LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

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-BF031115.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	1.241	29	31	34	rBV	765037	786034	61.16%	7.297%
2	1.367	38	42	45	rVB	64549	119668	9.31%	1.111%
3	1.527	54	56	59	rVB	71841	77828	6.06%	0.722%
4	1.641	61	66	70	rBV3	5848	13544	1.05%	0.126%
5	1.744	74	75	86	rBV	39765	62069	4.83%	0.576%
6	4.830	343	345	353	rBV	110429	140598	10.94%	1.305%
7	5.379	390	393	396	rBV	728567	864680	67.28%	8.027%
8	6.670	504	506	509	rBV	899512	888947	69.17%	8.252%
9	6.807	515	518	520	rBV	1002413	981193	76.34%	9.109%
10	7.093	540	543	545	rBV	219060	199796	15.55%	1.855%
11	7.276	557	559	562	rBV	812635	740995	57.65%	6.879%
12	7.790	601	604	606	rBV	625431	593233	46.16%	5.507%
13	8.670	678	681	683	rBV	302103	277423	21.59%	2.575%
14	10.019	796	799	801	rBV	1116207	1099136	85.52%	10.203%
15	10.522	841	843	846	rBV	73242	68891	5.36%	0.640%
16	10.831	869	870	873	rVB	223591	308637	24.01%	2.865%
17	11.425	920	922	925	rVB	13649	14027	1.09%	0.130%
18	11.814	953	956	959	rBV	653746	641019	49.88%	5.951%
19	11.871	959	961	966	rVB	8165	12872	1.00%	0.119%
20	12.019	972	974	982	rVB	20621	28603	2.23%	0.266%
21	12.579	1020	1023	1024	rBV	16492	16485	1.28%	0.153%
22	12.671	1029	1031	1034	rBV	366263	345216	26.86%	3.205%
23	14.671	1203	1206	1208	rBV	1143252	1285238	100.00%	11.931%
24	15.745	1298	1300	1304	rBV	22293	26922	2.09%	0.250%
25	15.860	1307	1310	1315	rBV	36615	92551	7.20%	0.859%
26	15.951	1315	1318	1320	rVV	321571	395669	30.79%	3.673%
27	16.740	1384	1387	1389	rBV2	10259	16672	1.30%	0.155%
28	17.231	1425	1430	1435	rBV2	21133	79058	6.15%	0.734%
29	17.357	1435	1441	1442	rVV	15191	44477	3.46%	0.413%
30	17.391	1442	1444	1449	rVB2	17839	44185	3.44%	0.410%
31	17.631	1462	1465	1467	rBV	276866	403403	31.39%	3.745%
32	18.580	1545	1548	1551	rBV3	11278	30967	2.41%	0.287%
33	19.140	1594	1597	1601	rBV5	40598	72228	5.62%	0.670%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

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-BF031115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

