LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

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-BF101015.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	4.320	188	191	199	rBV	252876	376361	12.37%	2.290%
2	5.017	247	252	254	rBV	1595055	3043384	100.00%	18.519%
3	5.417	284	287	298	rVB	93329	115940	3.81%	0.705%
4	6.457	376	378	380	rBV	639287	671209	22.05%	4.084%
5	6.583	387	389	392	rBV	266118	248418	8.16%	1.512%
6	6.823	407	410	412	rBV	442812	400416	13.16%	2.436%
7	6.880	414	415	421	rVB2	32909	38254	1.26%	0.233%
8	6.971	421	423	426	rBV	885929	1189414	39.08%	7.237%
9	7.394	457	460	462	rBV	927940	946217	31.09%	5.758%
10	8.023	513	515	520	rBV	18696	32958	1.08%	0.201%
11	8.114	520	523	525	rBV	546270	563678	18.52%	3.430%
12	9.063	602	606	608	rBV	34914	43486	1.43%	0.265%
13	9.189	614	617	620	rBV	1754722	1932049	63.48%	11.756%
14	9.589	650	652	654	rBV	197684	168247	5.53%	1.024%
15	9.795	668	670	674	rBV	32889	50305	1.65%	0.306%
16	9.875	674	677	679	rBV	581736	703669	23.12%	4.282%
17	10.275	707	712	713	rBV	28758	35263	1.16%	0.215%
18	10.778	754	756	760	rVB	32466	52183	1.71%	0.318%
19	10.869	763	764	766	rVV2	32498	35466	1.17%	0.216%
20	11.223	793	795	796	rBV	45924	40595	1.33%	0.247%
21	11.360	805	807	809	rBV	792450	736138	24.19%	4.479%
22	11.589	824	827	830	rBV2	25786	45578	1.50%	0.277%
23	12.835	934	936	940	rVV2	29996	46530	1.53%	0.283%
24	12.972	945	948	950	rBV	1615828	2318646	76.19%	14.109%
25	13.201	964	968	970	rBV3	23832	38381	1.26%	0.234%
26	13.475	988	992	994	rBV	235197	332041	10.91%	2.020%
27	13.566	997	1000	1004	rVB	17579	36295	1.19%	0.221%
28	13.921	1028	1031	1038	rBV	304813	459999	15.11%	2.799%
29	14.092	1043	1046	1048	rBV	471486	704924	23.16%	4.289%
30	14.286	1061	1063	1066	rBV3	15897	39347	1.29%	0.239%
31	14.641	1091	1094	1097	rBV2	29734	70688	2.32%	0.430%
32	14.961	1119	1122	1126	rBV	273261	345062	11.34%	2.100%
33	15.658	1180	1183	1186	rBV	364562	498303	16.37%	3.032%
34	16.195	1227	1230	1234	rBV	35097	74706	2.45%	0.455%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

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-BF101015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 16434150

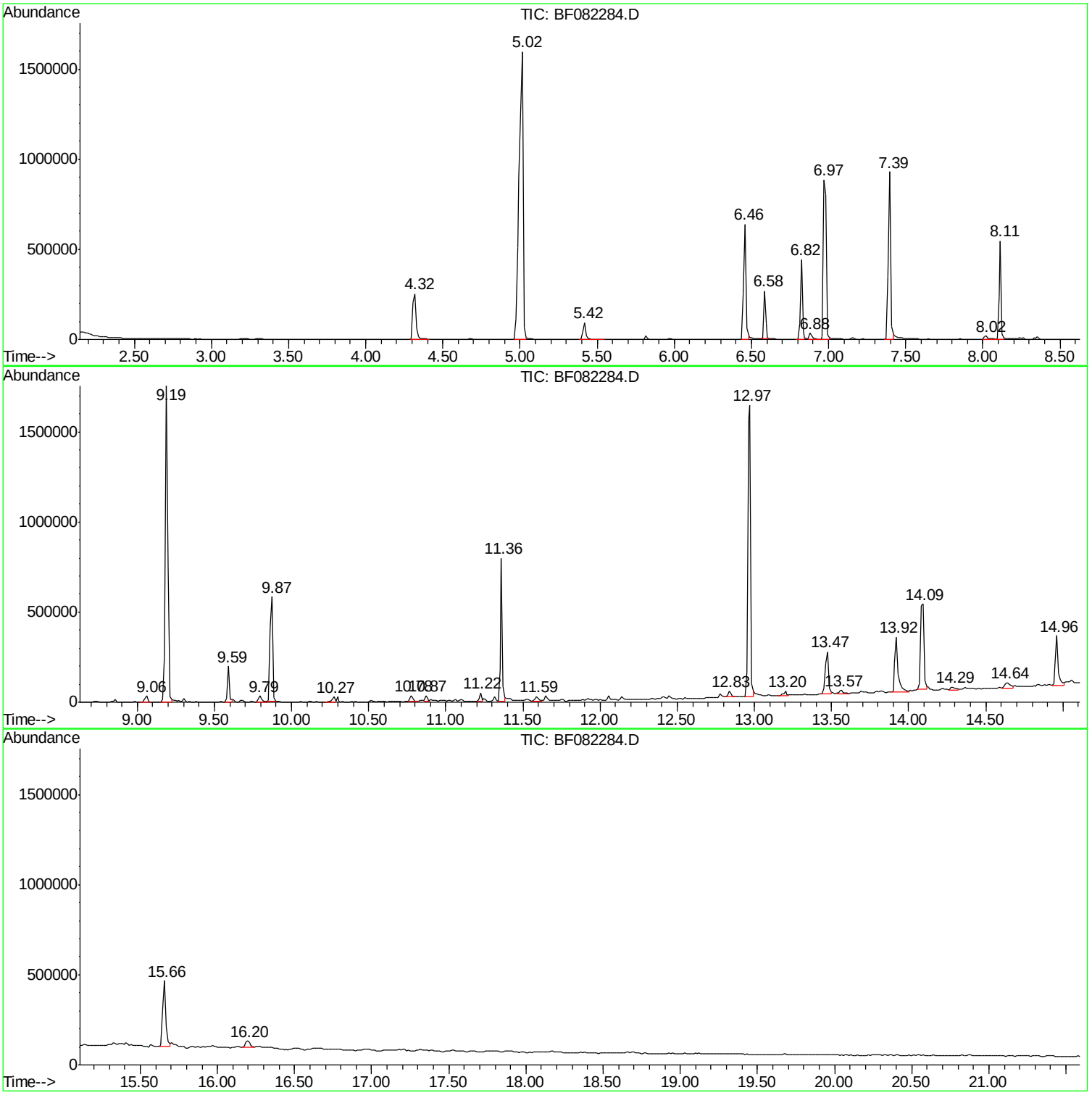
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

