LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
Data File : BF077466.D
Acq On : 26 Feb 2015 15:43
Operator : TP/IZ
Sample : G1384-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 41A-B-022515

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: CENTROID

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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	1.424	45	47	50	rBV	3634532	4071068	100.00%	20.548%
2	1.561	55	59	62	rVB	118699	187823	4.61%	0.948%
3	1.733	72	74	77	rVB	52671	66030	1.62%	0.333%
4	1.847	81	84	96	rVB2	84626	177475	4.36%	0.896%
5	5.047	362	364	372	rVB	236507	270581	6.65%	1.366%
6	5.562	406	409	411	rBV	1024427	1243427	30.54%	6.276%
7	6.819	517	519	522	rBV	1096285	1260747	30.97%	6.364%
8	6.979	530	533	535	rBV	1451819	1393926	34.24%	7.036%
9	7.265	556	558	560	rBV	366403	345600	8.49%	1.744%
10	7.459	572	575	577	rBV	828165	1074883	26.40%	5.425%
11	7.950	616	618	621	rBV	572935	794669	19.52%	4.011%
12	8.842	694	696	699	rBV	566676	481364	11.82%	2.430%
13	10.191	811	814	816	rBV	1961498	1754128	43.09%	8.854%
14	10.693	856	858	860	rBV	57442	47992	1.18%	0.242%
15	11.014	884	886	889	rVB2	514407	556564	13.67%	2.809%
16	11.916	963	965	967	rBV	86803	81285	2.00%	0.410%
17	11.996	969	972	975	rBV	1129257	1082091	26.58%	5.462%
18	12.865	1045	1048	1050	rBV	484061	600735	14.76%	3.032%
19	14.854	1220	1222	1225	rBV	1816463	2105944	51.73%	10.630%
20	15.494	1275	1278	1281	rBV	69383	87620	2.15%	0.442%
21	16.020	1322	1324	1333	rBV	348067	455848	11.20%	2.301%
22	16.145	1333	1335	1338	rBV	677783	703255	17.27%	3.550%
23	17.311	1434	1437	1439	rBV	66522	99772	2.45%	0.504%
24	17.871	1483	1486	1489	rBV	586428	703807	17.29%	3.552%
25	18.500	1538	1541	1546	rBV	62101	123024	3.02%	0.621%
26	19.631	1638	1640	1645	rVB5	21703	42403	1.04%	0.214%

Sum of corrected areas: 19812061

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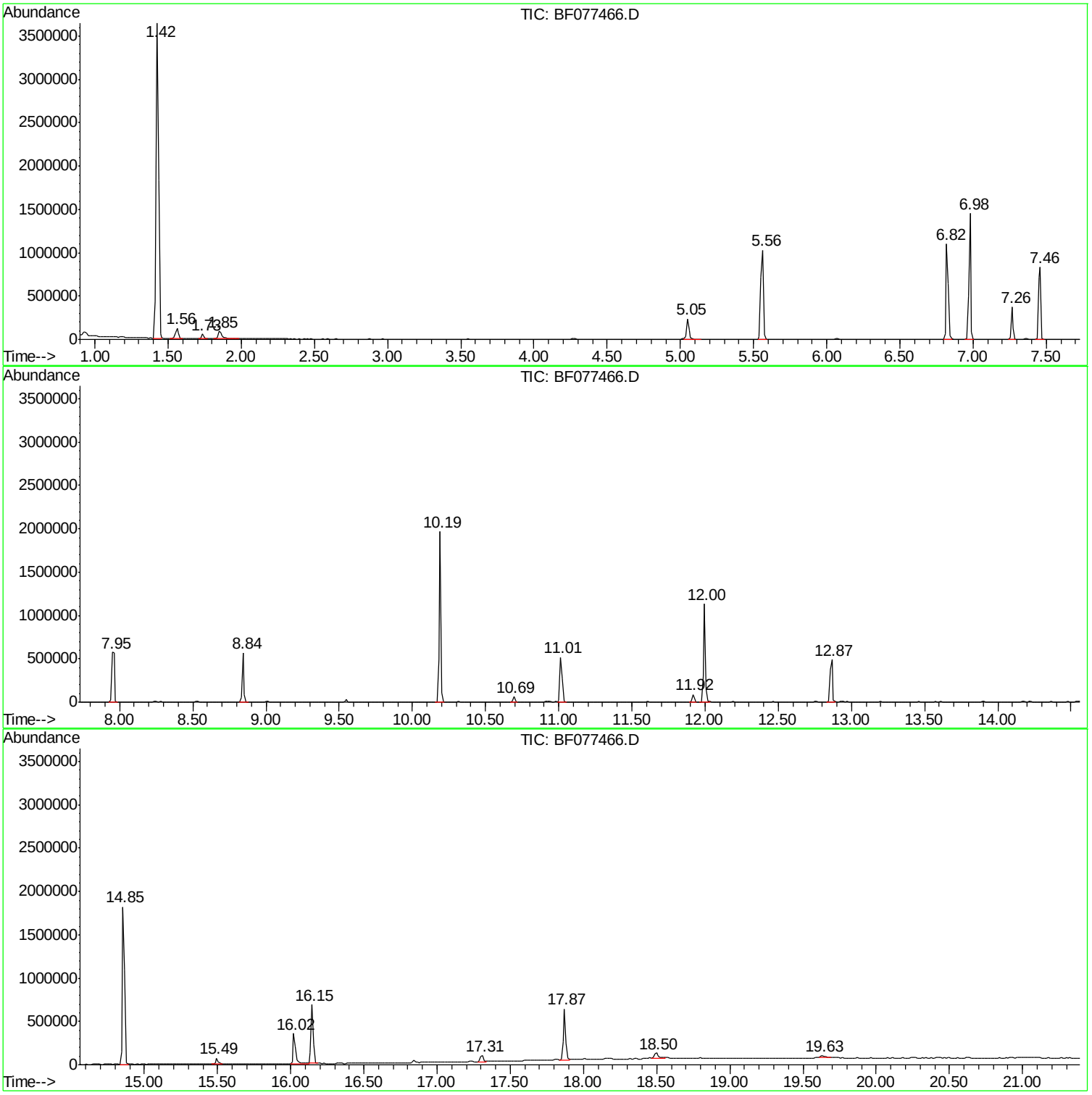
Instrument :
BNA_F
ClientSampleId :
41A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
Data File : BF077466.D
Acq On : 26 Feb 2015 15:43
Operator : TP/IZ
Sample : G1384-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 41A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

