LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080439.D
Acq On : 13 Jul 2015 21:31
Operator : TP/UM
Sample : G2945-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-PMW-11M

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:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.155	4	6	14	rBV	200605	332204	33.21%	5.378%
2	2.270	14	16	32	rVB	422105	594751	59.46%	9.628%
3	2.681	50	52	56	rVB	29012	42788	4.28%	0.693%
4	5.356	283	286	296	rBV	59308	88491	8.85%	1.433%
5	5.767	320	322	331	rBB	233620	235318	23.53%	3.809%
6	6.156	354	356	359	rBB	13637	19534	1.95%	0.316%
7	6.773	409	410	420	rBB	93147	138649	13.86%	2.245%
8	6.910	420	422	424	rBV	543077	438550	43.85%	7.099%
9	7.127	440	441	444	rBB	84040	99548	9.95%	1.612%
10	7.287	453	455	458	rBB	380599	383256	38.32%	6.204%
11	7.699	489	491	493	rBV	400340	320728	32.07%	5.192%
12	8.419	552	554	557	rBV	183701	148833	14.88%	2.409%
13	9.493	646	648	650	rVB	927266	721675	72.15%	11.683%
14	9.893	681	683	684	rBV	13394	13111	1.31%	0.212%
15	10.179	706	708	710	rVB	218694	176598	17.66%	2.859%
16	10.545	739	740	742	rBV	52816	61950	6.19%	1.003%
17	10.888	768	770	772	rBB	16296	12406	1.24%	0.201%
18	10.968	775	777	780	rBV	483911	417931	41.79%	6.766%
19	11.665	837	838	841	rBB	157344	190486	19.04%	3.084%
20	12.168	881	882	885	rBV	16581	16911	1.69%	0.274%
21	13.299	978	981	983	rBV	1123781	1000193	100.00%	16.192%
22	14.282	1065	1067	1071	rBV	24000	41707	4.17%	0.675%
23	14.465	1080	1083	1085	rBV	32816	41824	4.18%	0.677%
24	14.511	1085	1087	1090	rVV	268464	260607	26.06%	4.219%
25	15.528	1174	1176	1179	rBV	78263	98418	9.84%	1.593%
26	16.260	1237	1240	1243	rBV	218110	280732	28.07%	4.545%

Sum of corrected areas: 6177199

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
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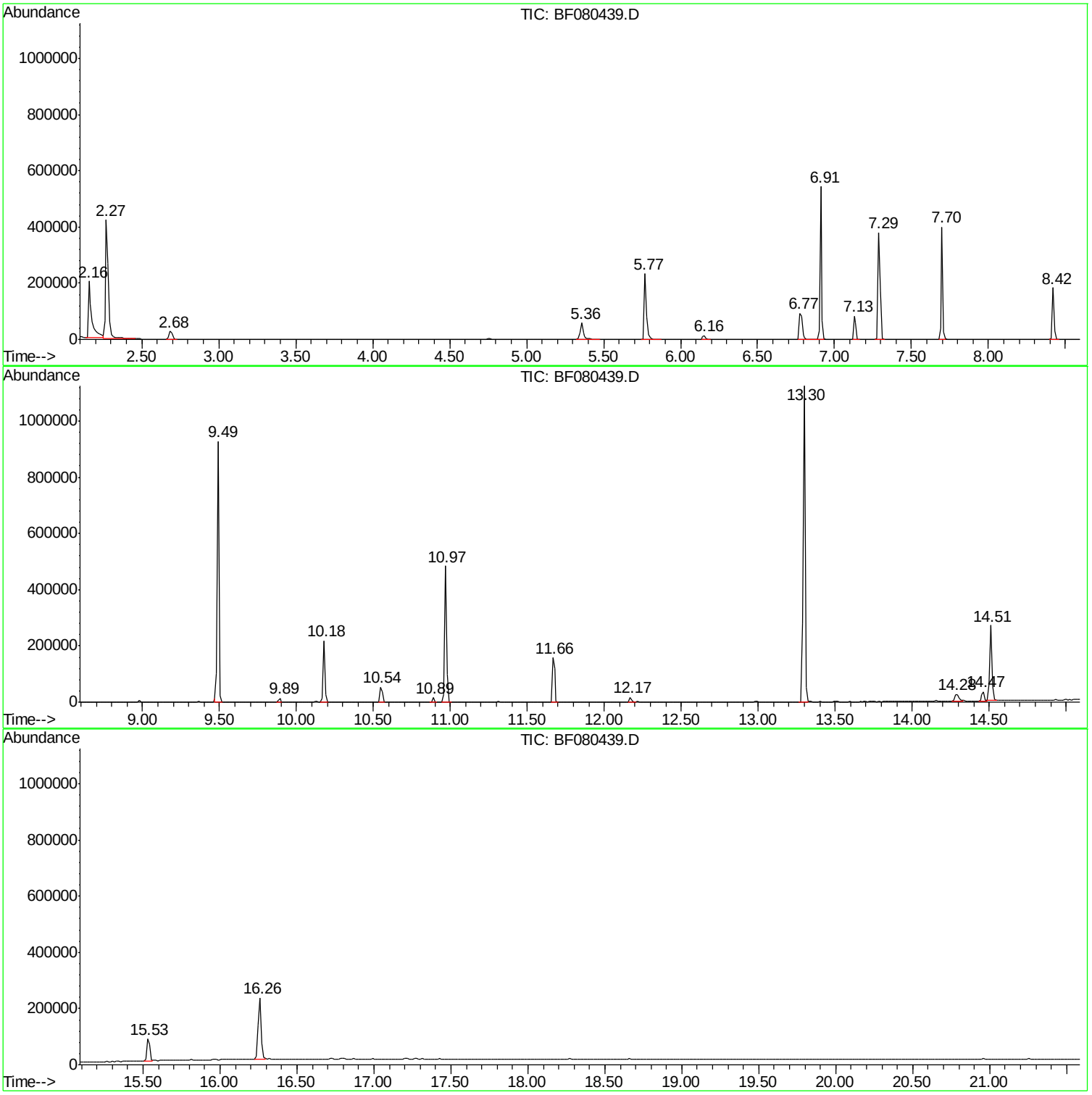
Operator : TP/UM
Sample : G2945-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-PMW-11M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080439.D
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Operator : TP/UM
Sample : G2945-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-PMW-11M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

