LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

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-BF121315.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	2.213	9	11	28	rVB2	62195	188315	5.07%	0.551%
2	5.116	261	265	270	rBV	809499	1118033	30.08%	3.274%
3	5.527	298	301	304	rBV	2902053	3193695	85.91%	9.352%
4	5.927	334	336	339	rBB	57236	49505	1.33%	0.145%
5	6.545	387	390	393	rVB	2615475	3155553	84.89%	9.240%
6	6.682	399	402	405	rBV	2506881	3688639	99.23%	10.801%
7	6.922	420	423	425	rBV	629080	762088	20.50%	2.232%
8	7.070	434	436	439	rVB	2035377	2843239	76.49%	8.326%
9	7.482	468	472	474	rBV	2109087	2586127	69.57%	7.573%
10	7.573	477	480	482	rBV	67618	100028	2.69%	0.293%
11	8.202	532	535	537	rBV	1112310	1019399	27.42%	2.985%
12	9.276	626	629	632	rBV	3736047	3717327	100.00%	10.885%
13	9.665	661	663	666	rBV	961369	843799	22.70%	2.471%
14	9.893	681	683	686	rBV	82597	66104	1.78%	0.194%
15	9.951	686	688	691	rVB	1228308	1125223	30.27%	3.295%
16	10.396	723	727	728	rBV	71340	110667	2.98%	0.324%
17	10.614	743	746	749	rBV	33129	51706	1.39%	0.151%
18	10.739	754	757	759	rBV	2505021	2610624	70.23%	7.645%
19	10.865	765	768	772	rVB	96907	119440	3.21%	0.350%
20	11.311	803	807	808	rBV	86331	78447	2.11%	0.230%
21	11.436	815	818	820	rVV	806862	1054228	28.36%	3.087%
22	11.482	820	822	825	rVB	25257	37557	1.01%	0.110%
23	11.734	842	844	849	rVB	40853	39444	1.06%	0.116%
24	12.134	876	879	882	rBV3	44237	69113	1.86%	0.202%
25	12.842	939	941	944	rBV	249596	216069	5.81%	0.633%
26	12.922	944	948	950	rVB2	58314	95722	2.58%	0.280%
27	13.014	953	956	959	rBV	3166116	3304370	88.89%	9.676%
28	13.551	1001	1003	1005	rBV	123133	136435	3.67%	0.400%
29	13.597	1005	1007	1011	rVB2	35507	54064	1.45%	0.158%
30	13.905	1032	1034	1041	rBV2	106219	175539	4.72%	0.514%
31	14.054	1045	1047	1050	rBV	819452	800434	21.53%	2.344%
32	14.237	1061	1063	1068	rVB	50368	47616	1.28%	0.139%
33	14.545	1088	1090	1092	rBV	32881	39945	1.07%	0.117%
34	15.494	1170	1173	1176	rBV	556320	651318	17.52%	1.907%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

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-BF121315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