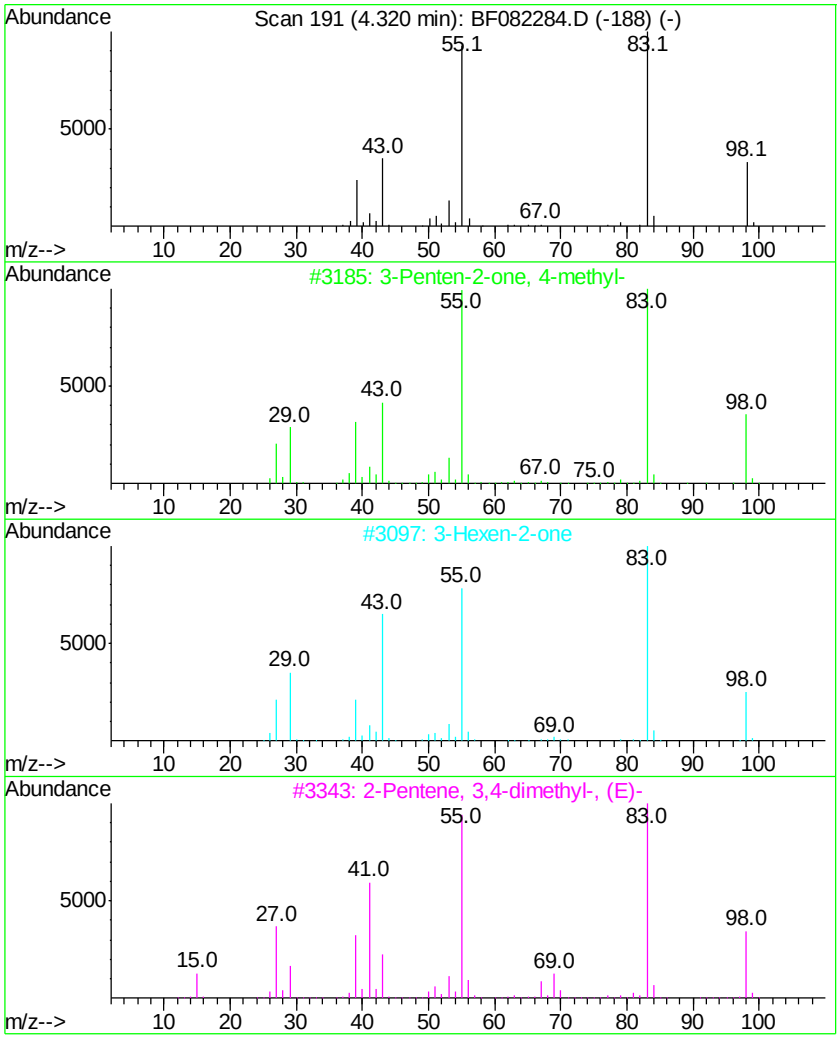
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

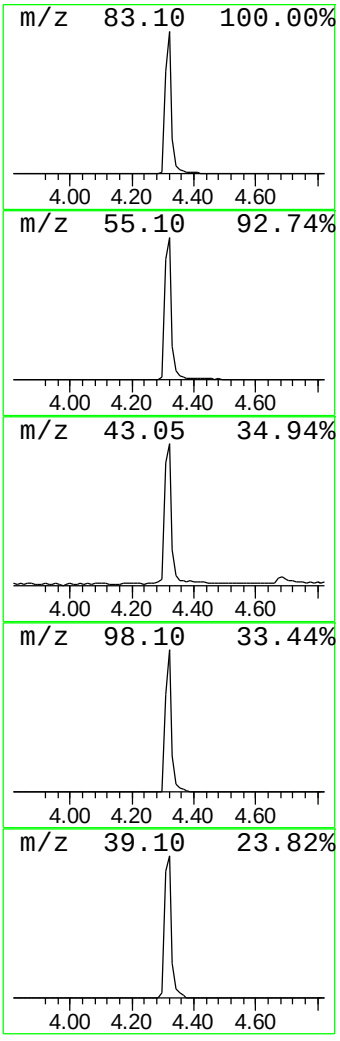
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	18.80 ng	376361	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