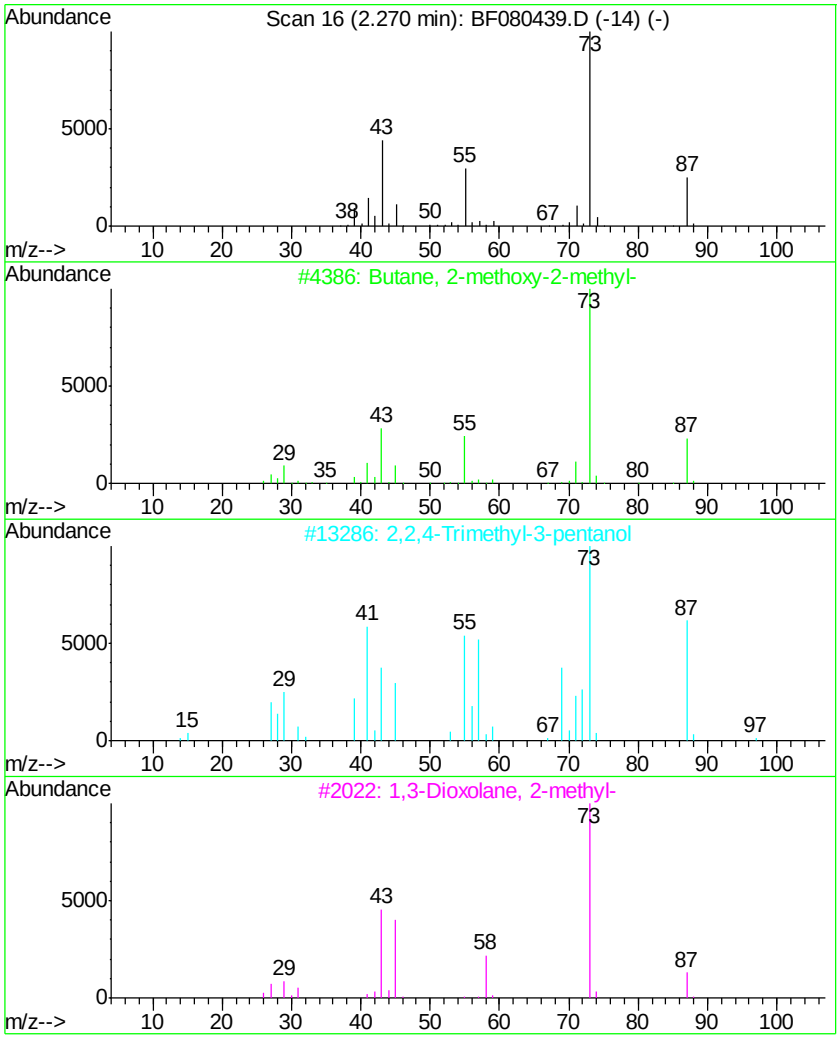
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