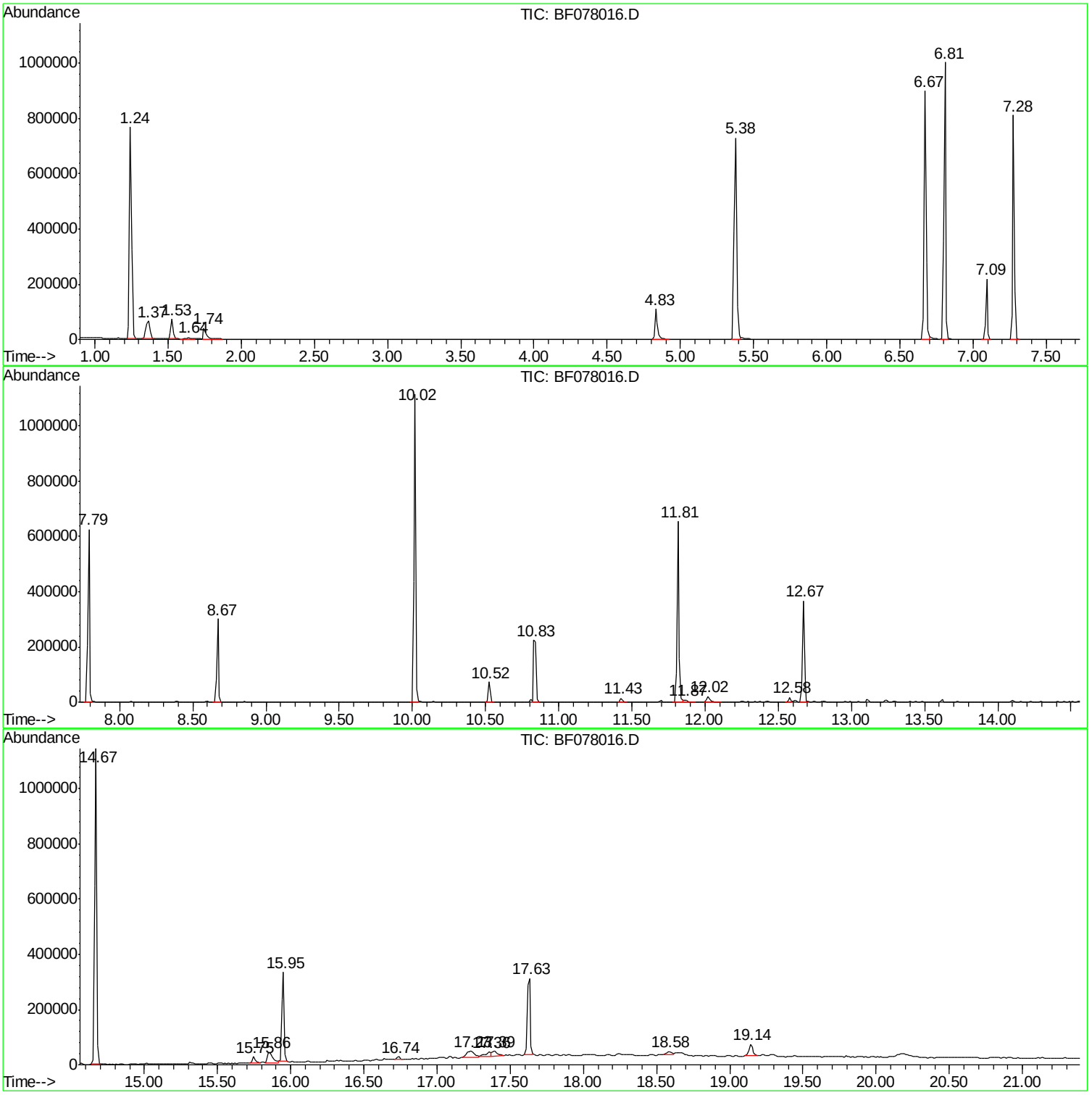
Sum of corrected areas: 10772264

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

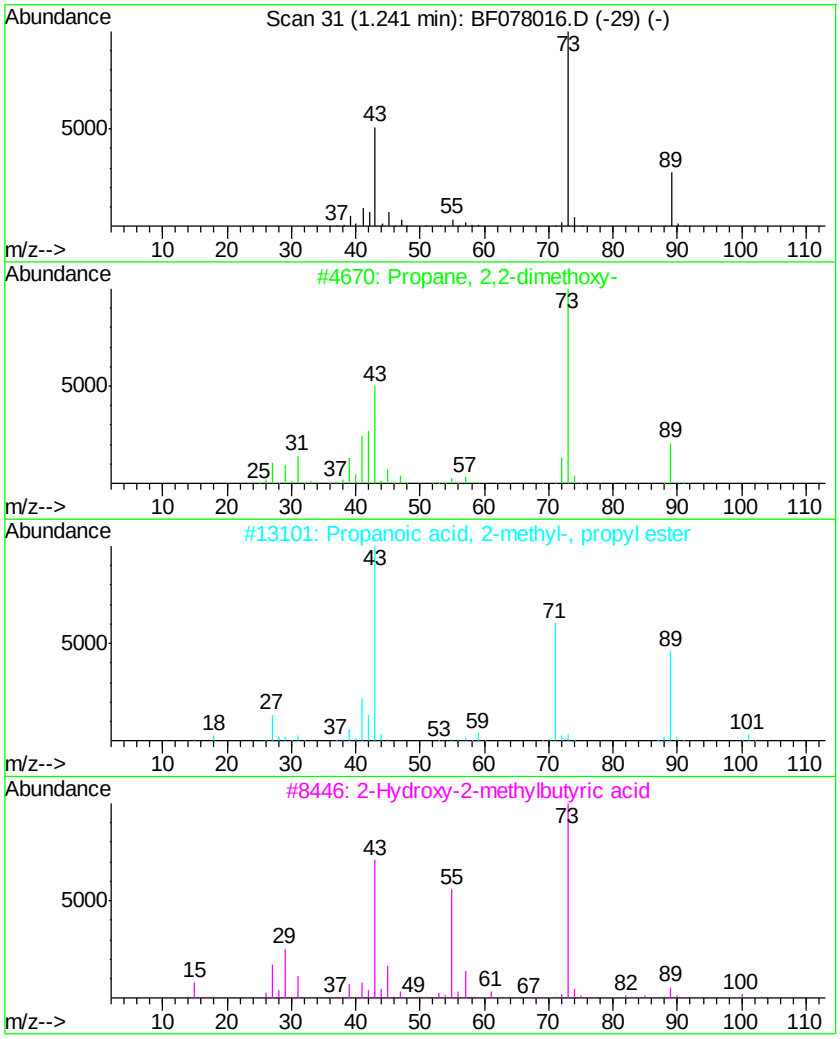
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

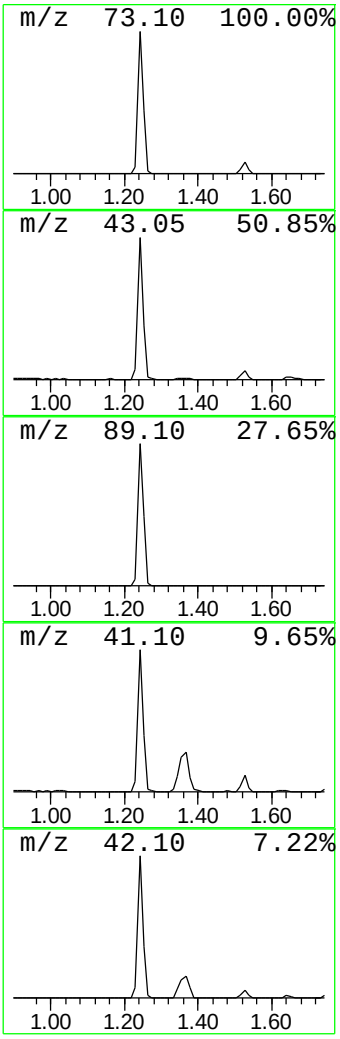
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.24	78.68 ng	786034	1,4-Dichlorobenzene-d4	7.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