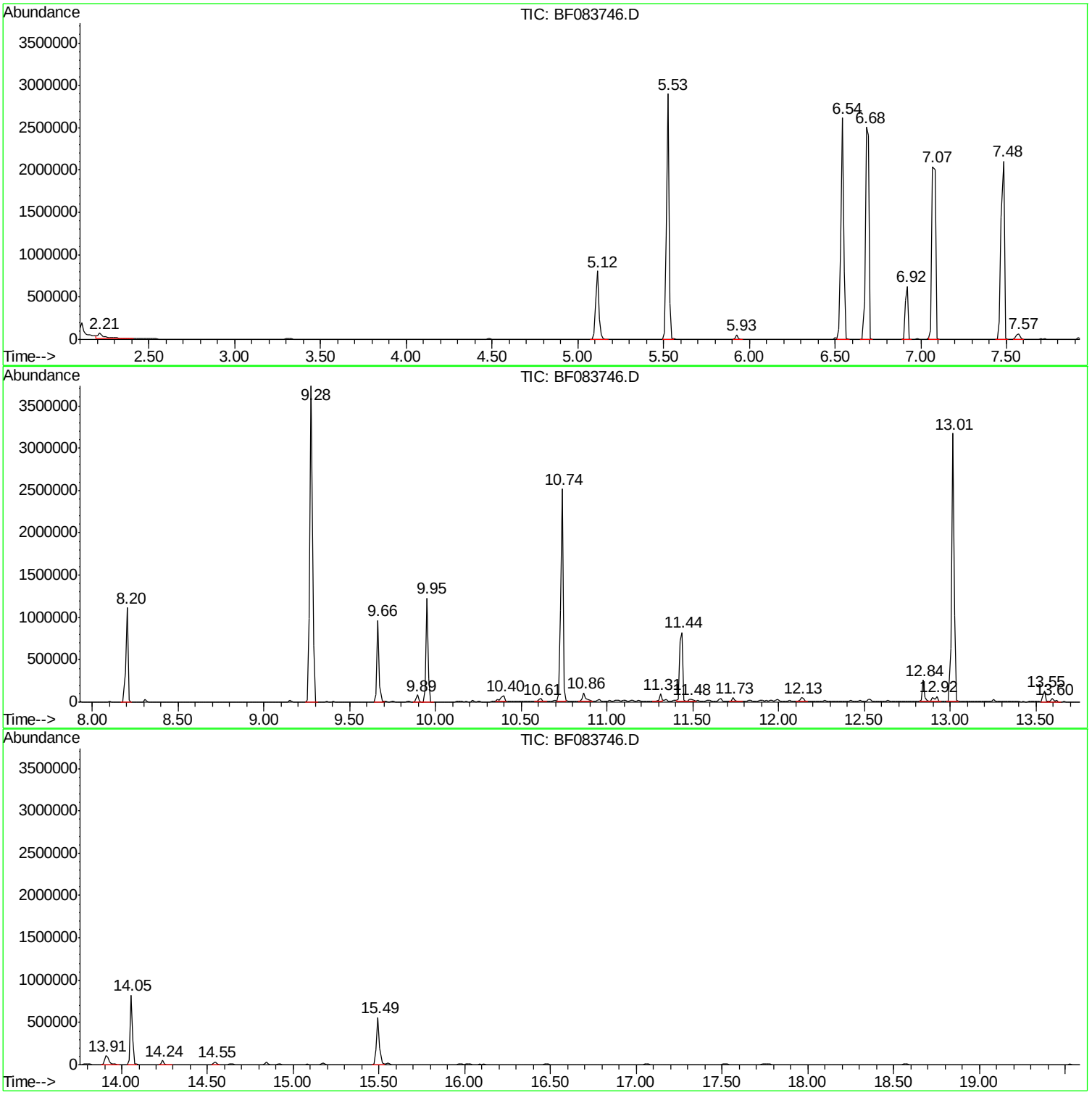
Sum of corrected areas: 34149812

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOUTHWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

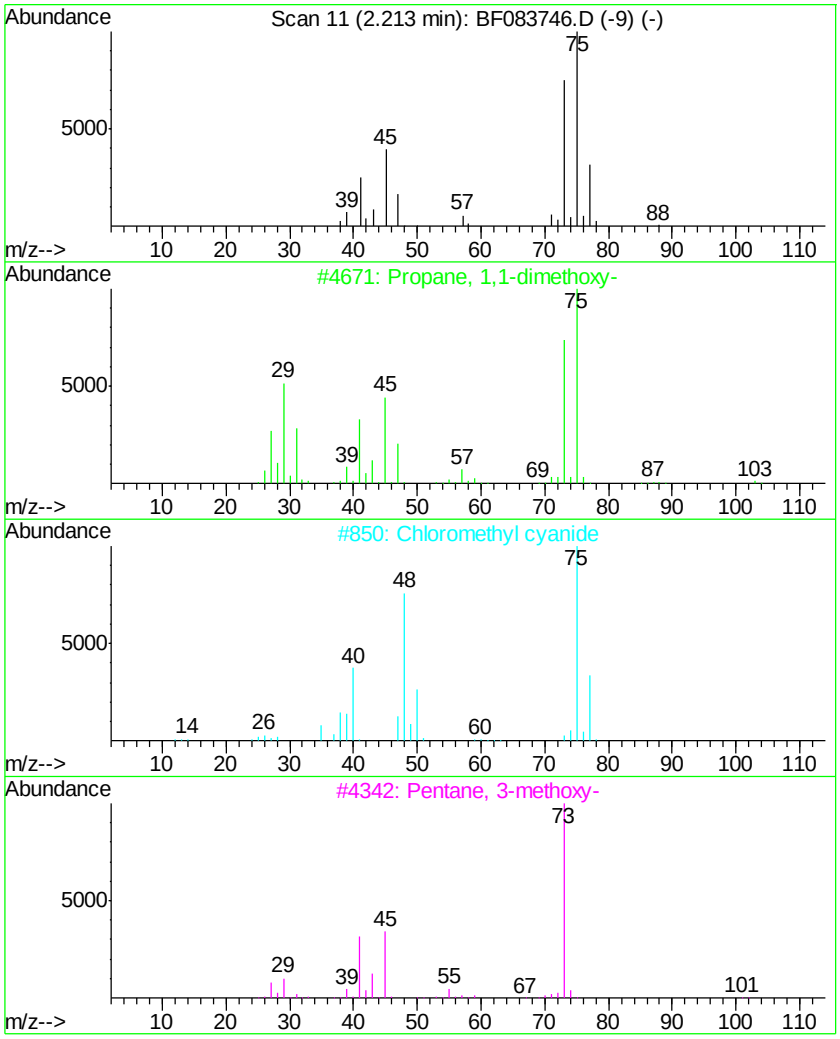
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

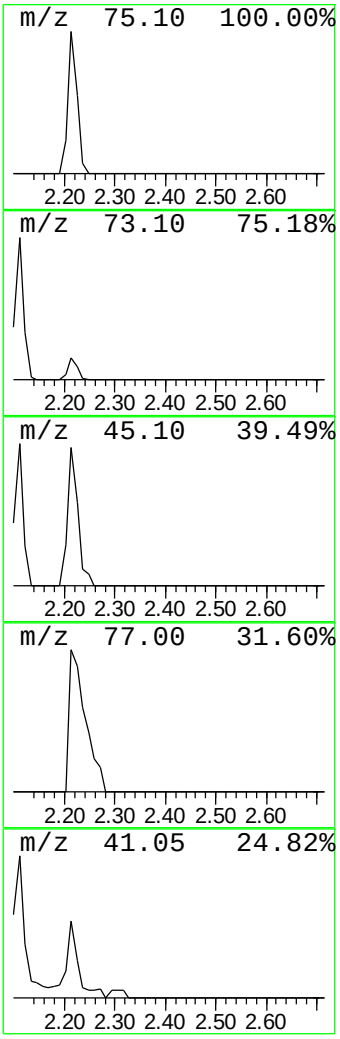
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	4.94 ng	188315	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2	Chloromethyl cyanide	75	C2H2ClN	000107-14-2	47
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5	Glycine	75	C2H5NO2	000056-40-6	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