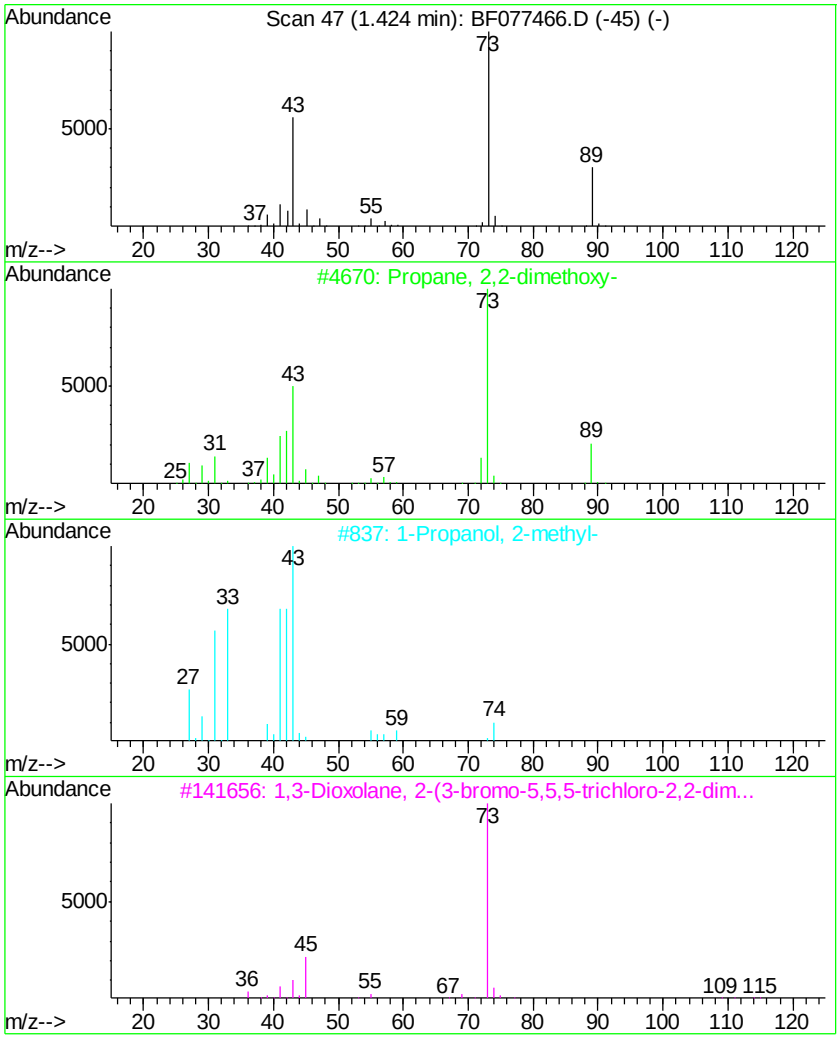
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

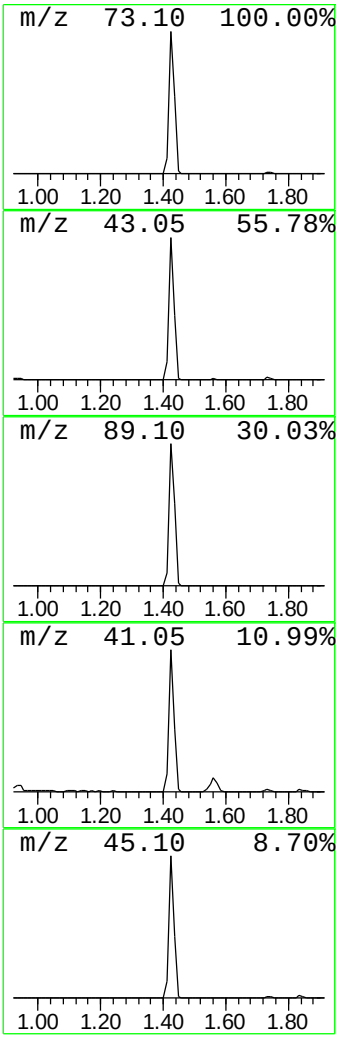
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.42	235.59 ng	4071070	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Operator : TP/IZ
Sample : G1384-05
Misc :
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Instrument : BNA_F
ClientSampleId : 41A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