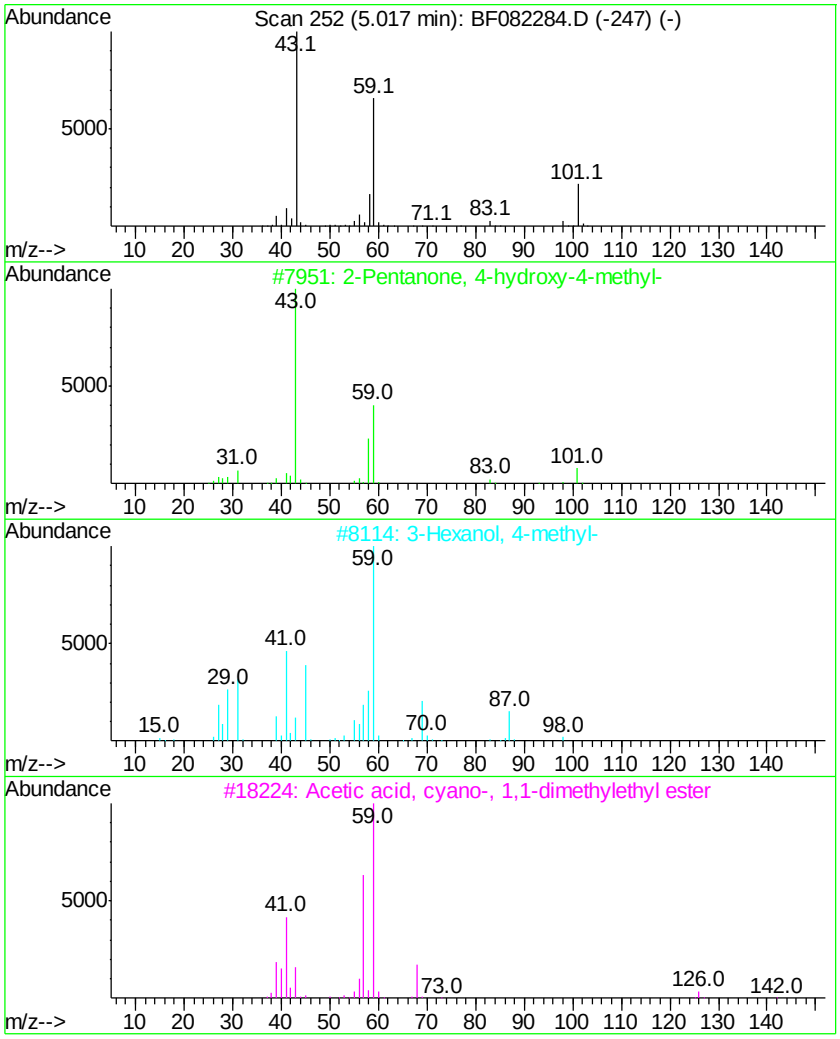
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

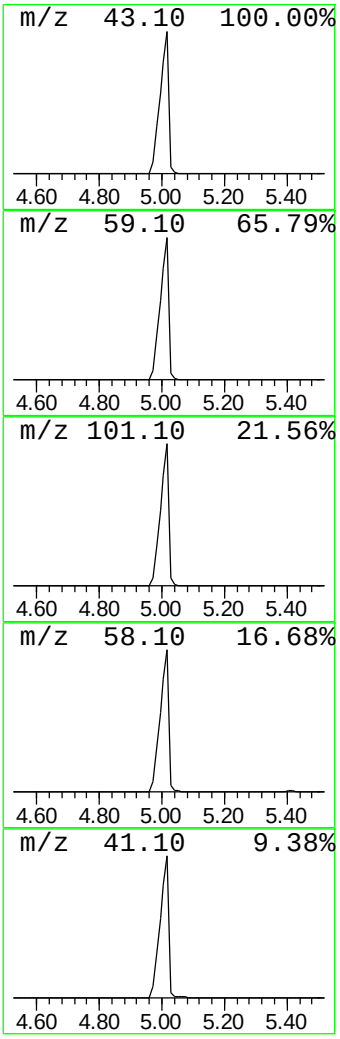
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	152.01 ng	3043380	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