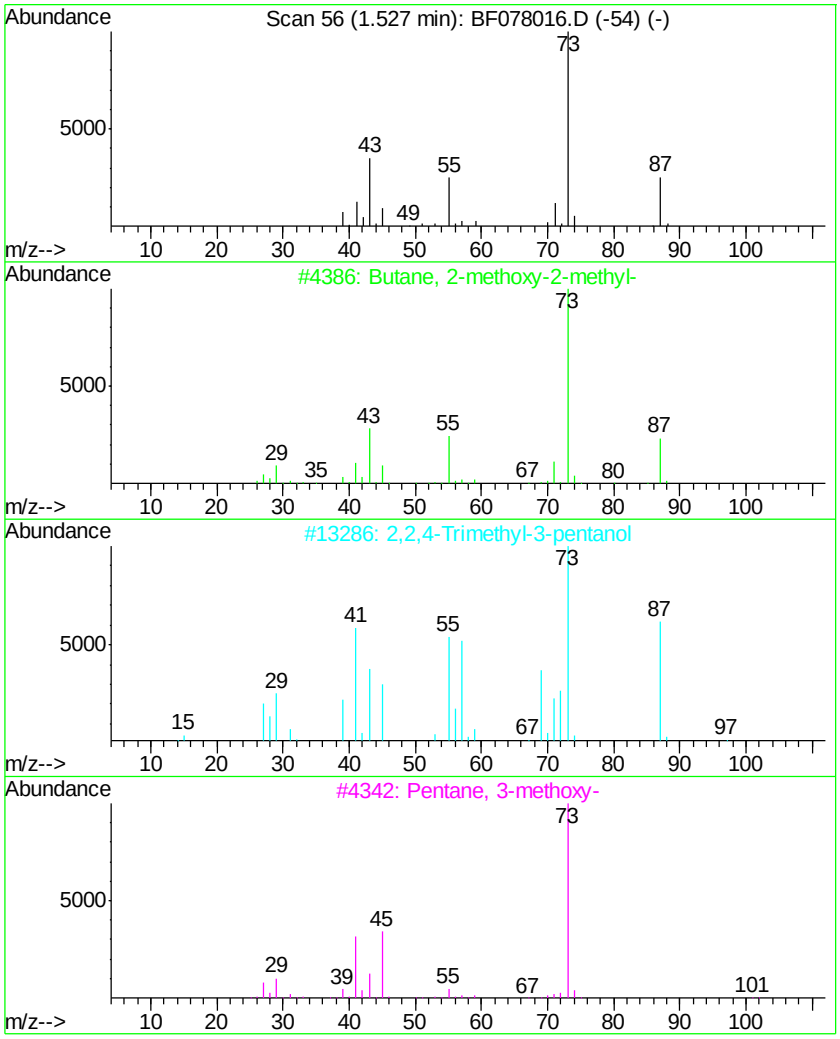
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

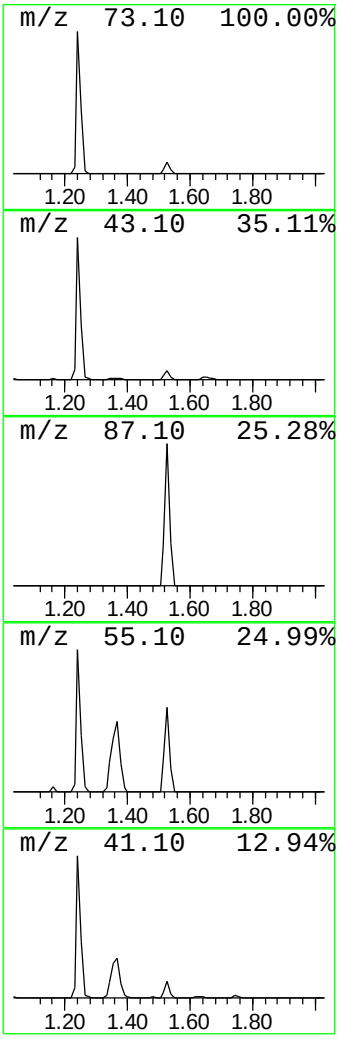
****

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.53	7.79 ng	77828	1,4-Dichlorobenzene-d4	7.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	56
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

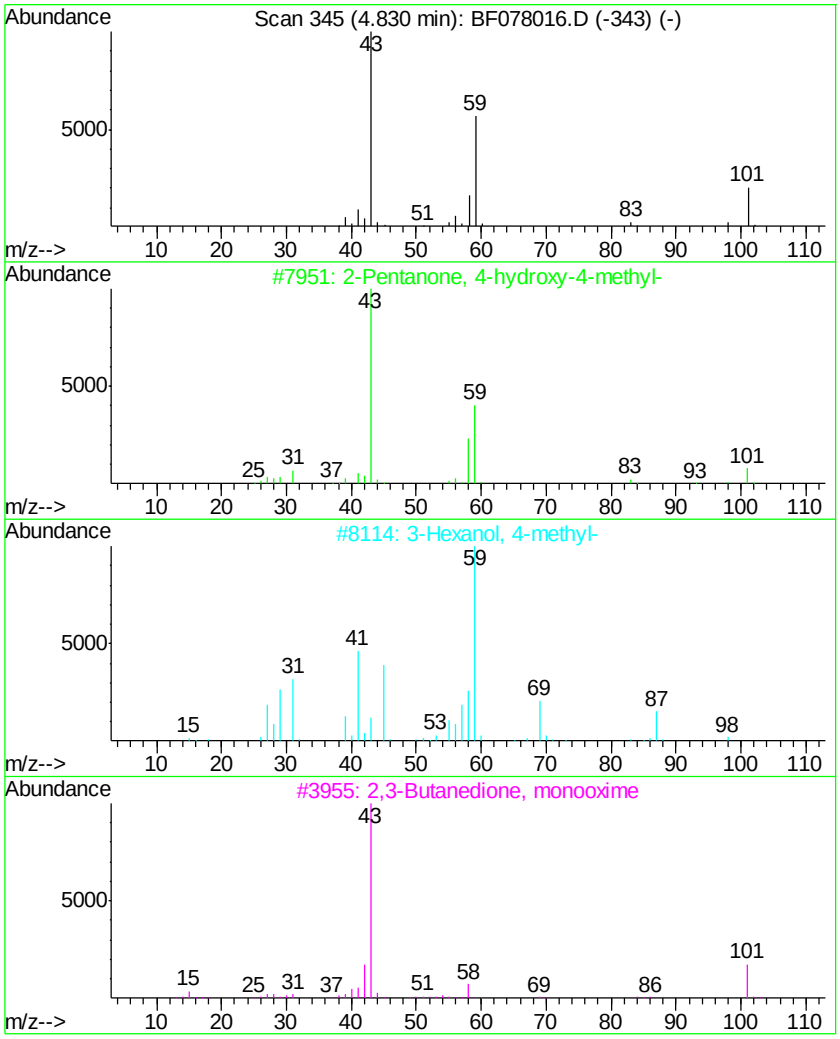
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