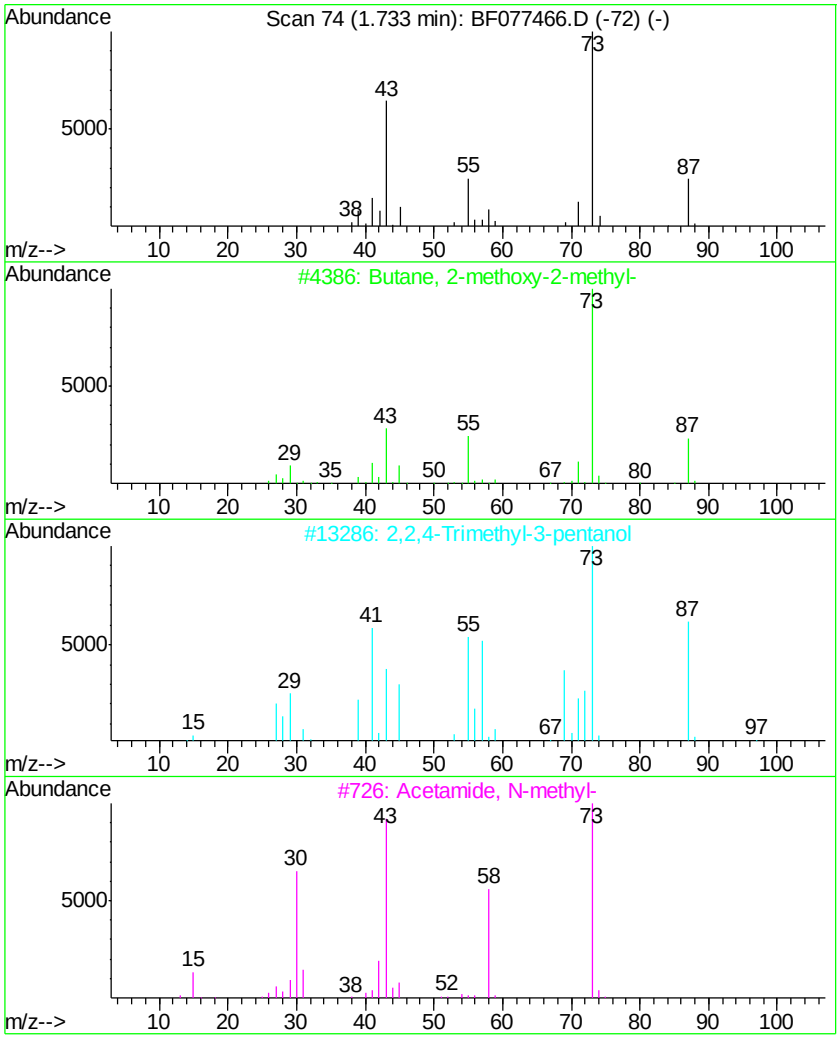
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

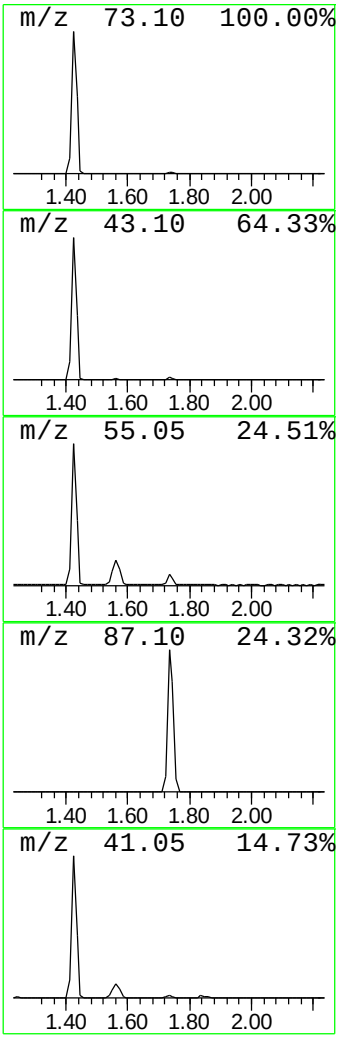
****

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.73	3.82 ng	66030	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	10
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BF077466.D
Acq On : 26 Feb 2015 15:43
Operator : TP/IZ
Sample : G1384-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 41A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

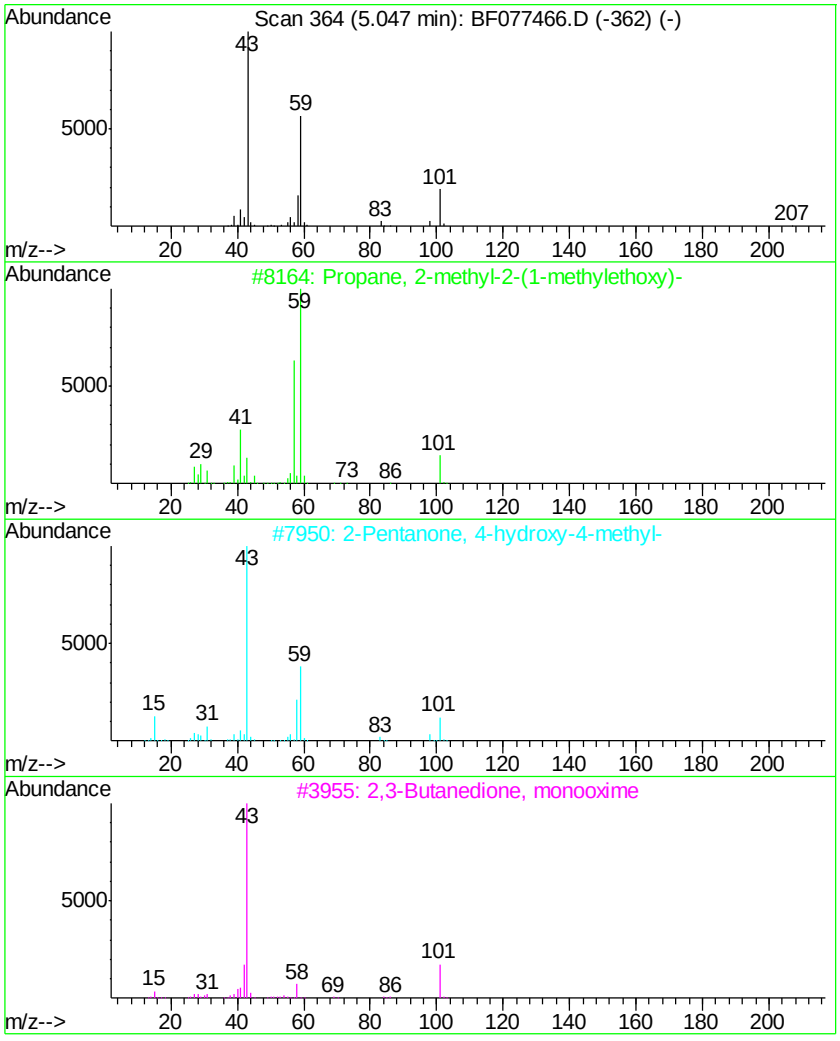
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