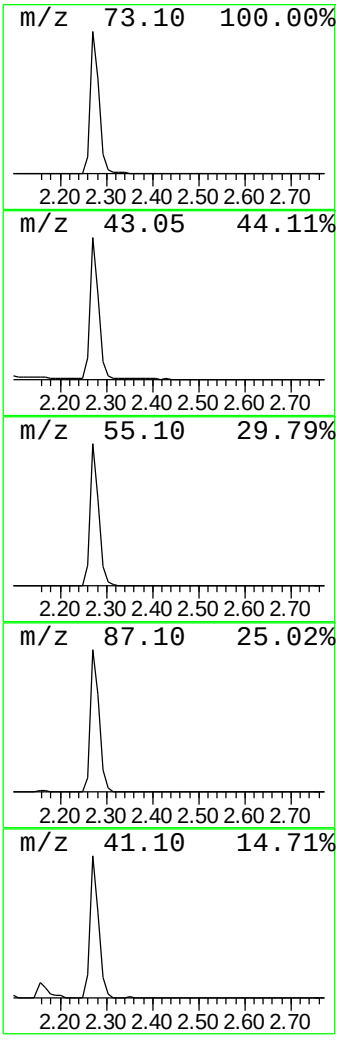
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	119.49 ng	594751	1,4-Dichlorobenzene-d4	7.14

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BF080439.D
Acq On : 13 Jul 2015 21:31
Operator : TP/UM
Sample : G2945-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-PMW-11M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

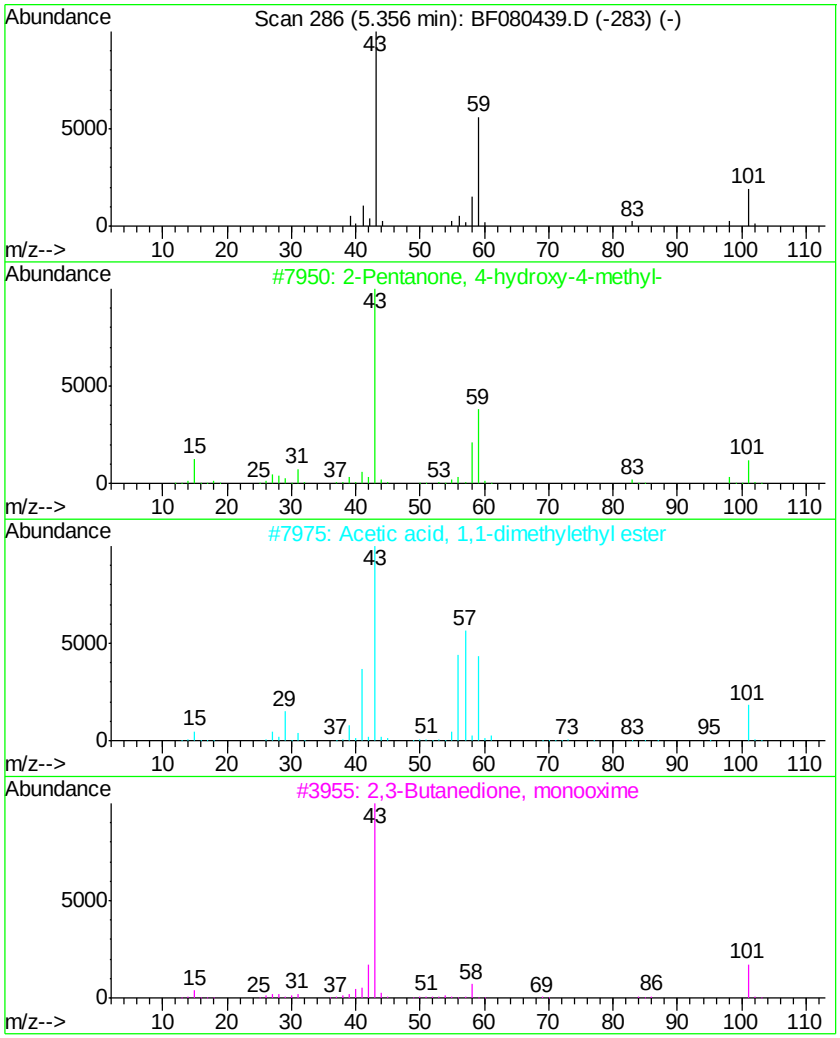
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