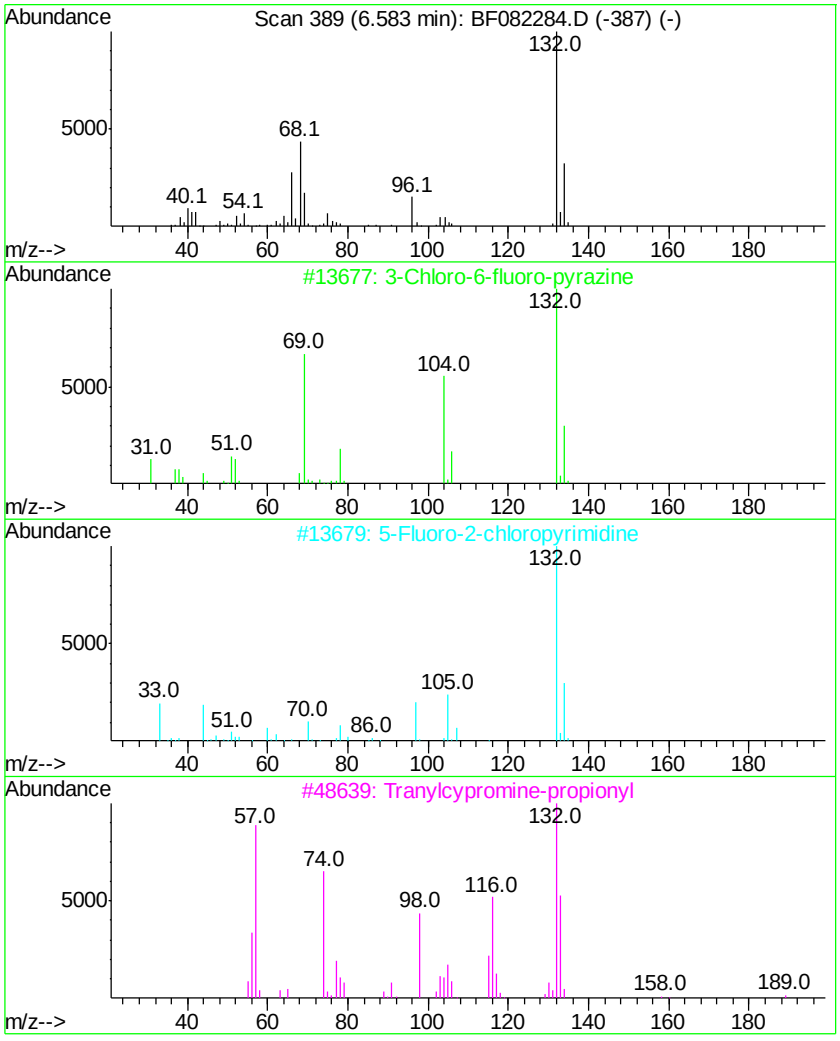
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

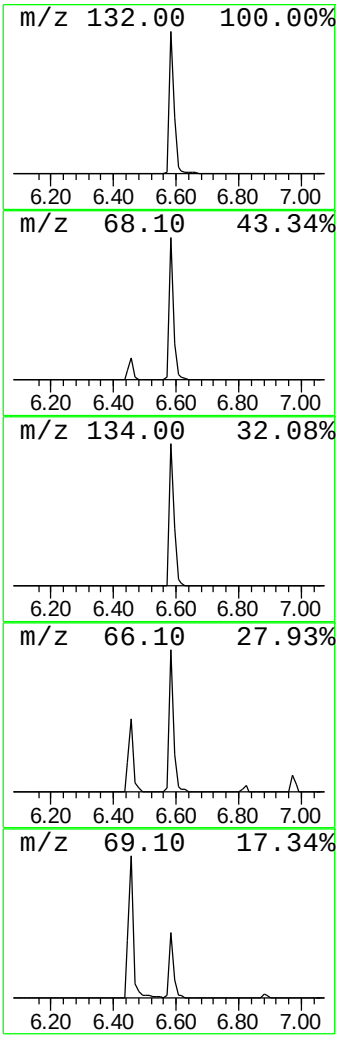
****

Peak Number 3 unknown6.58 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	12.41 ng	248418	1,4-Dichlorobenzene-d4	6.82

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	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

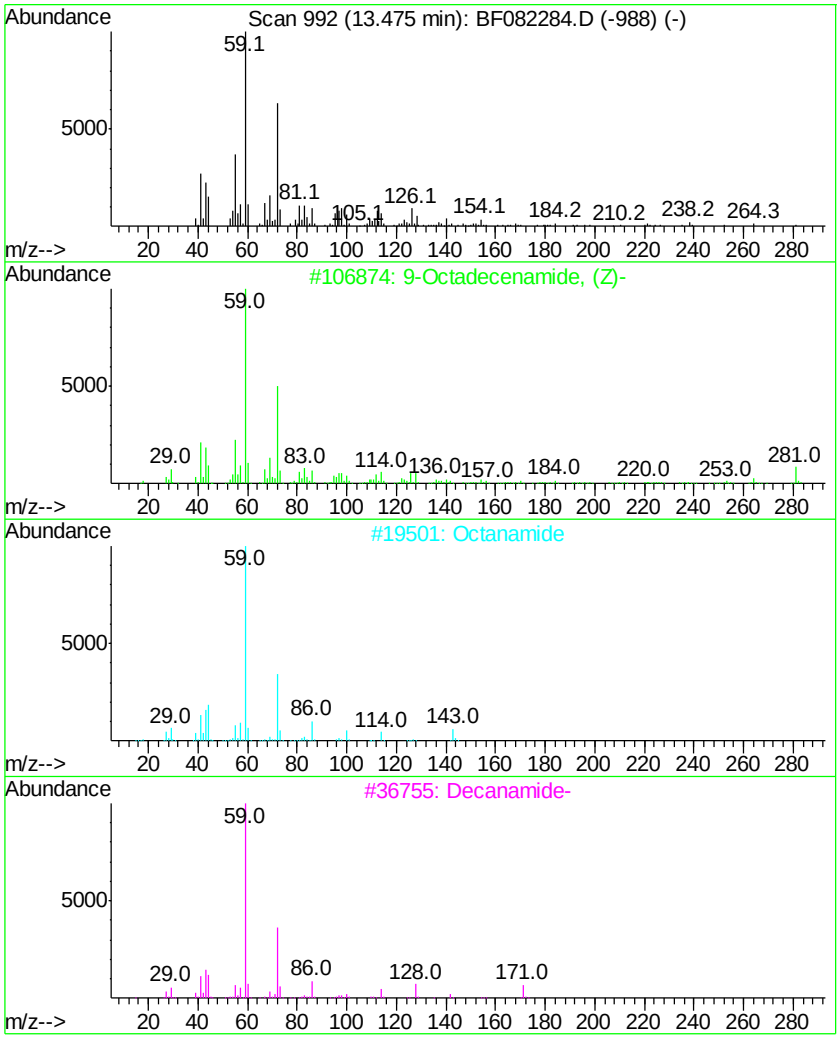
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