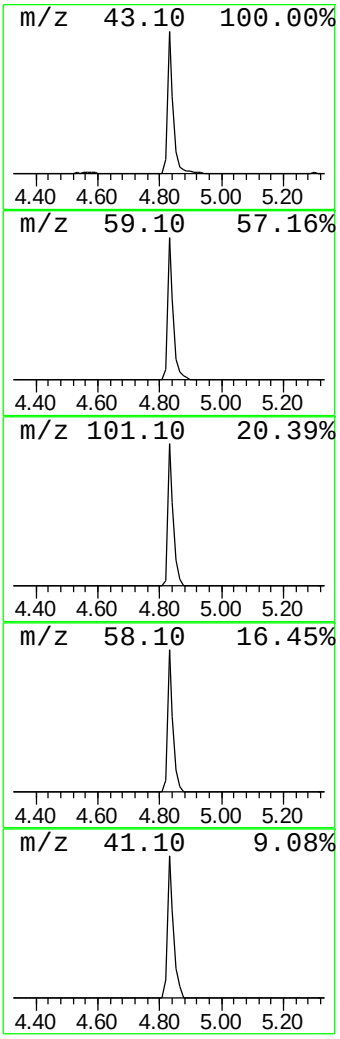
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	14.07 ng	140598	1,4-Dichlorobenzene-d4	7.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
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	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

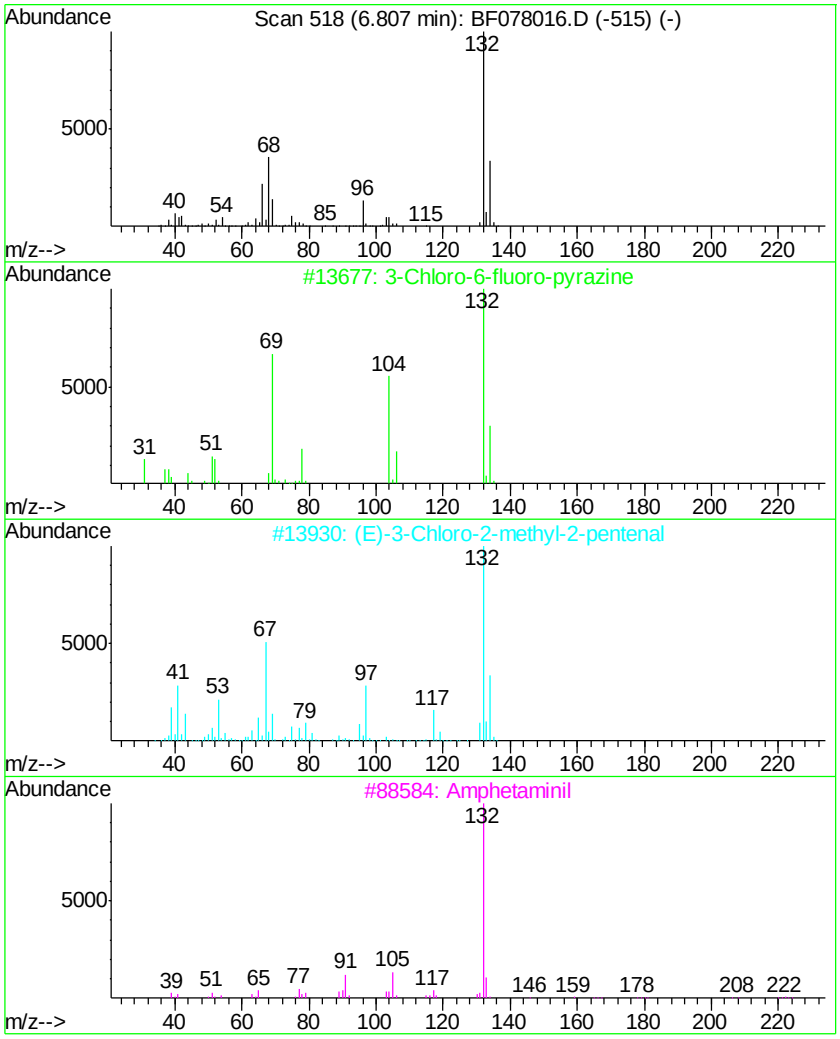
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

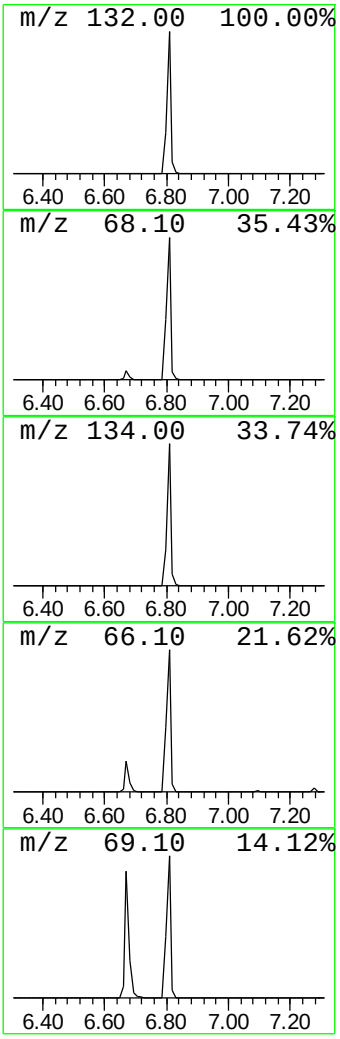
****

Peak Number 6 unknown6.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.81	98.22 ng	981193	1,4-Dichlorobenzene-d4	7.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