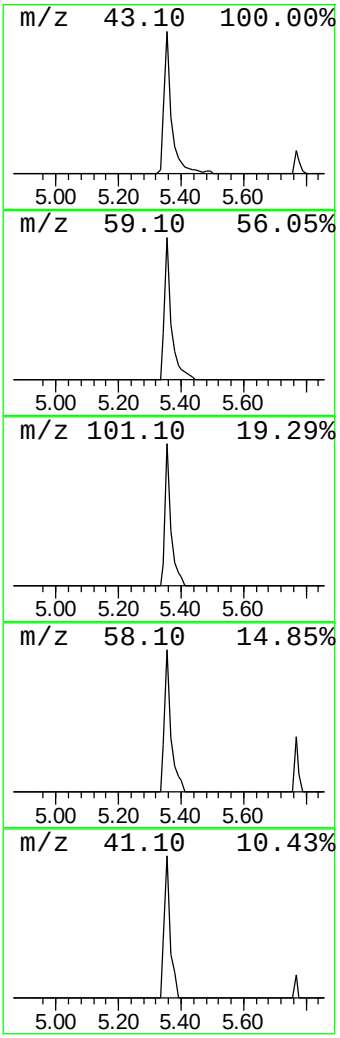
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.36	17.78 ng	88491	1,4-Dichlorobenzene-d4	7.14

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080439.D
Acq On : 13 Jul 2015 21:31
Operator : TP/UM
Sample : G2945-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-PMW-11M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

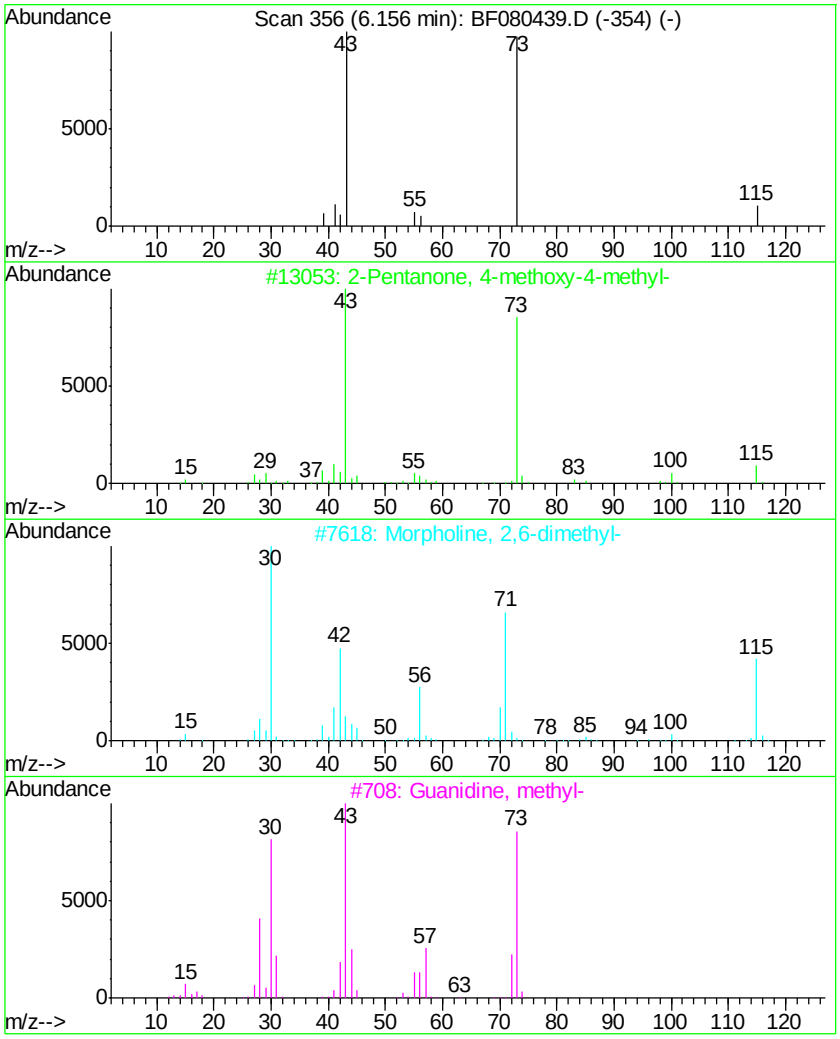
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

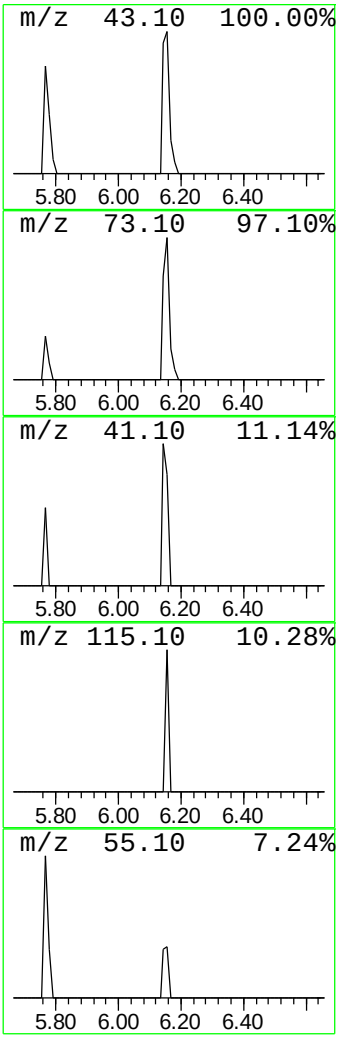
****

Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	3.92 ng	19534	1,4-Dichlorobenzene-d4	7.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	4
3	Guanidine, methyl-	73	C2H7N3	000471-29-4	4
4	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	4
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	4