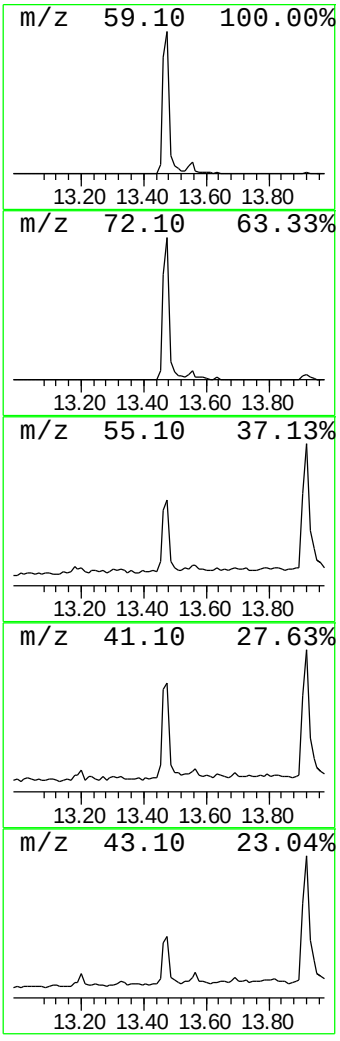
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	9.42 ng	332041	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Octanamide	143	C8H17NO	000629-01-6	59
3	Decanamide-	171	C10H21NO	002319-29-1	59
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
5	Hexadecanamide	255	C16H33NO	000629-54-9	59





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

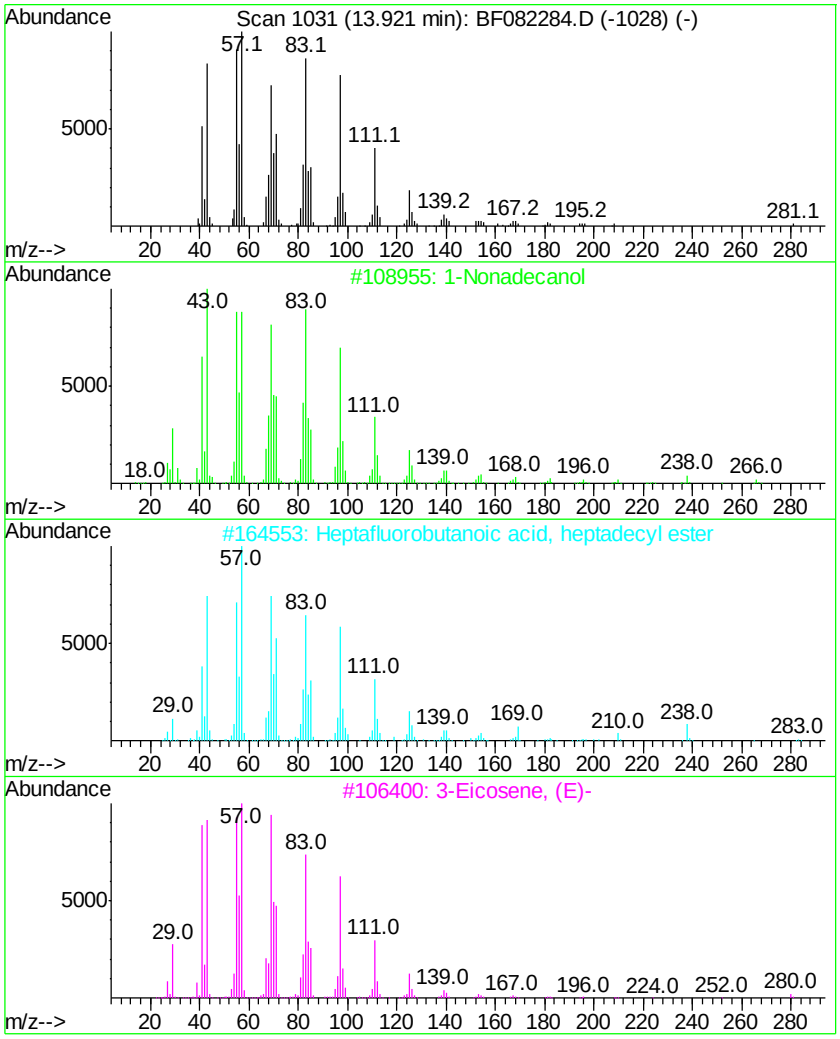
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