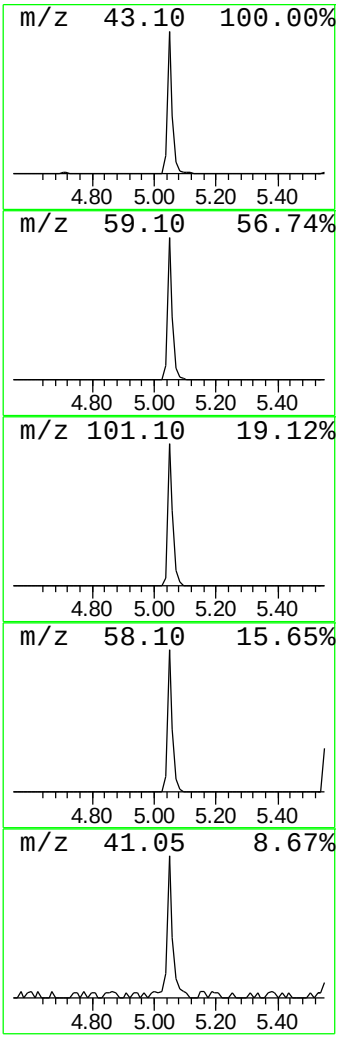
****

Peak Number 5 unknown5.05 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	15.66 ng	270581	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 26 Feb 2015 15:43
Operator : TP/IZ
Sample : G1384-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 41A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

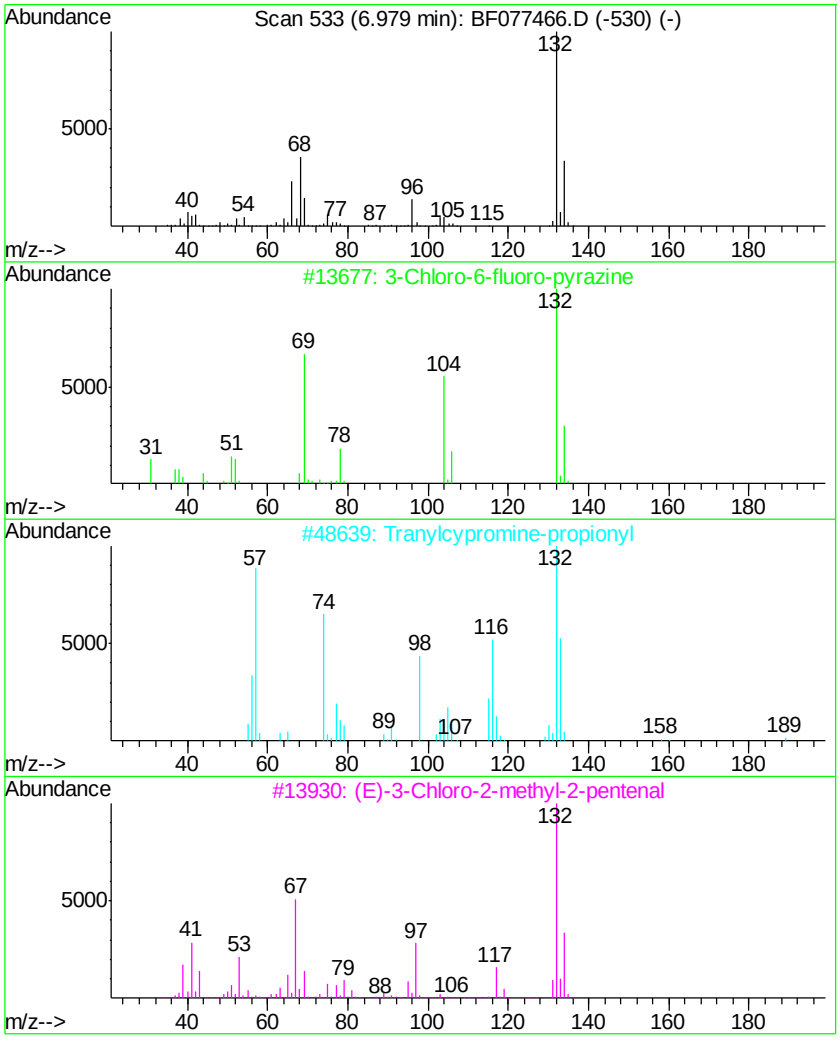
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

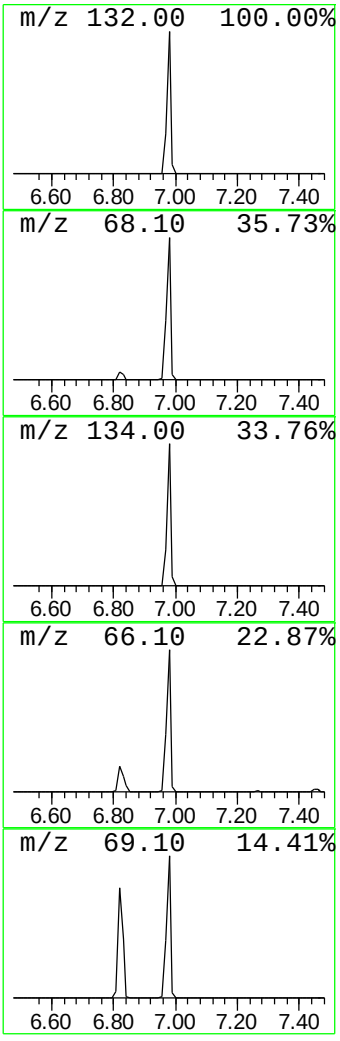
****

Peak Number 6 unknown6.98 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	80.67 ng	1393930	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Xenon	132	Xe	007440-63-3	9