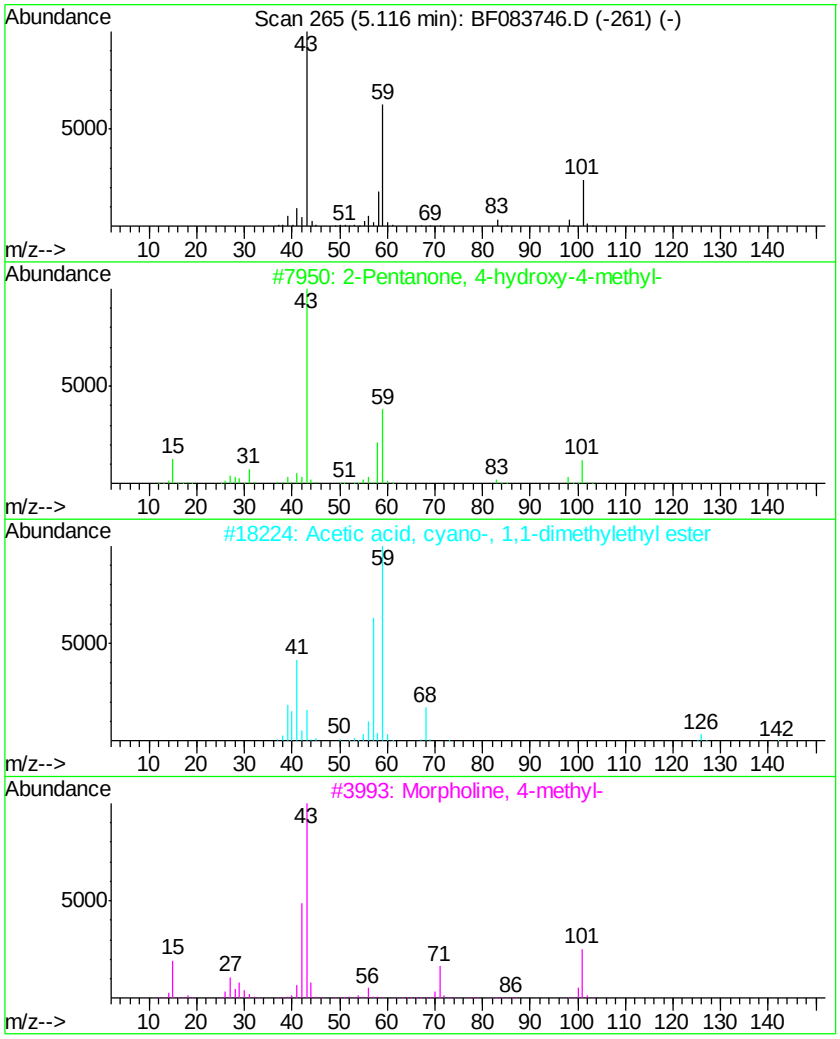
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

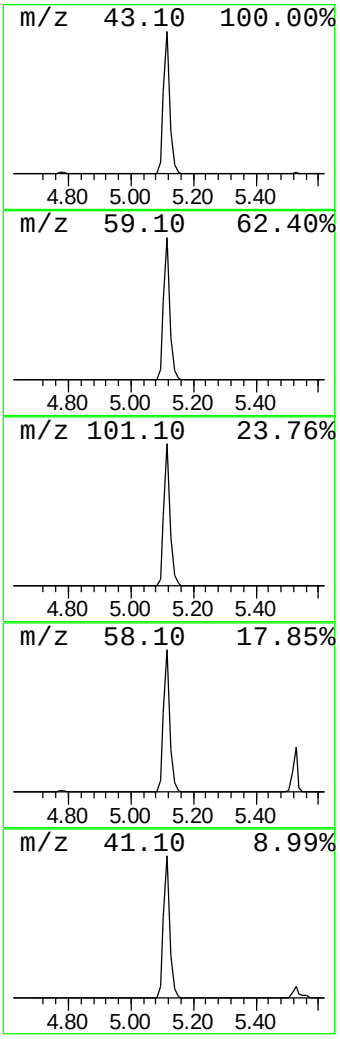
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	29.34 ng	1118030	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