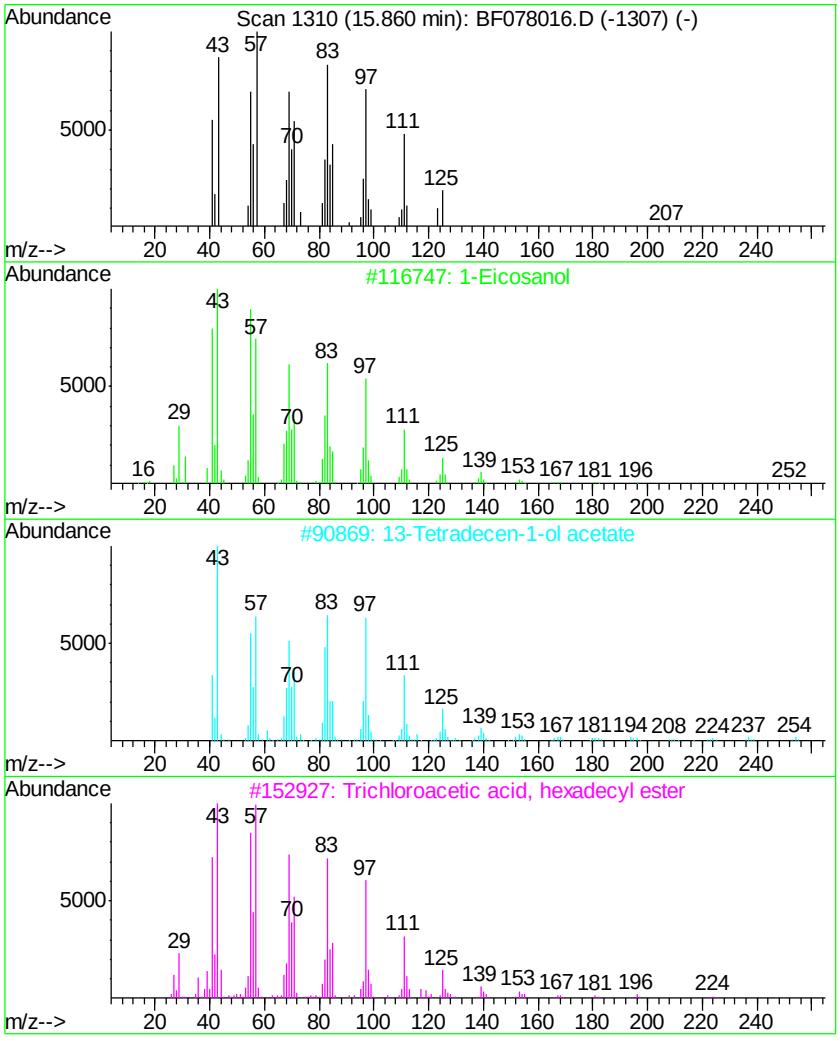
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

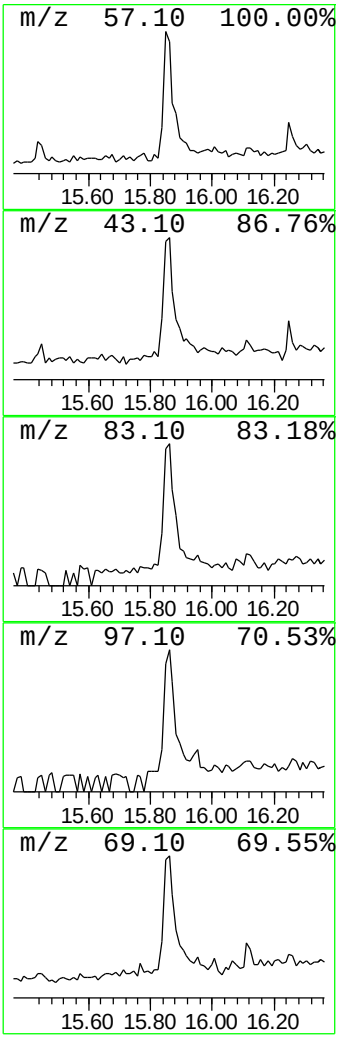
****

Peak Number 8 1-Eicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	4.68 ng	92551	Chrysene-d12	15.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	90
2	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	90
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	86
5	1-Nonadecene	266	C19H38	018435-45-5	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