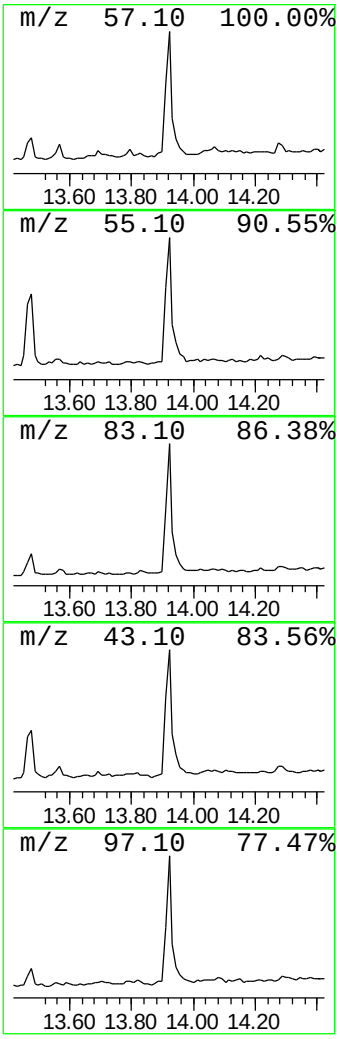
****

Peak Number 6 1-Nonadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	13.05 ng	459999	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecanol	284	C19H40O	001454-84-8	95
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

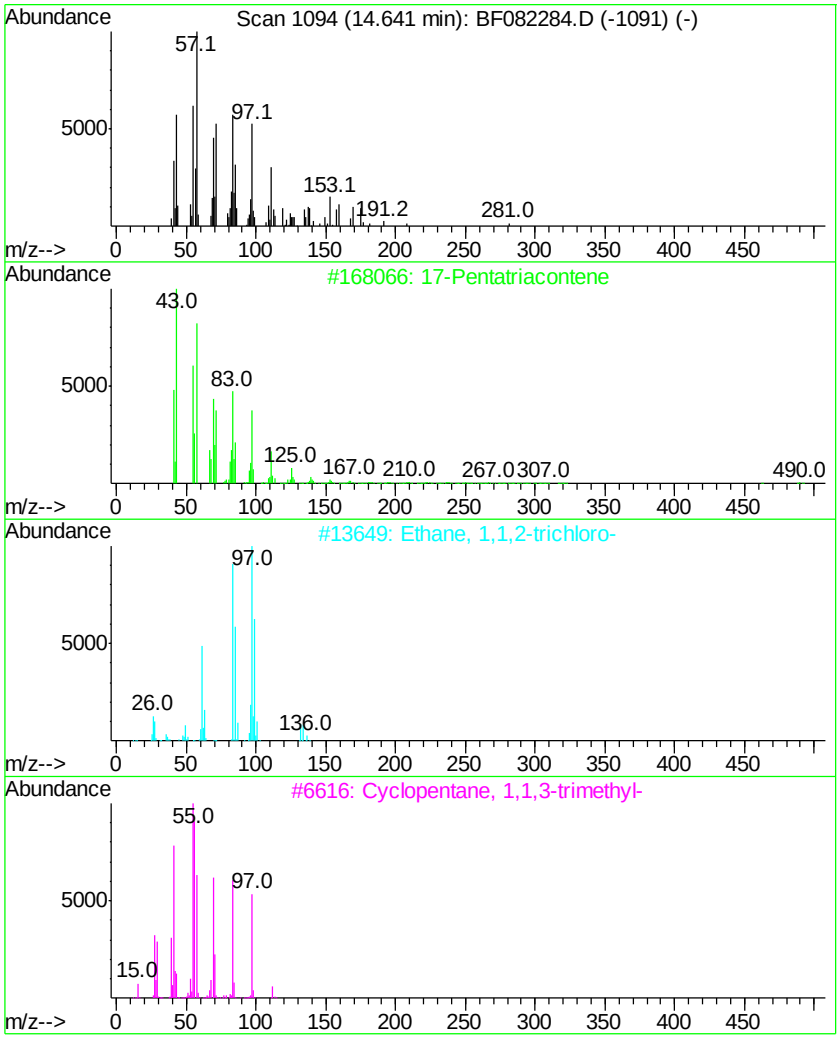
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