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Data File : BF077466.D
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Operator : TP/IZ
Sample : G1384-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 41A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

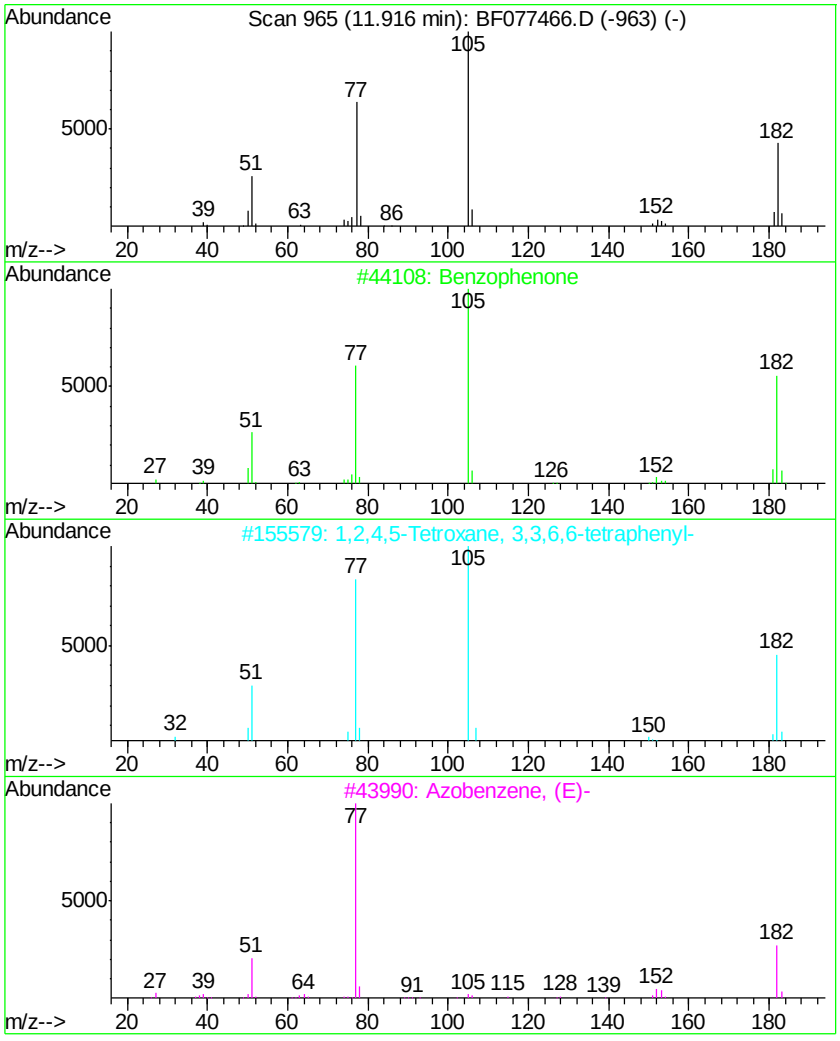
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

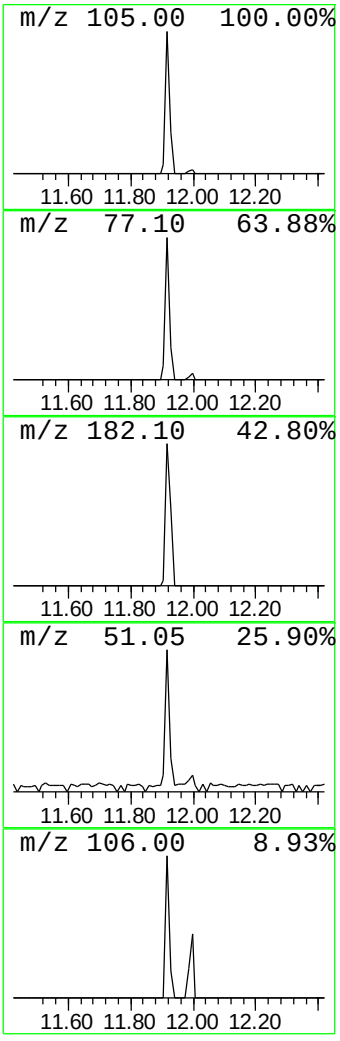
****

Peak Number 8 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	2.92 ng	81285	Acenaphthene-d10	11.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3	Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





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Instrument : BNA_F
ClientSampleId : 41A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