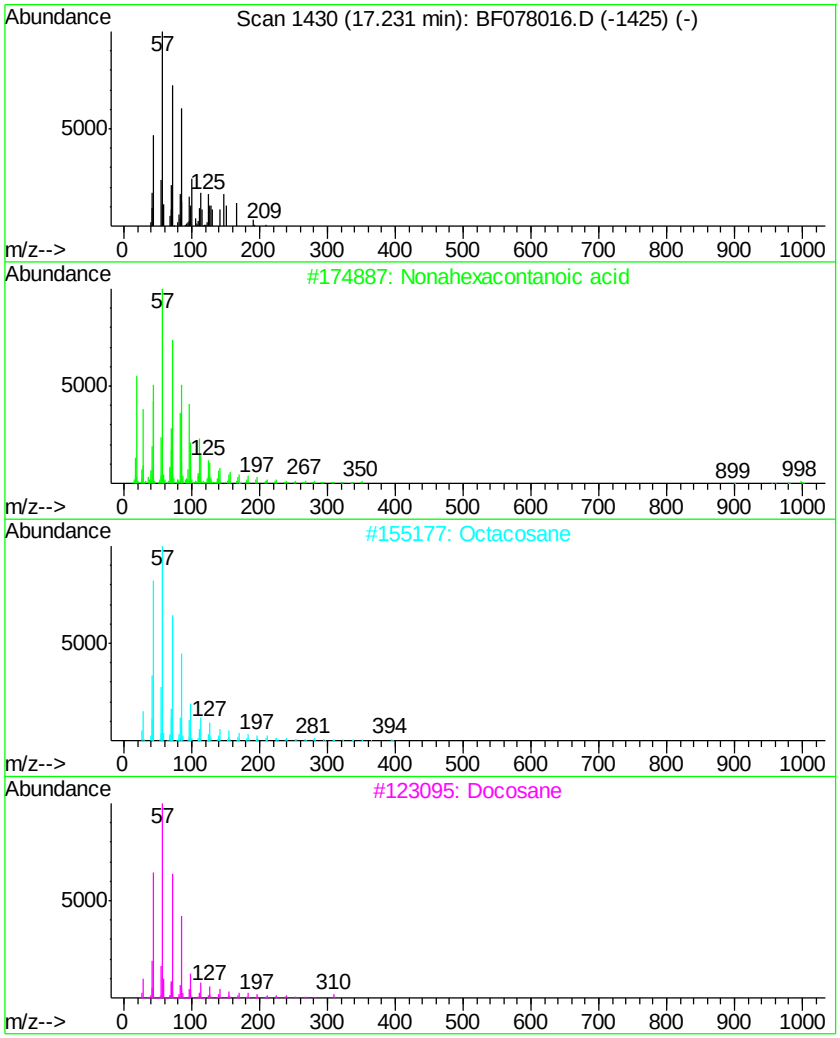
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

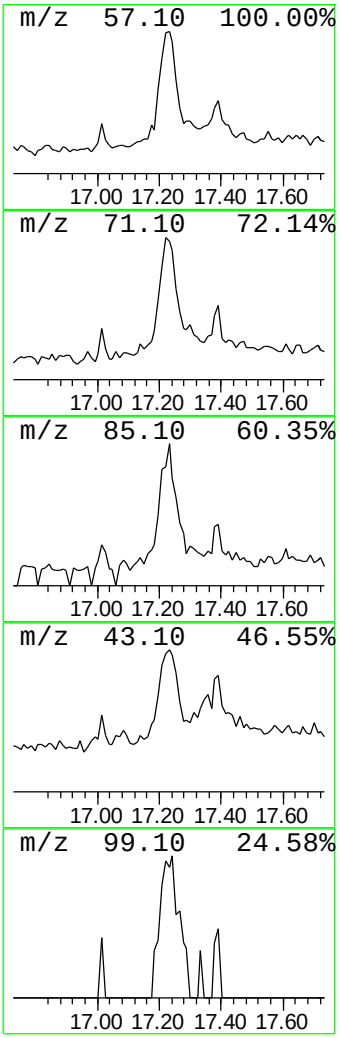
****

Peak Number 9 Nonahexacontanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.23	3.92 ng	79058	Perylene-d12	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	59
2	Octacosane	394	C28H58	000630-02-4	58
3	Docosane	310	C22H46	000629-97-0	53
4	Pentacosane	352	C25H52	000629-99-2	53
5	Triacontane	422	C30H62	000638-68-6	53





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

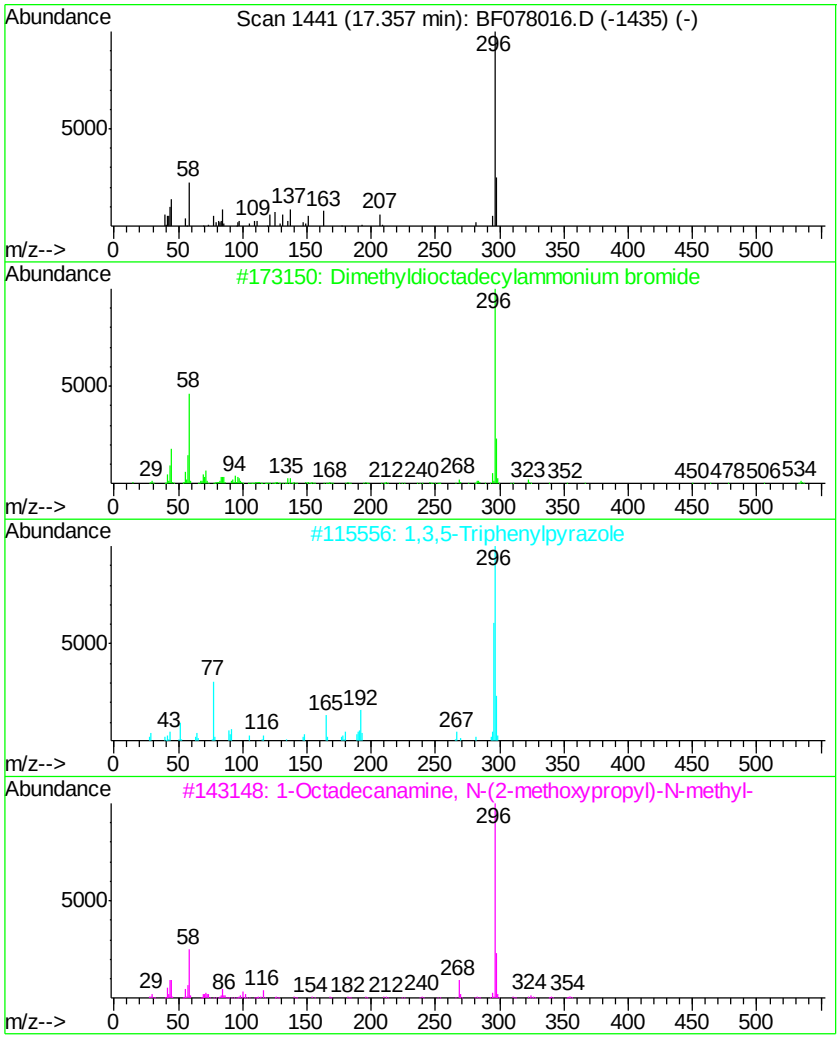
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