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
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Acq On : 13 Jul 2015 21:31
Operator : TP/UM
Sample : G2945-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-PMW-11M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

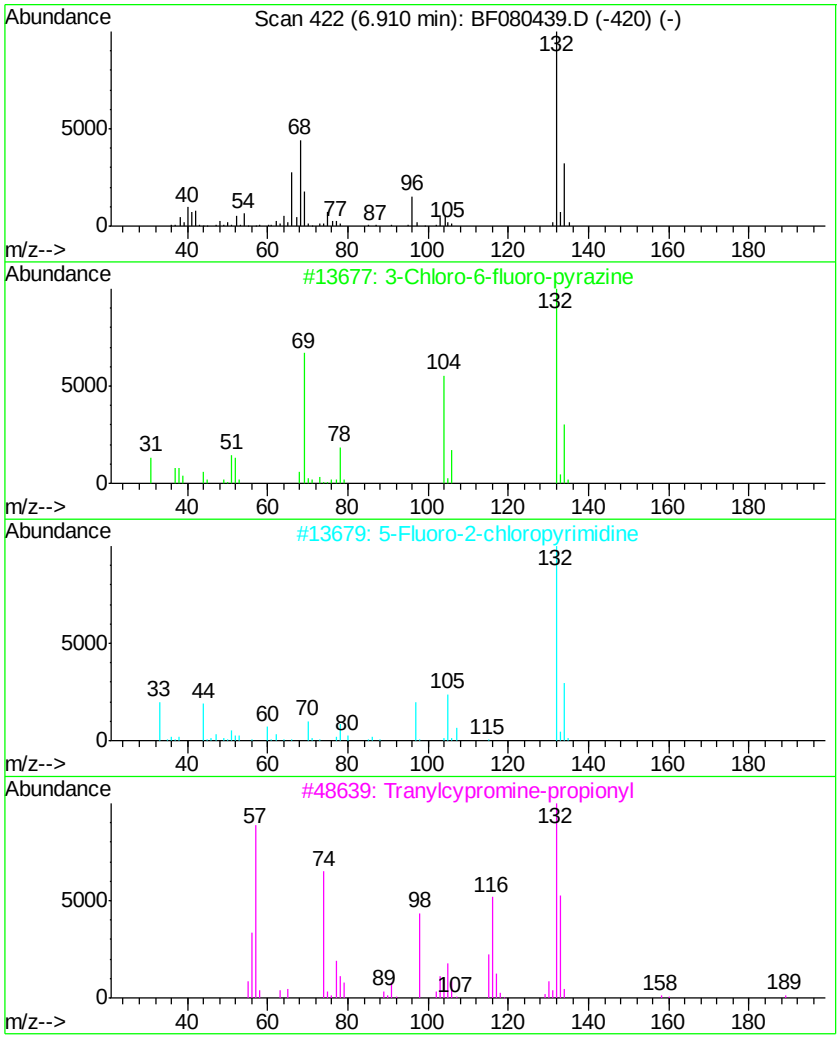
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

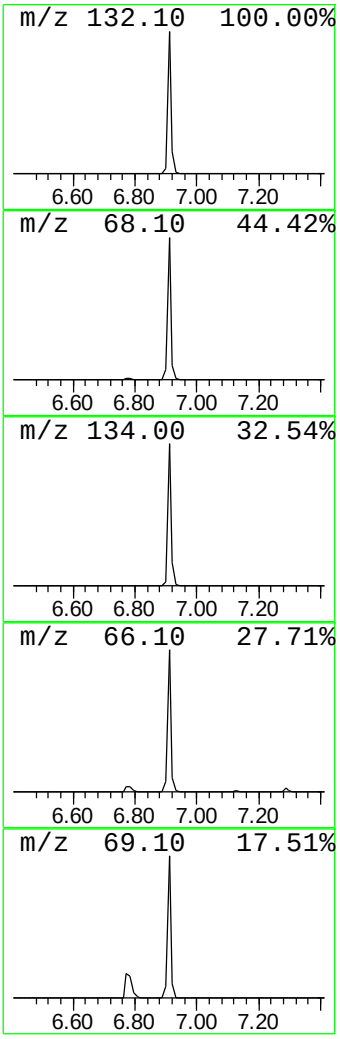
****

Peak Number 6 unknown6.91 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.91	88.11 ng	438550	1,4-Dichlorobenzene-d4	7.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
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Operator : TP/UM
Sample : G2945-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-PMW-11M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