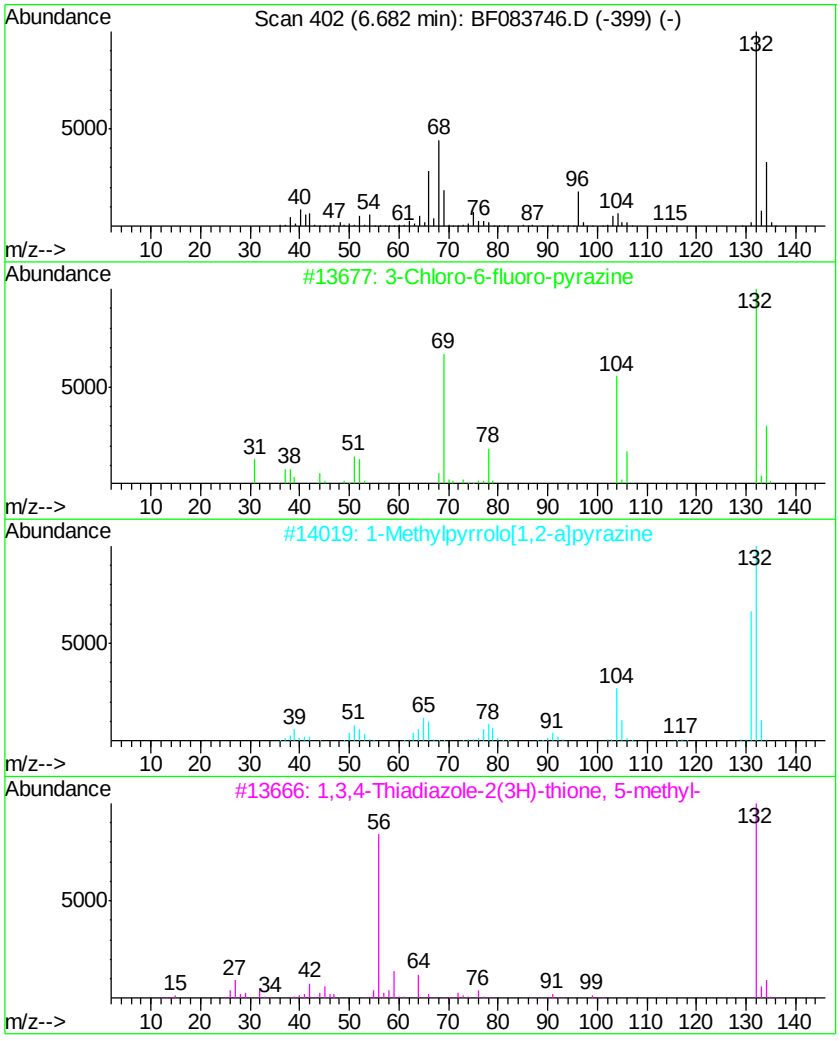
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

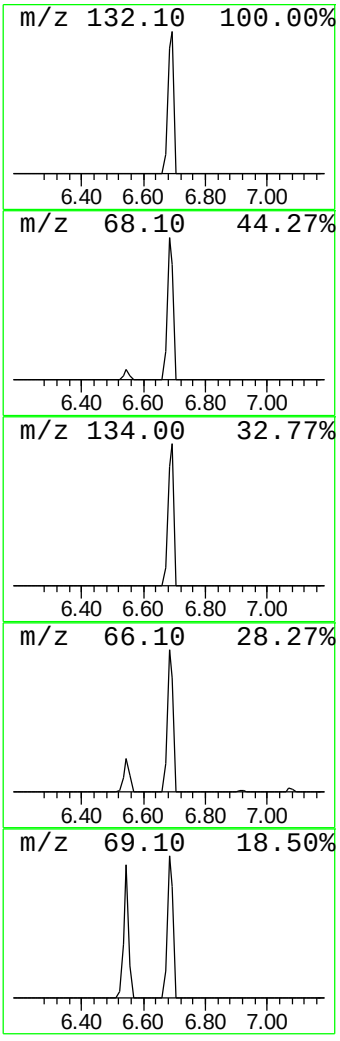
****

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	96.80 ng	3688640	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
3	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

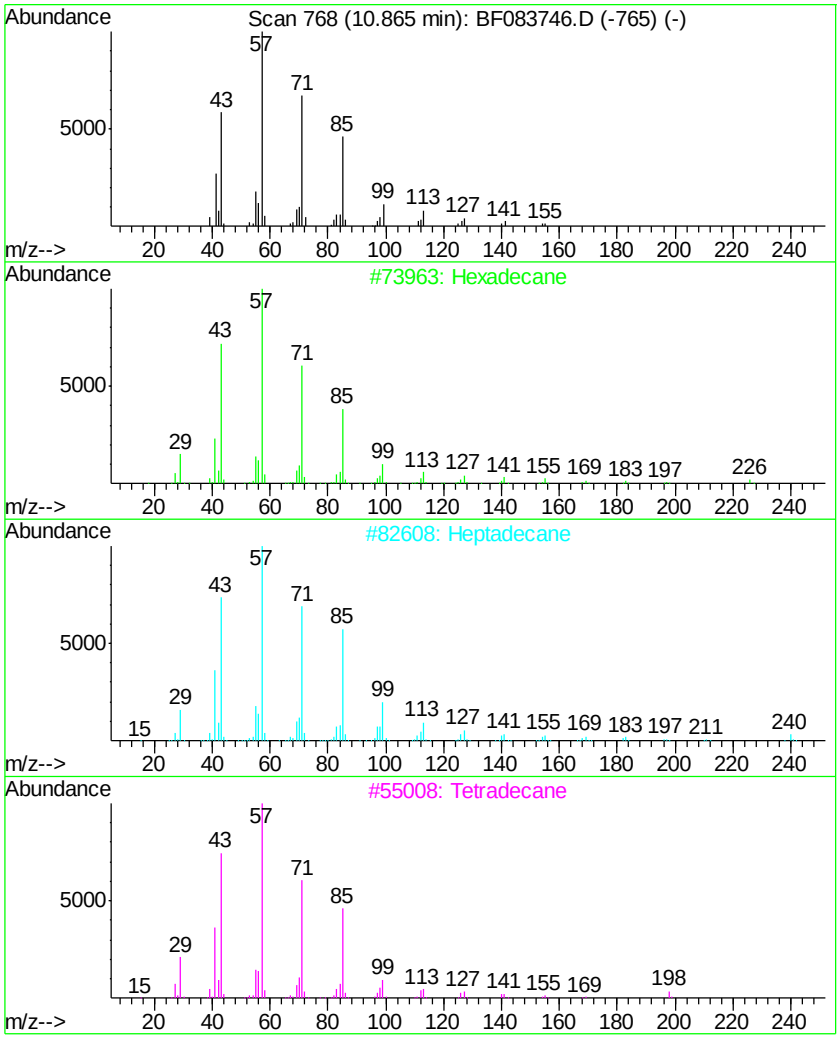
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