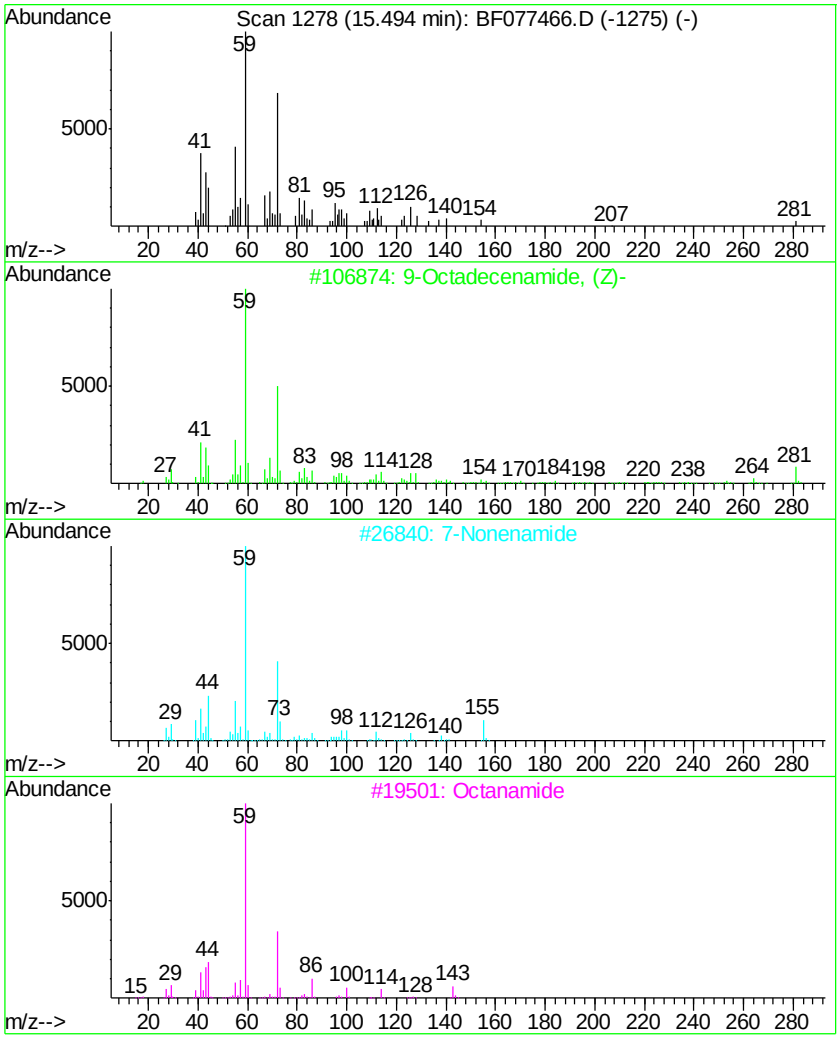
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

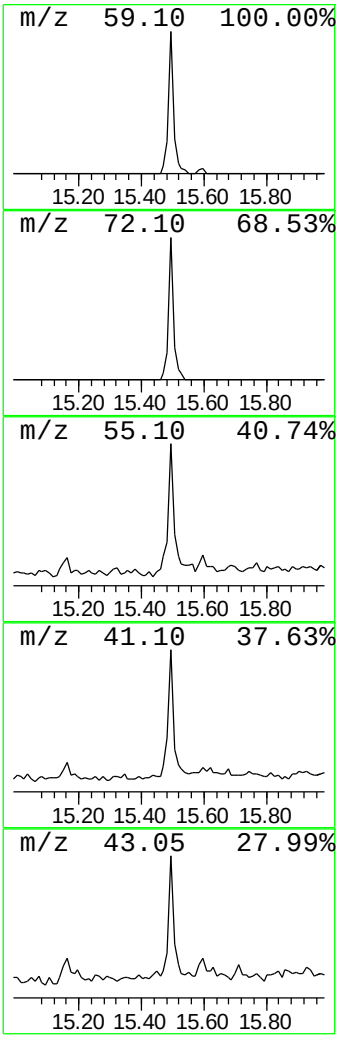
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	2.49 ng	87620	Chrysene-d12	16.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
2	7-Nonenamide	155	C9H17NO	090949-53-4	59
3	Octanamide	143	C8H17NO	000629-01-6	53
4	Tetradecanamide	227	C14H29NO	000638-58-4	53
5	Diazene, [1-(2,2-dimethylhydrazi...	172	C8H20N4	061940-94-1	47





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

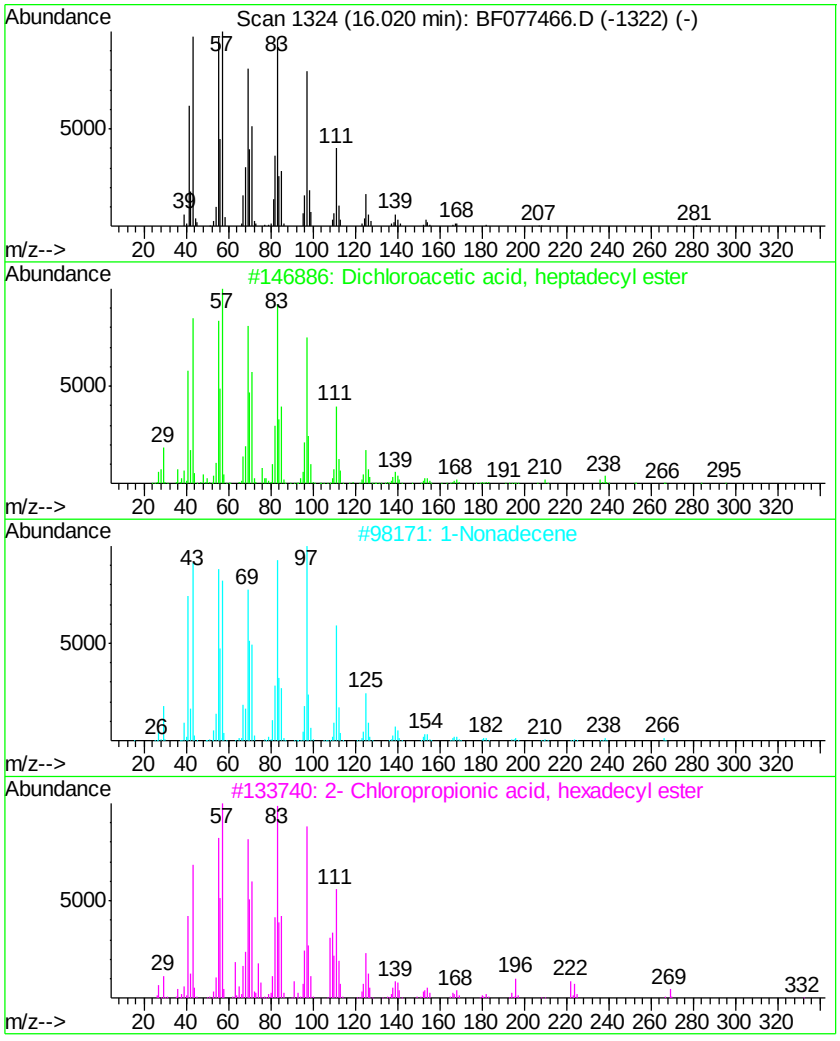
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