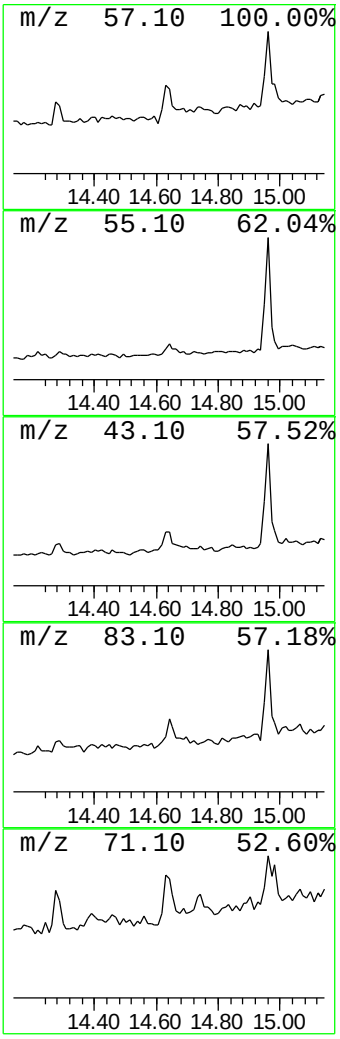
****

Peak Number 7 17-Pentatriacontene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.01 ng	70688	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	58
2	Ethane, 1,1,2-trichloro-	132	C2H3Cl3	000079-00-5	38
3	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	30
4	2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	15
5	Cycloheptane, methyl-	112	C8H16	004126-78-7	15





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

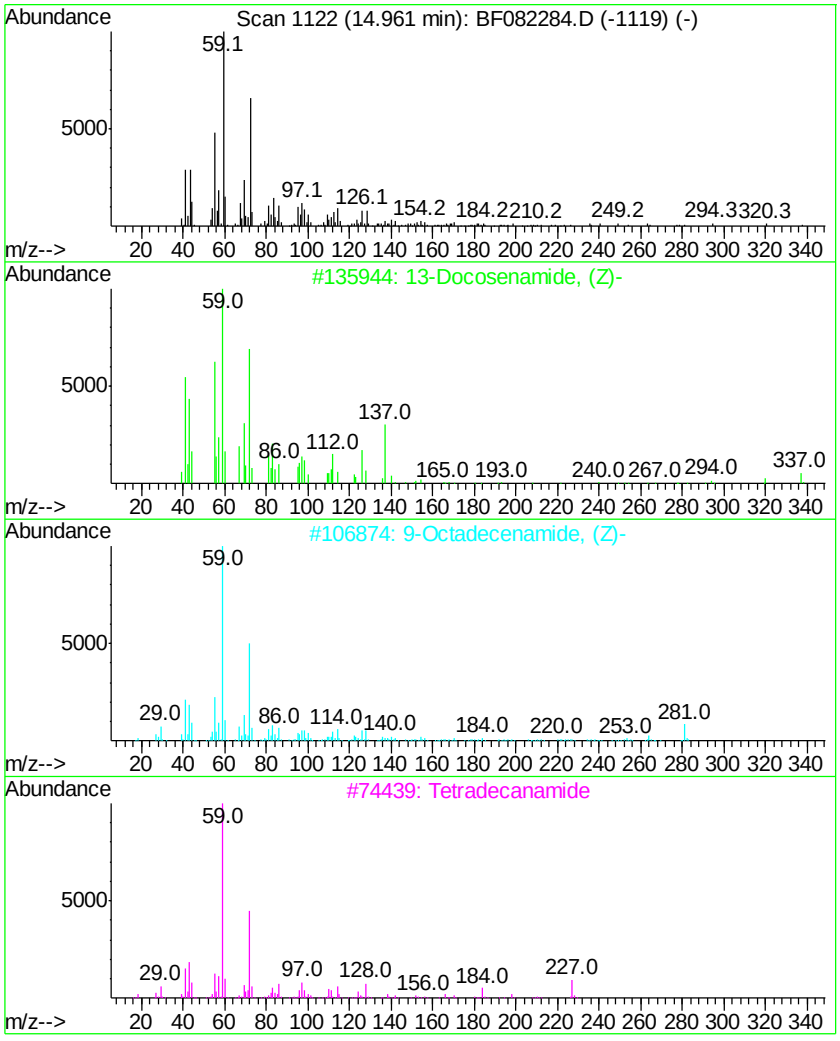
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

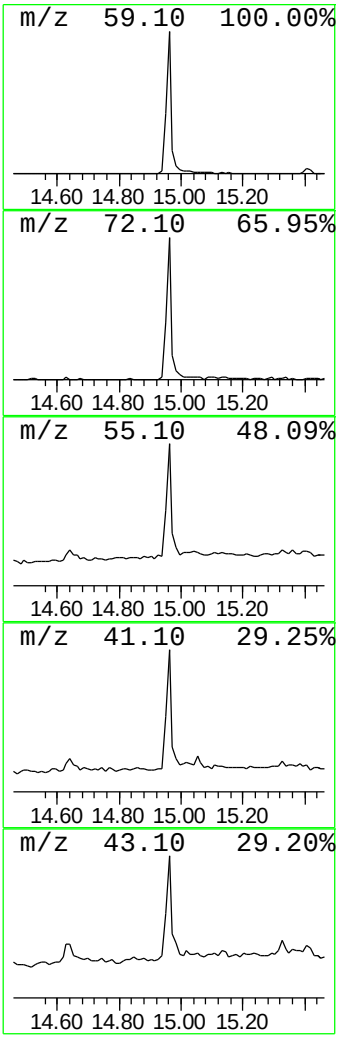
****

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	13.85 ng	345062	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3	Tetradecanamide	227	C14H29NO	000638-58-4	78
4	Hexadecanamide	255	C16H33NO	000629-54-9	72
5	Dodecanamide	199	C12H25NO	001120-16-7	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