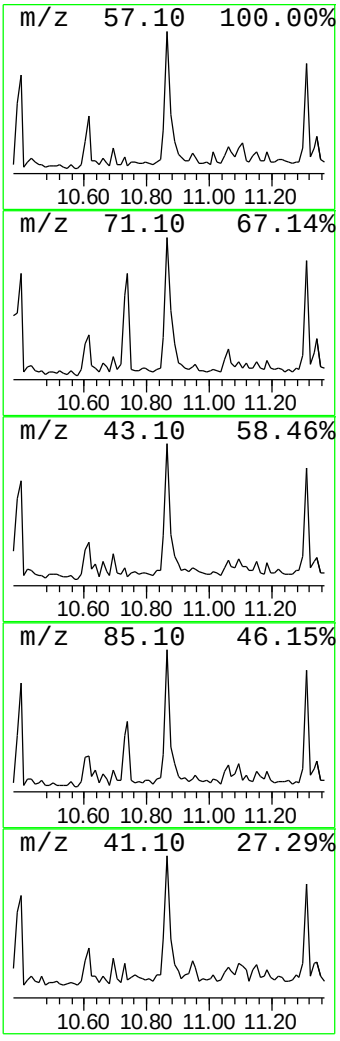
****

Peak Number 5 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	2.27 ng	119440	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heptadecane	240	C17H36	000629-78-7	87
3	Tetradecane	198	C14H30	000629-59-4	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Tritetracontane	605	C43H88	007098-21-7	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

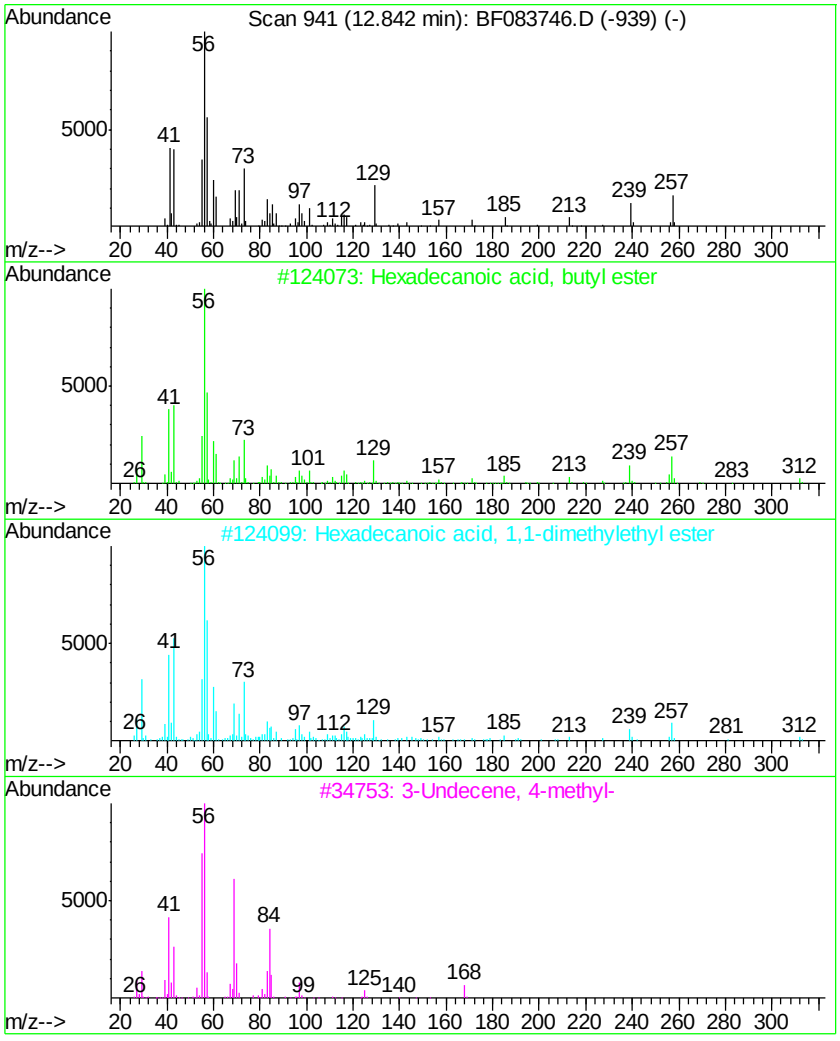
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