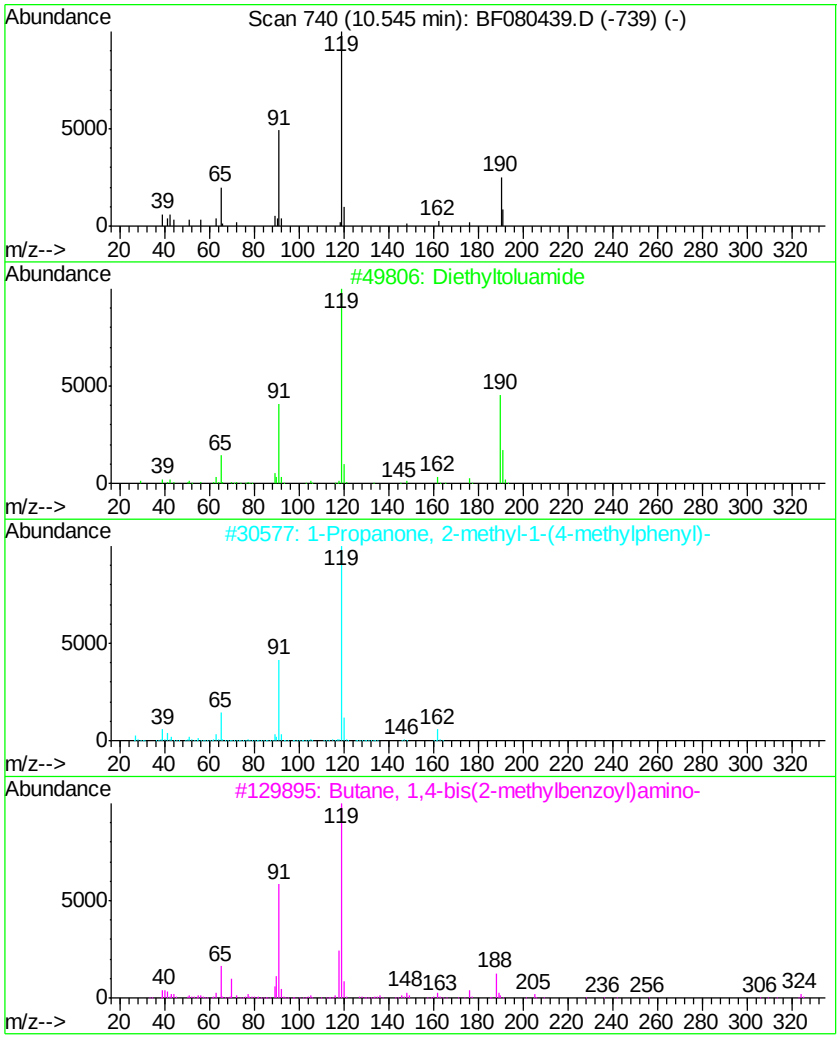
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

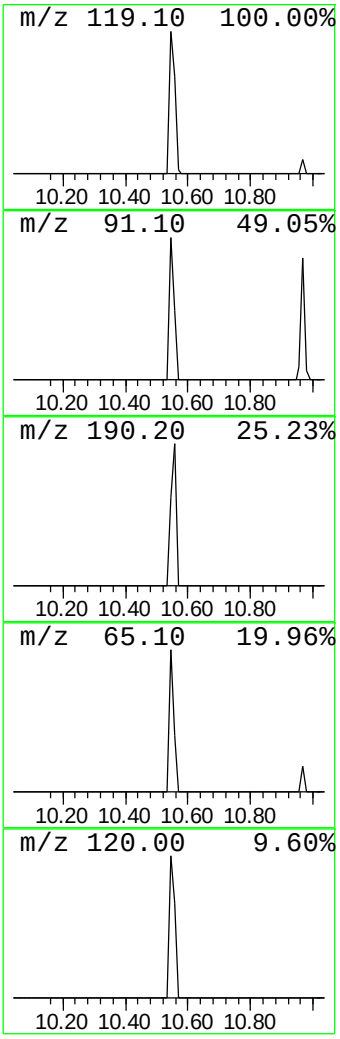
****

Peak Number 8 Diethyltoluamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	7.02 ng	61950	Acenaphthene-d10	10.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	94
2	1-Propanone, 2-methyl-1-(4-methy...	162	C11H14O	050390-51-7	74
3	Butane, 1,4-bis(2-methylbenzoyl)...	324	C20H24N2O2	341936-40-1	64
4	1-Propanone, 2-methyl-1-(2-methy...	162	C11H14O	002040-21-3	64
5	Benzoic acid, 4-methyl-, 3-methy...	206	C13H18O2	212261-12-6	64