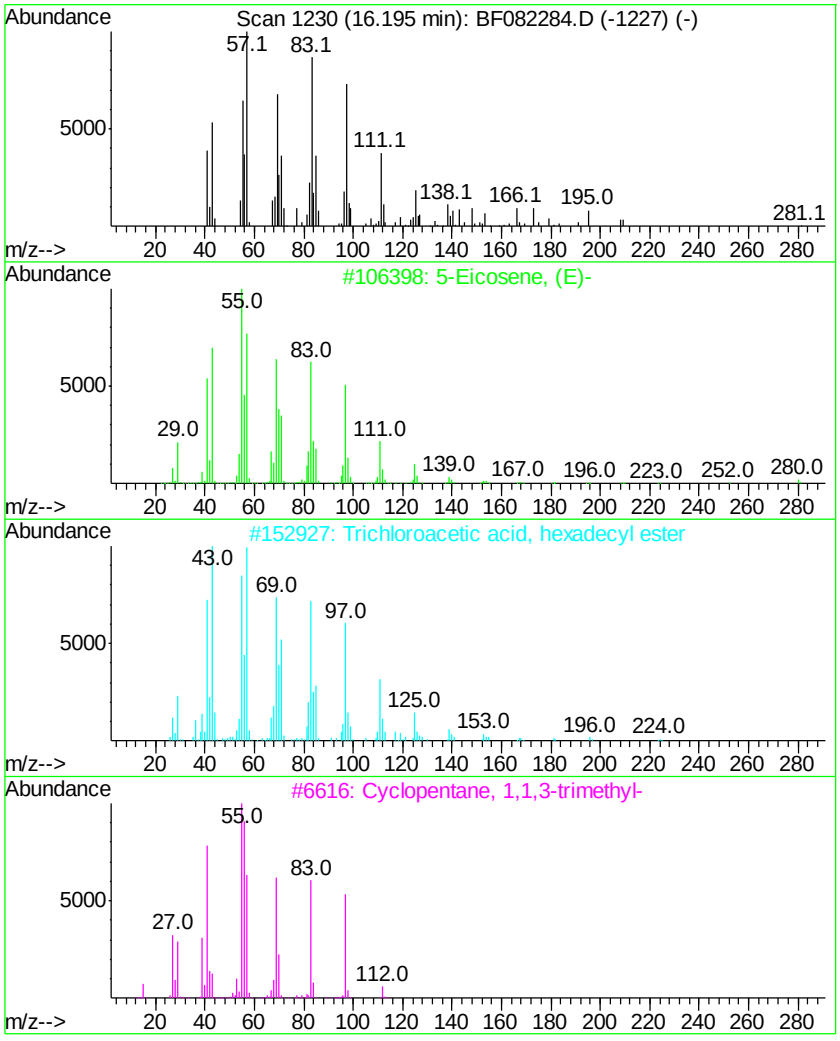
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

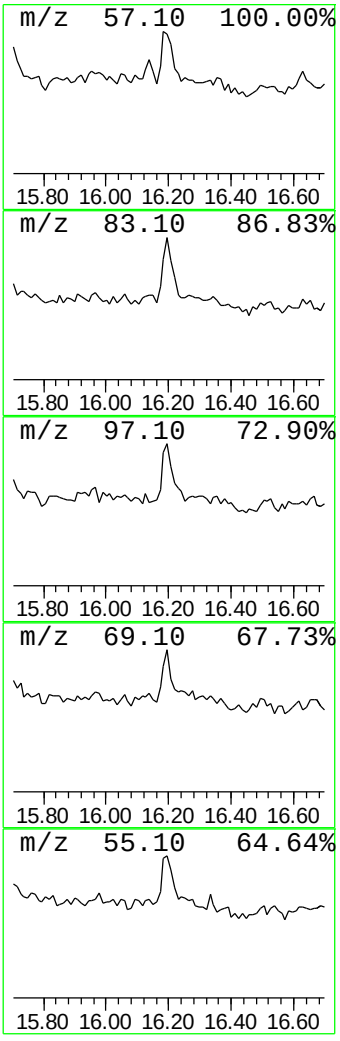
****

Peak Number 9 5-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	3.00 ng	74706	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	64
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	49
3	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	49
4	17-Pentatriacontene	491	C35H70	006971-40-0	47
5	1-Docosene	308	C22H44	001599-67-3	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101515\
Data File : BF082284.D
Acq On : 14 Oct 2015 17:43
Operator : UM/IZ
Sample : G4015-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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
3-Penten-2-one, 4...	4.32	18.8	ng	376361	1	6.82	400416	20.0
2-Pentanone, 4-hy...	5.02	152.0	ng	3043380	1	6.82	400416	20.0
unknown6.58	6.58	12.4	ng	248418	1	6.82	400416	20.0
9-Octadecenamide,...	13.48	9.4	ng	332041	5	14.09	704924	20.0
1-Nonadecanol	13.92	13.1	ng	459999	5	14.09	704924	20.0
17-Pentatriacontene	14.64	2.0	ng	70688	5	14.09	704924	20.0
13-Docosenamide, ...	14.96	13.9	ng	345062	6	15.66	498303	20.0
5-Eicosene, (E)-	16.20	3.0	ng	74706	6	15.66	498303	20.0