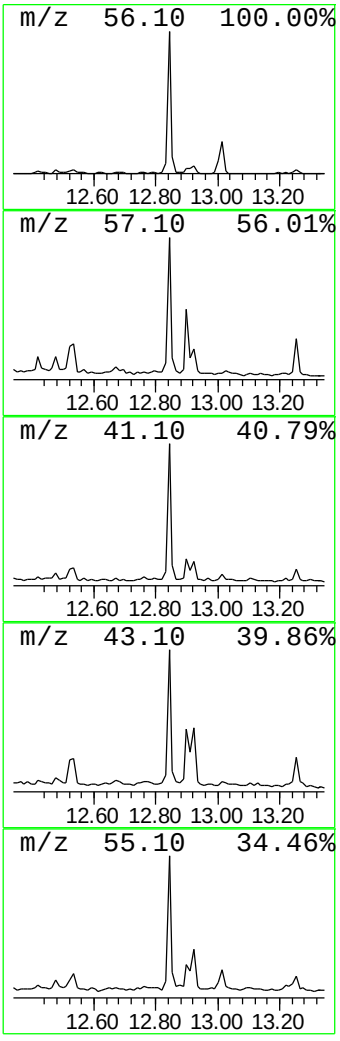
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	5.40 ng	216069	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	3-Undecene, 4-methyl-	168	C12H24	074630-68-5	32
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

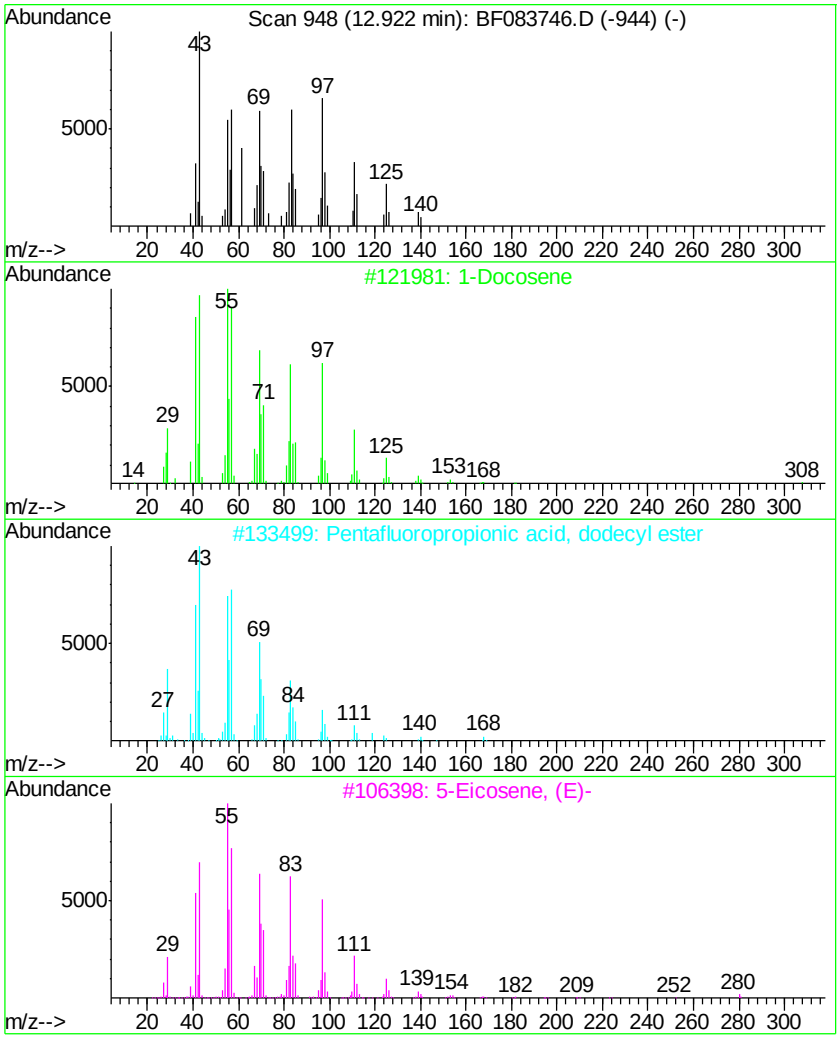
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