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Sample : G2945-11
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Instrument : BNA_F
ClientSampleId : TE-PMW-11M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

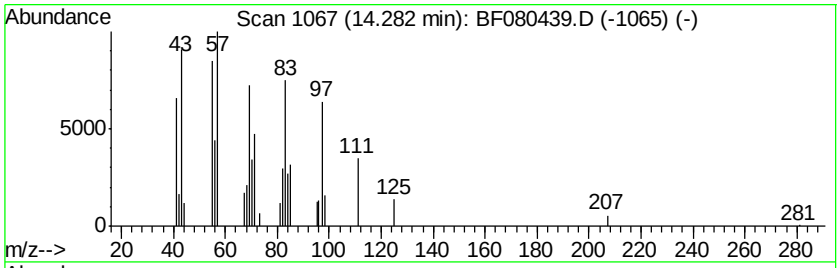
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

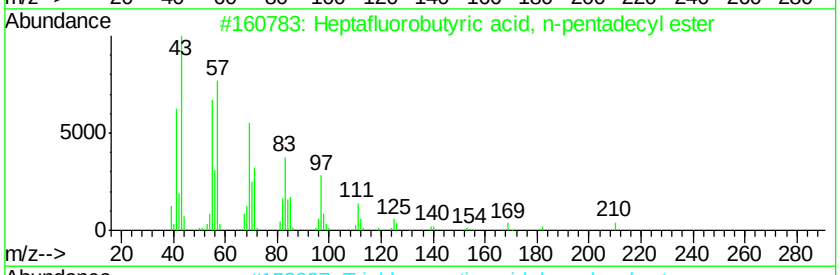
****

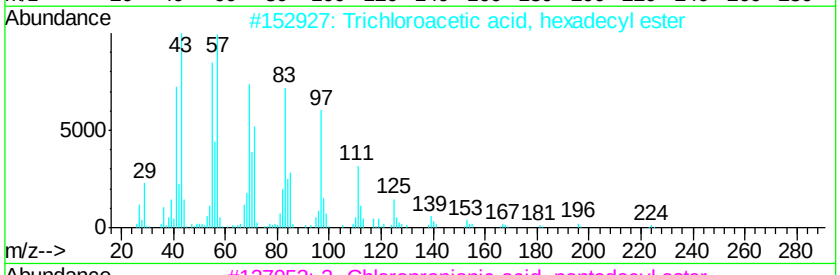
Peak Number 9 Heptafluorobutyric acid, n-... Concentration Rank 10

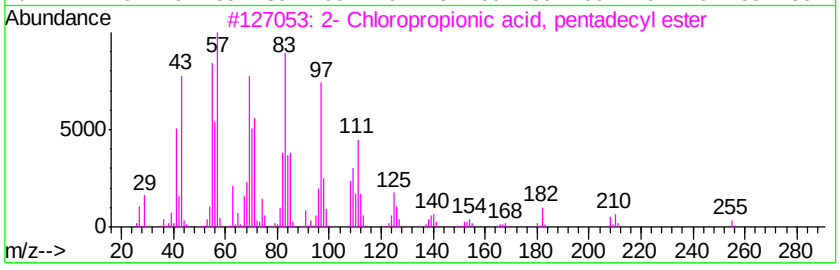
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	3.20 ng	41707	Chrysene-d12	14.51

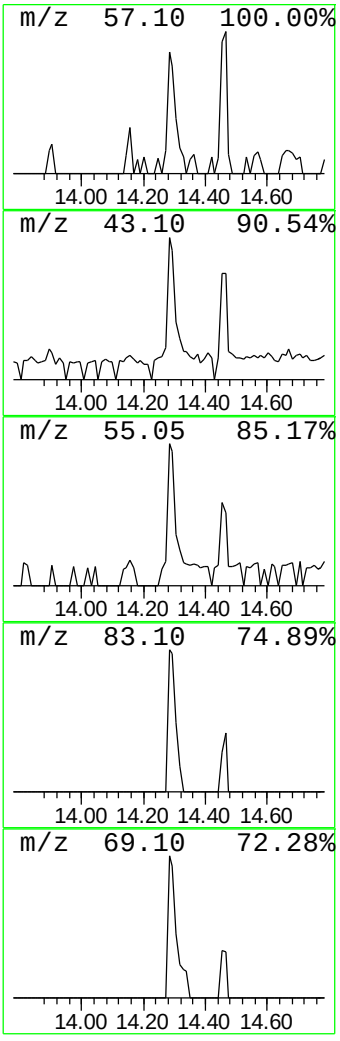
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
4	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91











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Instrument : BNA_F
ClientSampleId : TE-PMW-11M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