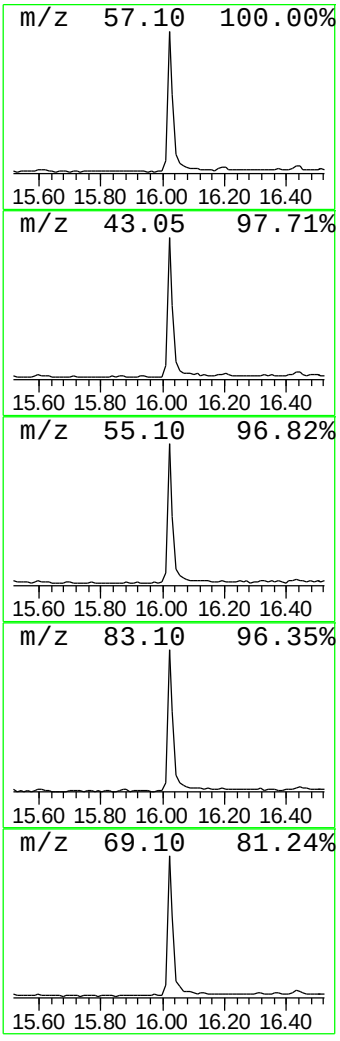
****

Peak Number 10 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	12.96 ng	455848	Chrysene-d12	16.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
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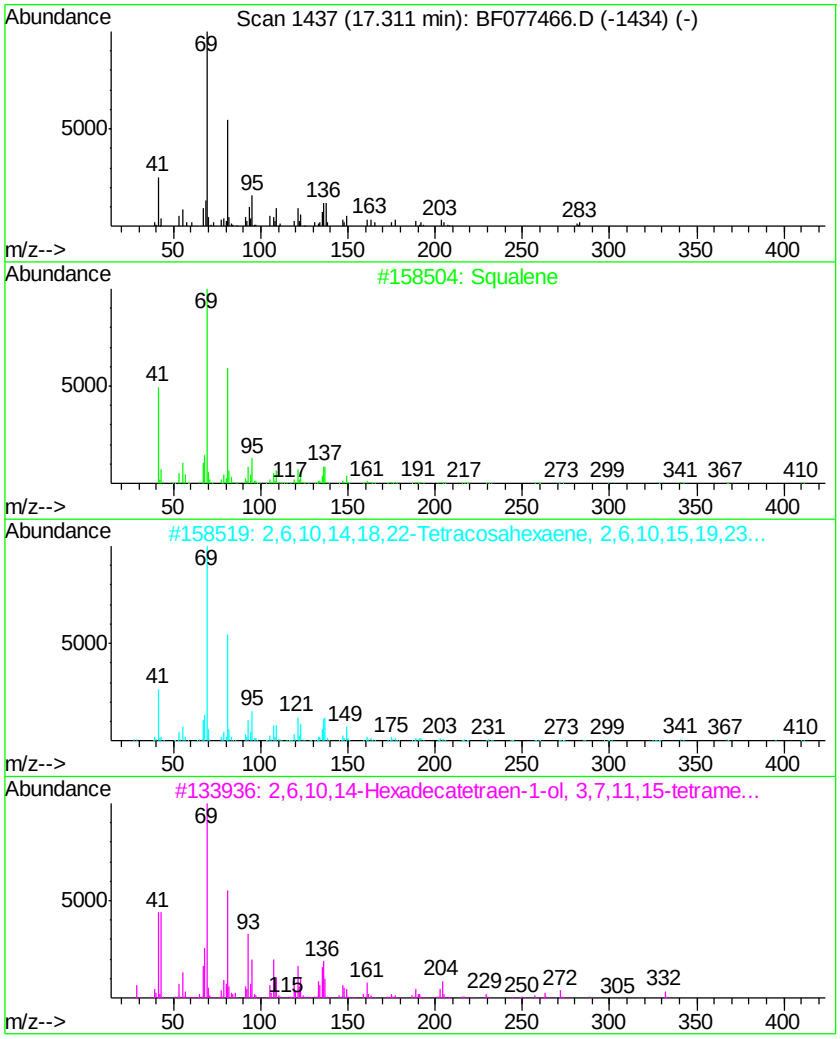
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

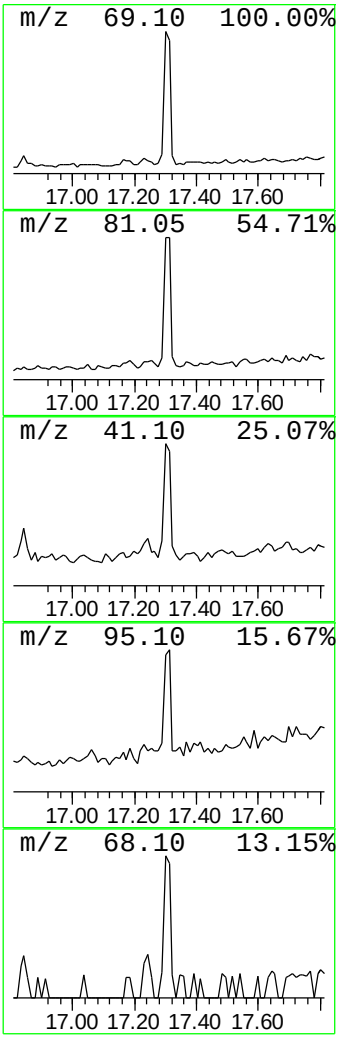
****

Peak Number 11 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.31	2.84 ng	99772	Perylene-d12	17.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	90
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87
3	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	78
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	2,7,11-Trimethyl-4-phenylthiodod...	314	C21H30S	1000190-11-3	64