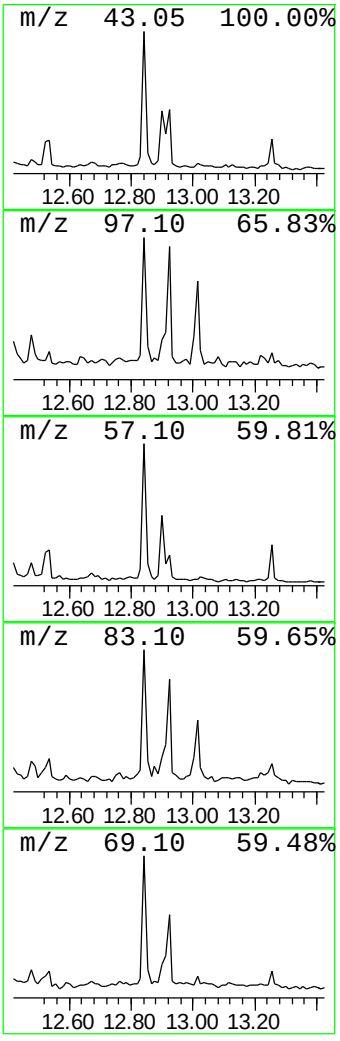
****

Peak Number 7 1-Docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	2.39 ng	95722	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	76
2	Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	62
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	58
4	1-Octadecene	252	C18H36	000112-88-9	58
5	1-Tridecanol	200	C13H28O	000112-70-9	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

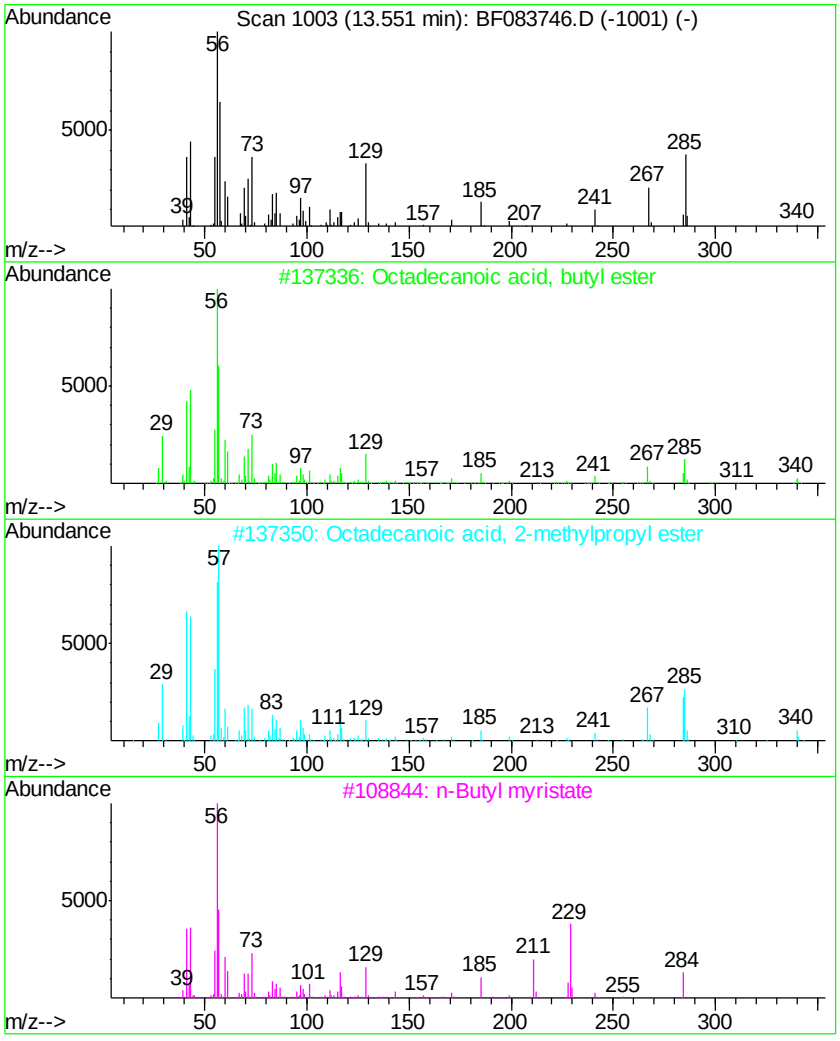
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

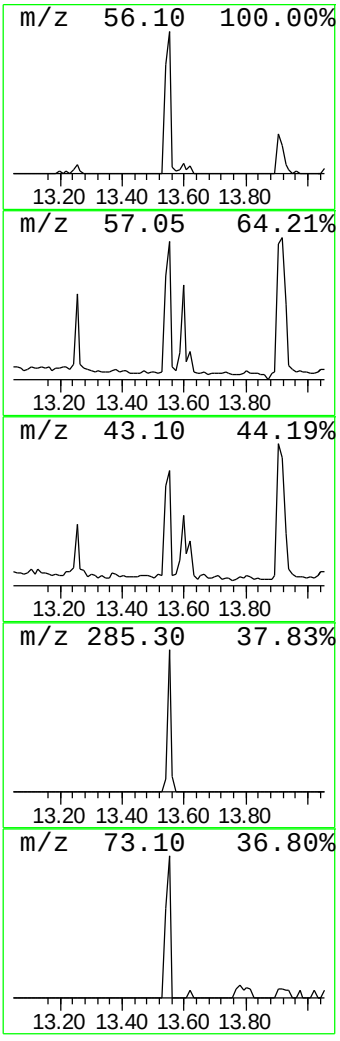
****

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	3.41 ng	136435	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	96
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	86
3	n-Butyl myristate	284	C18H36O2	000110-36-1	38
4	2-Methyl-1-octadecene	266	C19H38	061868-20-0	27
5	5-Methyl-2-hexene,c&t	98	C7H14	003404-62-4	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

