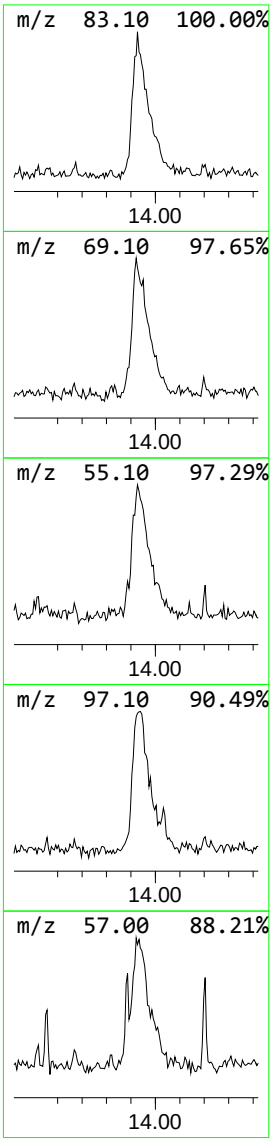
****

Peak Number 7 n-Nonadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	5.22 ng	286450	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	n-Pentadecanol	228	C15H32O	000629-76-5	87
5	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	81





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TIC Integration Parameters: LSCINT.P

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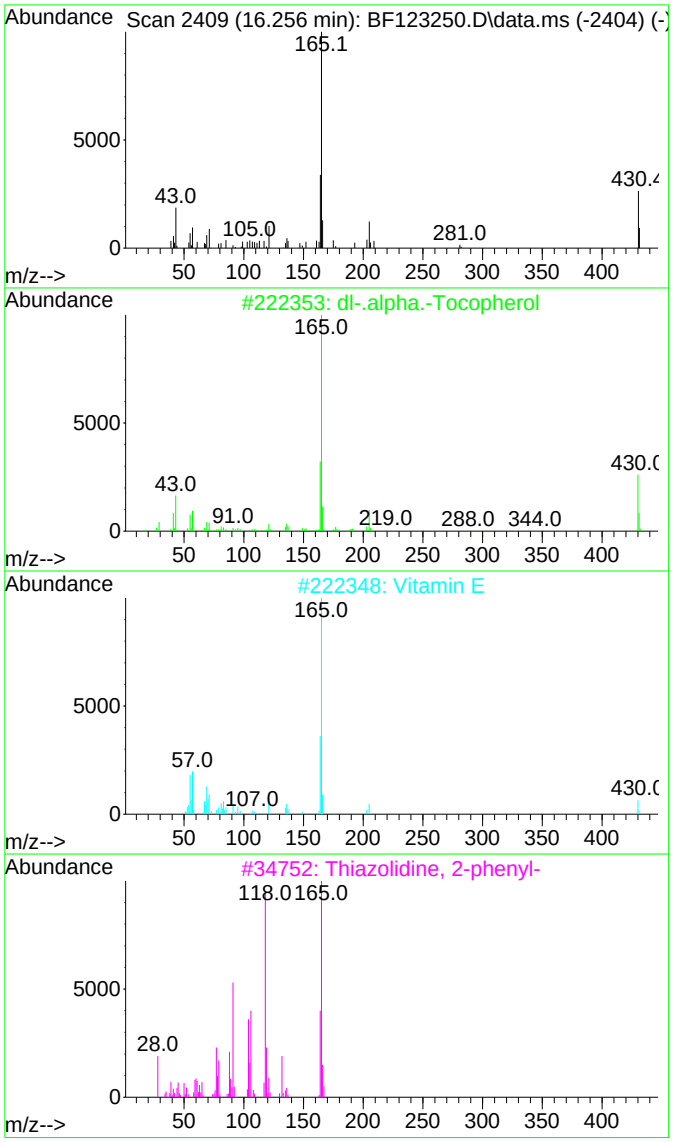
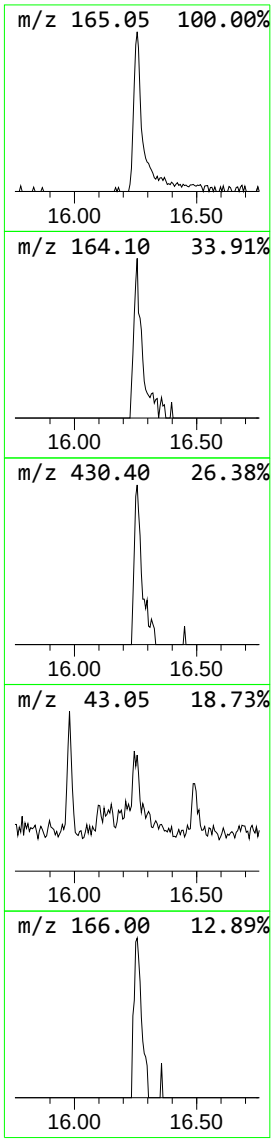
Peak Number 8 dl-.alpha.-Tocopherol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.256	2.14 ng	95998	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-.alpha.-Tocopherol	430	C29H50O2	010191-41-0	95
2	Vitamin E	430	C29H50O2	000059-02-9	94
3	Thiazolidine, 2-phenyl-	165	C9H11NS	004569-82-8	53
4	4-Amino-3-methoxypyrazolo[3,4-d]...	165	C6H7N5O	111375-22-5	50
5	3-Methoxy-6-methyl-6H-pyrazolo[4...	165	C6H7N5O	037526-57-1	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022021\
Data File : BF123250.D
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Operator : JU/CG
Sample : M1433-05
Misc :
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Instrument : BNA_F
ClientSampleId : FR-WEST

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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...	2.116	8.5	ng	383857	1	6.857	899234	20.0
4-Penten-2-one,...	3.557	2.1	ng	93623	1	6.857	899234	20.0
3-Penten-2-one,...	4.451	90.7	ng	4078170	1	6.857	899234	20.0
2-Pentanone, 4-...	5.069	34.2	ng	1538660	1	6.857	899234	20.0
n-Hexadecanoic ...	11.916	5.3	ng	313369	4	11.386	1176460	20.0
Octadecanoic acid	12.704	8.1	ng	478365	4	11.386	1176460	20.0
n-Nonadecanol-1	13.921	5.2	ng	286450	5	14.033	1097450	20.0
dl-.alpha.-Toco...	16.256	2.1	ng	95998	6	15.509	895394	20.0