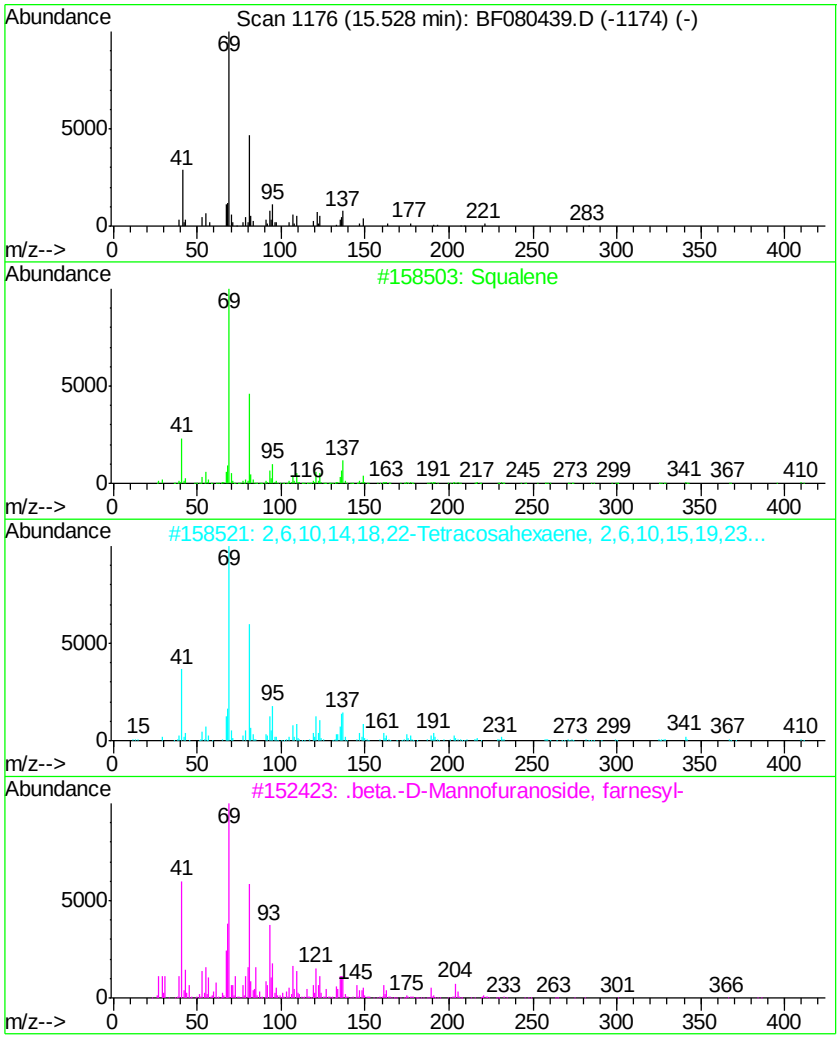
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

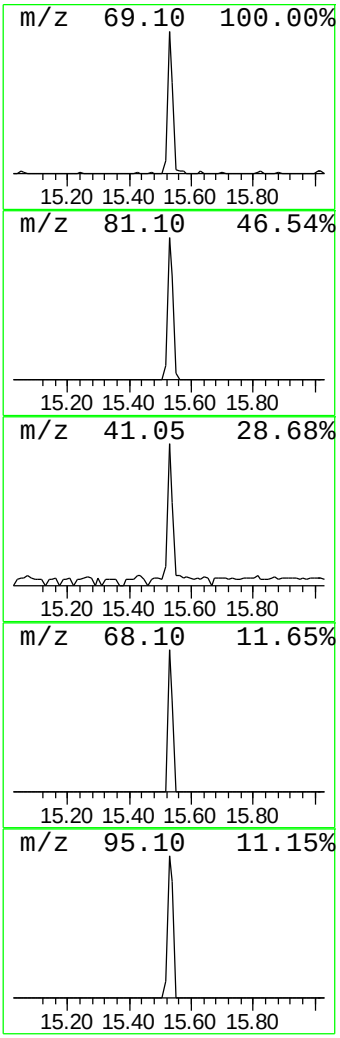
****

Peak Number 10 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.53	7.01 ng	98418	Perylene-d12	16.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	87
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	83
3	.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
5	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	64





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.27	119.5	ng	594751	1	7.14	99548	20.0
2-Pentanone, 4-hy...	5.36	17.8	ng	88491	1	7.14	99548	20.0
2-Pentanone, 4-me...	6.16	3.9	ng	19534	1	7.14	99548	20.0
unknown6.91	6.91	88.1	ng	438550	1	7.14	99548	20.0
Diethyltoluamide	10.54	7.0	ng	61950	3	10.18	176598	20.0
Heptafluorobutyri...	14.28	3.2	ng	41707	5	14.51	260607	20.0
Squalene	15.53	7.0	ng	98418	6	16.26	280732	20.0