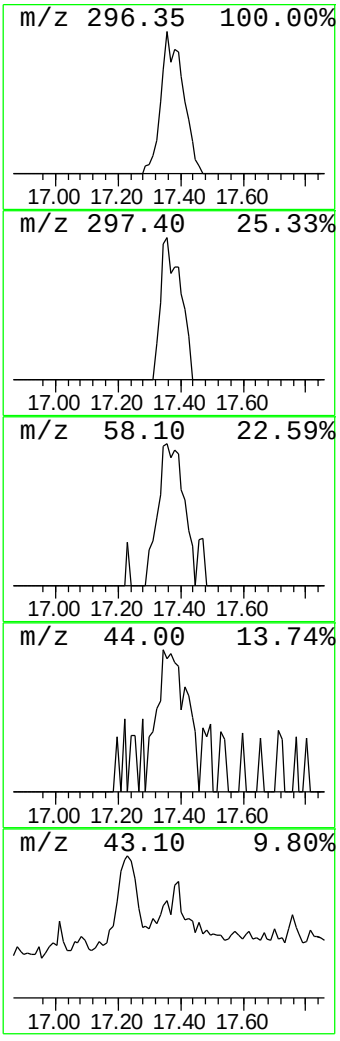
****

Peak Number 10 Dimethyldioctadecylammonium... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.36	2.21 ng	44477	Perylene-d12	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyldioctadecylammonium bromide	630	C38H80BrN	003700-67-2	64
2	1,3,5-Triphenylpyrazole	296	C21H16N2	002183-27-9	42
3	1-Octadecanamine, N-(2-methoxypr...	355	C23H49NO	1000196-18-5	39
4	Cobalt, (1,5-cyclooctadiene)(.et...	296	C18H21Co	1000151-80-3	9
5	Benzoic acid, 4-[[[4-(dimethylam...	296	C18H20N2O2	020534-73-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

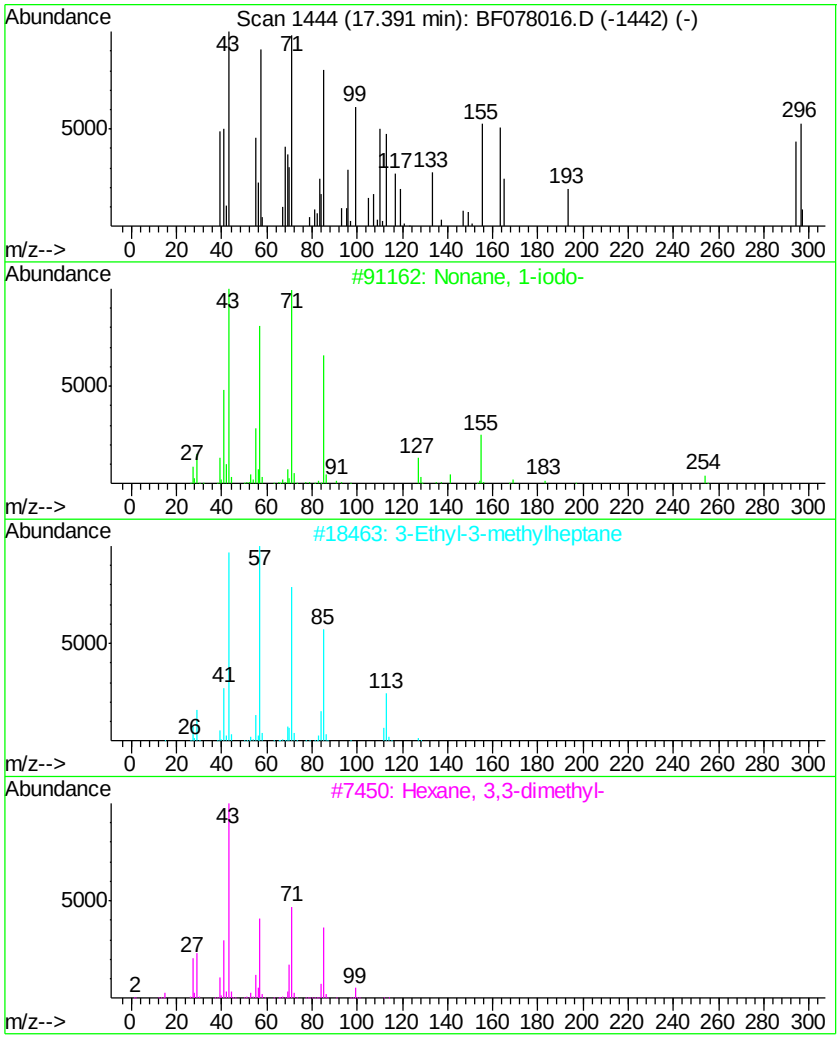
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

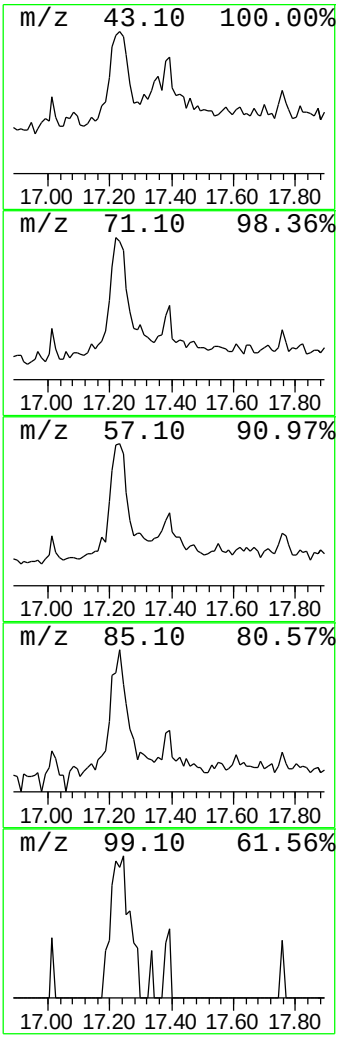
****

Peak Number 11 unknown17.39 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	2.19 ng	44185	Perylene-d12	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 1-iodo-	254	C9H19I	004282-42-2	27
2	3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	25
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	22
4	Tetradecane	198	C14H30	000629-59-4	16
5	Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	12