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Instrument : BNA_F
ClientSampleId : 41A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

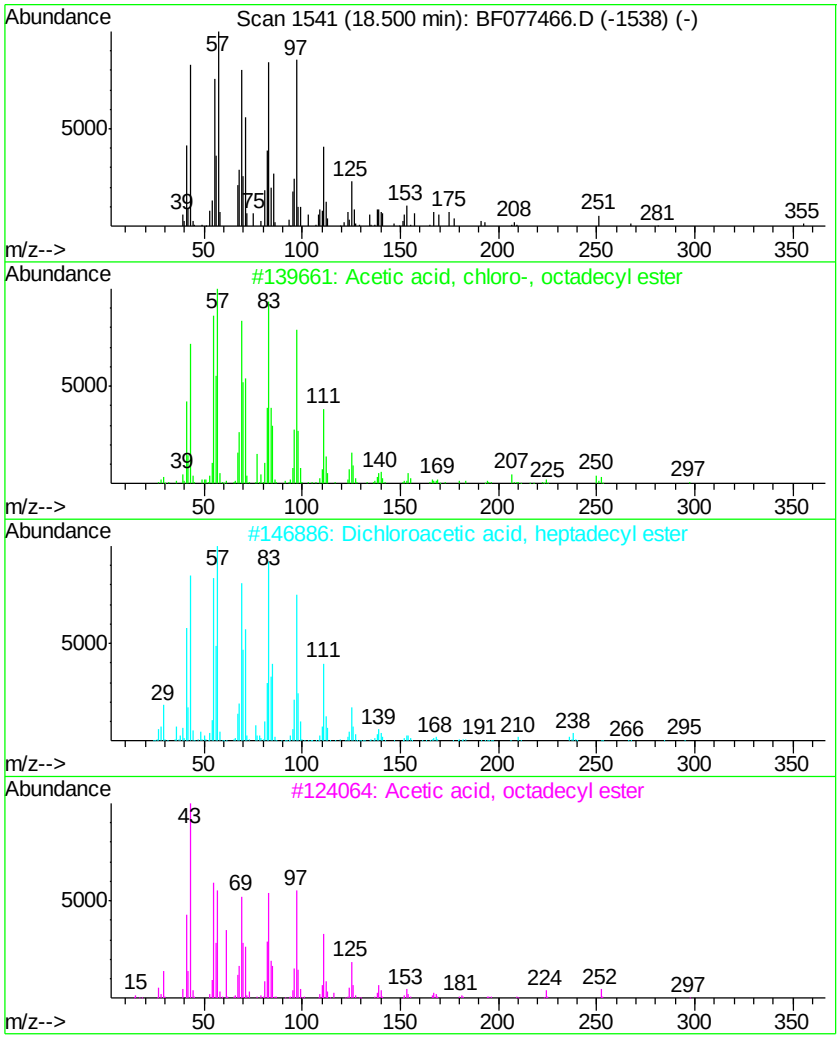
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

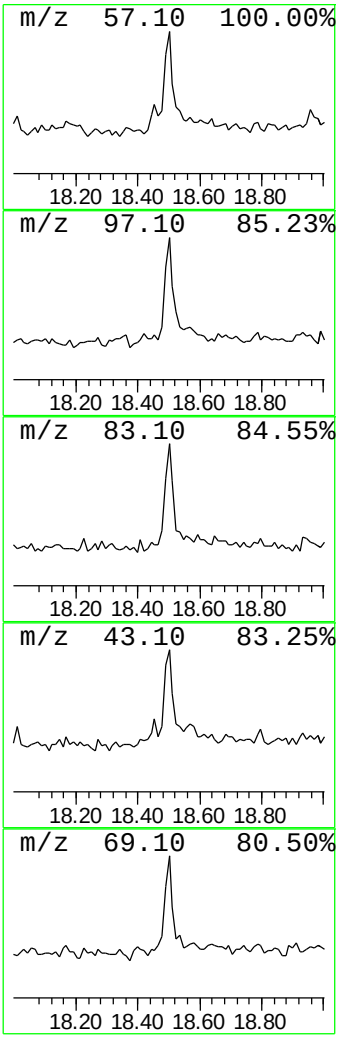
****

Peak Number 12 Acetic acid, chloro-, octad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	3.50 ng	123024	Perylene-d12	17.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	90
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
3	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	62
4	17-Pentatriacontene	491	C35H70	006971-40-0	60
5	1-Docosanol	326	C22H46O	000661-19-8	52





Tentatively Identified Compound (LSC) summary

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Data File : BF077466.D
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Operator : TP/IZ
Sample : G1384-05
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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
Propane, 2,2-dime...	1.42	235.6	ng	4071070	1	7.26	345600	20.0
Butane, 2-methoxy...	1.73	3.8	ng	66030	1	7.26	345600	20.0
unknown5.05	5.05	15.7	ng	270581	1	7.26	345600	20.0
unknown6.98	6.98	80.7	ng	1393930	1	7.26	345600	20.0
Benzophenone	11.92	2.9	ng	81285	3	11.01	556564	20.0
9-Octadecenamide,...	15.49	2.5	ng	87620	5	16.15	703255	20.0
Dichloroacetic ac...	16.02	13.0	ng	455848	5	16.15	703255	20.0
Squalene	17.31	2.8	ng	99772	6	17.87	703807	20.0
Acetic acid, chlo...	18.50	3.5	ng	123024	6	17.87	703807	20.0