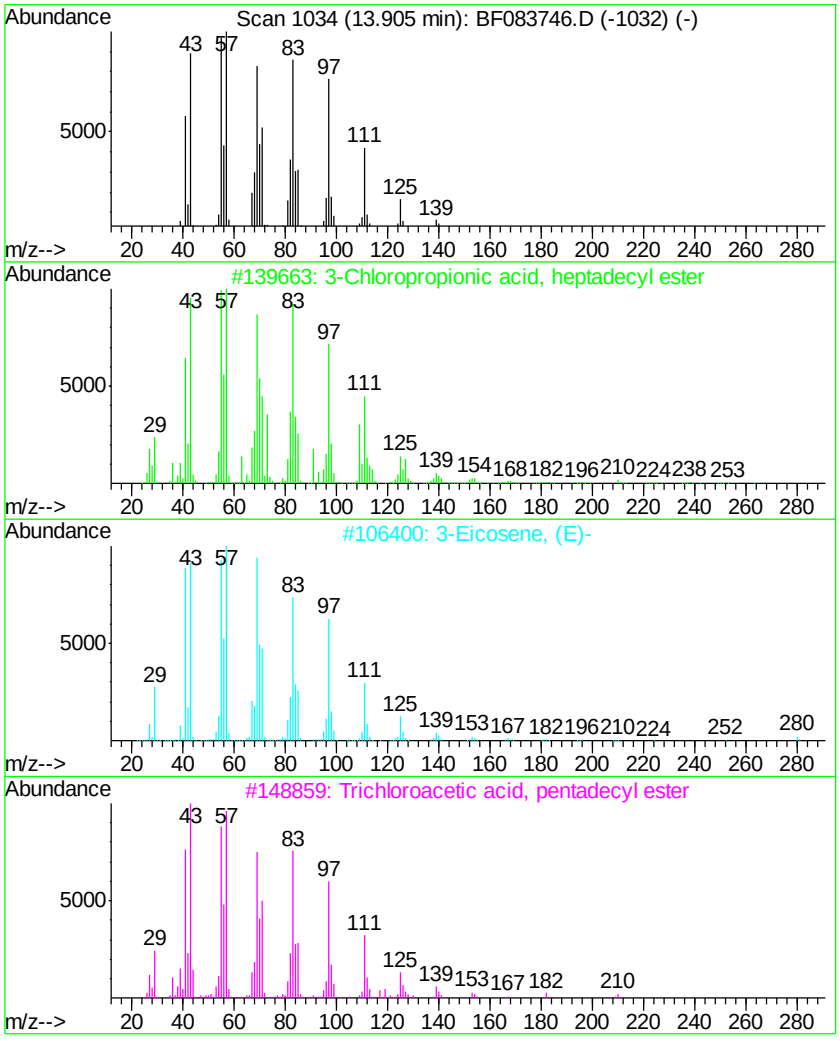
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

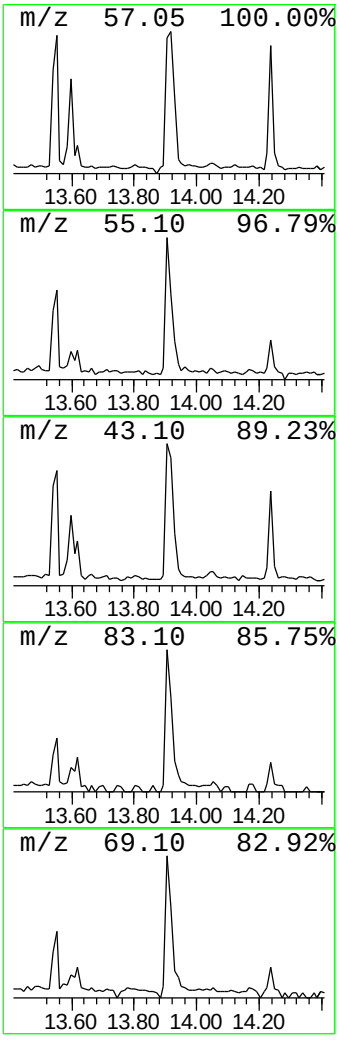
****

Peak Number 9 3-Chloropropionic acid, hep... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	4.39 ng	175539	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	1-Heptadecanol	256	C17H36O	001454-85-9	87
5	1-Tetracosanol	354	C24H50O	000506-51-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083746.D
Acq On : 13 Dec 2015 23:08
Operator : UM/IZ
Sample : G4743-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHWALL-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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, 1,1-dime...	2.21	4.9	ng	188315	1	6.92	762088	20.0
2-Pentanone, 4-hy...	5.12	29.3	ng	1118030	1	6.92	762088	20.0
unknown6.68	6.68	96.8	ng	3688640	1	6.92	762088	20.0
Hexadecane	10.87	2.3	ng	119440	4	11.44	1054230	20.0
Hexadecanoic acid...	12.84	5.4	ng	216069	5	14.05	800434	20.0
1-Docosene	12.92	2.4	ng	95722	5	14.05	800434	20.0
Octadecanoic acid...	13.55	3.4	ng	136435	5	14.05	800434	20.0
3-Chloropropionic...	13.91	4.4	ng	175539	5	14.05	800434	20.0