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

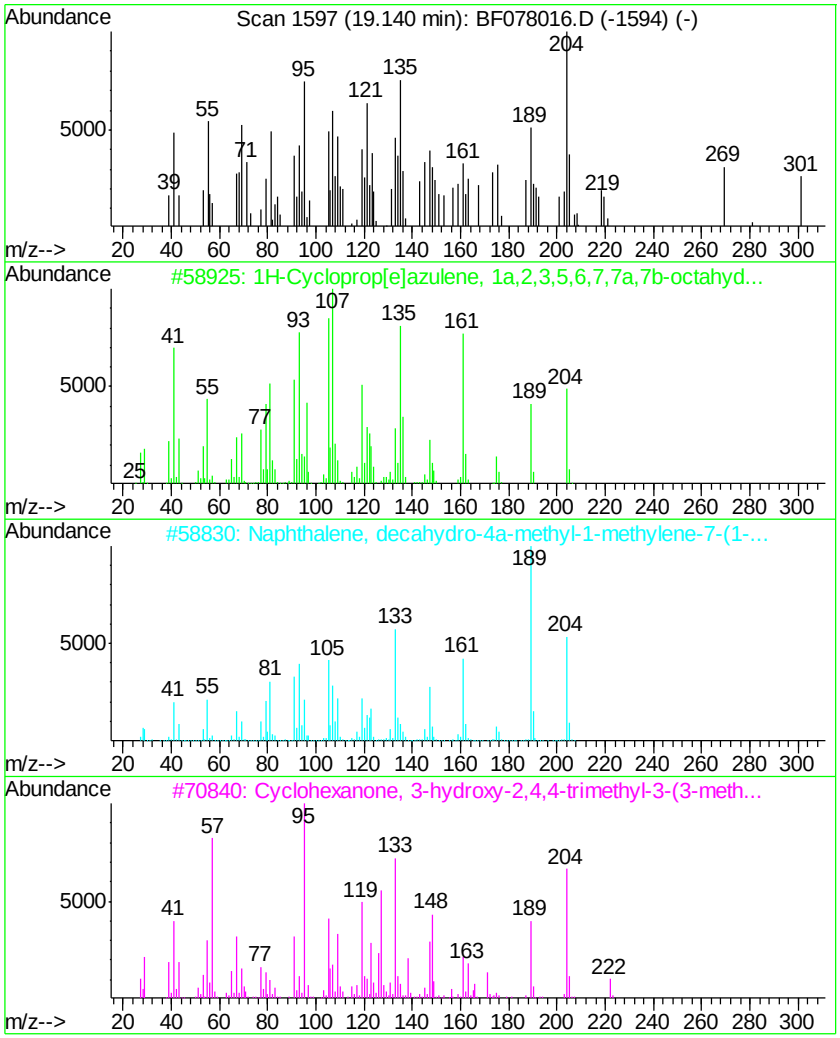
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

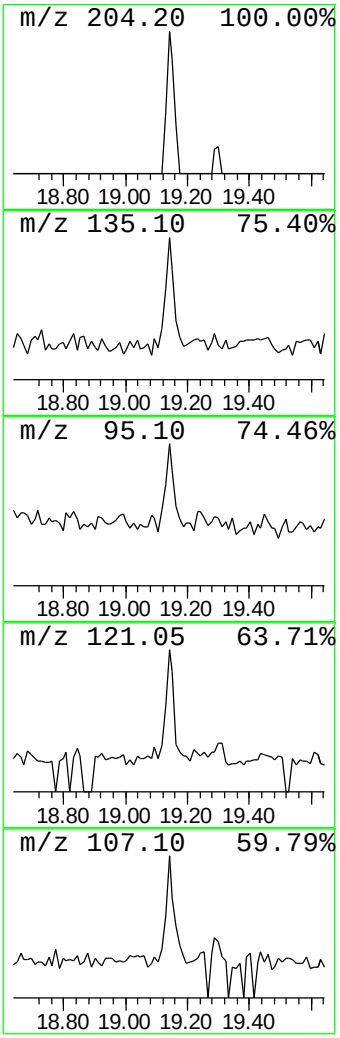
****

Peak Number 12 1H-Cycloprop[e]azulene, 1a,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.14	3.58 ng	72228	Perylene-d12	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	64
2	Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	60
3	Cyclohexanone, 3-hydroxy-2,4,4-t...	222	C14H22O2	088764-84-5	50
4	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	50
5	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032615\
Data File : BF078016.D
Acq On : 27 Mar 2015 2:38
Operator : TP/IZ
Sample : G1653-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
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...	1.24	78.7	ng	786034	1	7.09	199796	20.0
Butane, 2-methoxy...	1.53	7.8	ng	77828	1	7.09	199796	20.0
2-Pentanone, 4-hy...	4.83	14.1	ng	140598	1	7.09	199796	20.0
unknown6.81	6.81	98.2	ng	981193	1	7.09	199796	20.0
1-Eicosanol	15.86	4.7	ng	92551	5	15.95	395669	20.0
Nonahexacontanoic...	17.23	3.9	ng	79058	6	17.63	403403	20.0
Dimethyldioctadec...	17.36	2.2	ng	44477	6	17.63	403403	20.0
unknown17.39	17.39	2.2	ng	44185	6	17.63	403403	20.0
1H-Cycloprop[e]az...	19.14	3.6	ng	72228	6	17.63	403403	20.0