LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081464.D
Acq On : 5 Sep 2015 14:47
Operator : UM/IZ
Sample : G3526-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-16(0-0.16)

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-BF090115.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	4.399	243	246	257	rVB	458398	749002	59.88%	6.385%
2	4.902	288	290	302	rBV	1146381	1165150	93.14%	9.933%
3	6.022	386	388	395	rBV	1244017	1135312	90.76%	9.679%
4	6.125	395	397	399	rBV	1315633	1250939	100.00%	10.664%
5	6.353	415	417	420	rVB	459900	385840	30.84%	3.289%
6	6.513	429	431	433	rBV	852974	827860	66.18%	7.058%
7	6.936	465	468	470	rBV	687703	794878	63.54%	6.776%
8	7.645	528	530	532	rBV	584724	493498	39.45%	4.207%
9	8.730	622	625	627	rBV	1090349	1087693	86.95%	9.273%
10	9.131	658	660	663	rBV	286518	239676	19.16%	2.043%
11	9.382	680	682	685	rVB	552240	506692	40.50%	4.320%
12	10.171	748	751	753	rBV	669415	747843	59.78%	6.375%
13	10.319	762	764	767	rBB	11989	13395	1.07%	0.114%
14	10.845	808	810	813	rBV	501012	507402	40.56%	4.326%
15	11.428	859	861	867	rBV	45043	58241	4.66%	0.497%
16	12.297	934	937	938	rVB	33328	41599	3.33%	0.355%
17	12.365	938	943	946	rBV2	9710	13808	1.10%	0.118%
18	12.434	946	949	951	rBV	927754	838171	67.00%	7.145%
19	12.994	995	998	1000	rBV	33260	33330	2.66%	0.284%
20	13.360	1028	1030	1036	rBV	17513	42295	3.38%	0.361%
21	13.451	1036	1038	1041	rBV	353667	407730	32.59%	3.476%
22	13.680	1056	1058	1060	rBV	11619	12541	1.00%	0.107%
23	13.977	1082	1084	1092	rBV3	10701	25814	2.06%	0.220%
24	14.274	1106	1110	1112	rVB	10290	13675	1.09%	0.117%
25	14.331	1112	1115	1117	rBV	41726	39380	3.15%	0.336%
26	14.548	1132	1134	1139	rBV2	7959	13661	1.09%	0.116%
27	14.765	1151	1153	1155	rBV	254153	284632	22.75%	2.427%

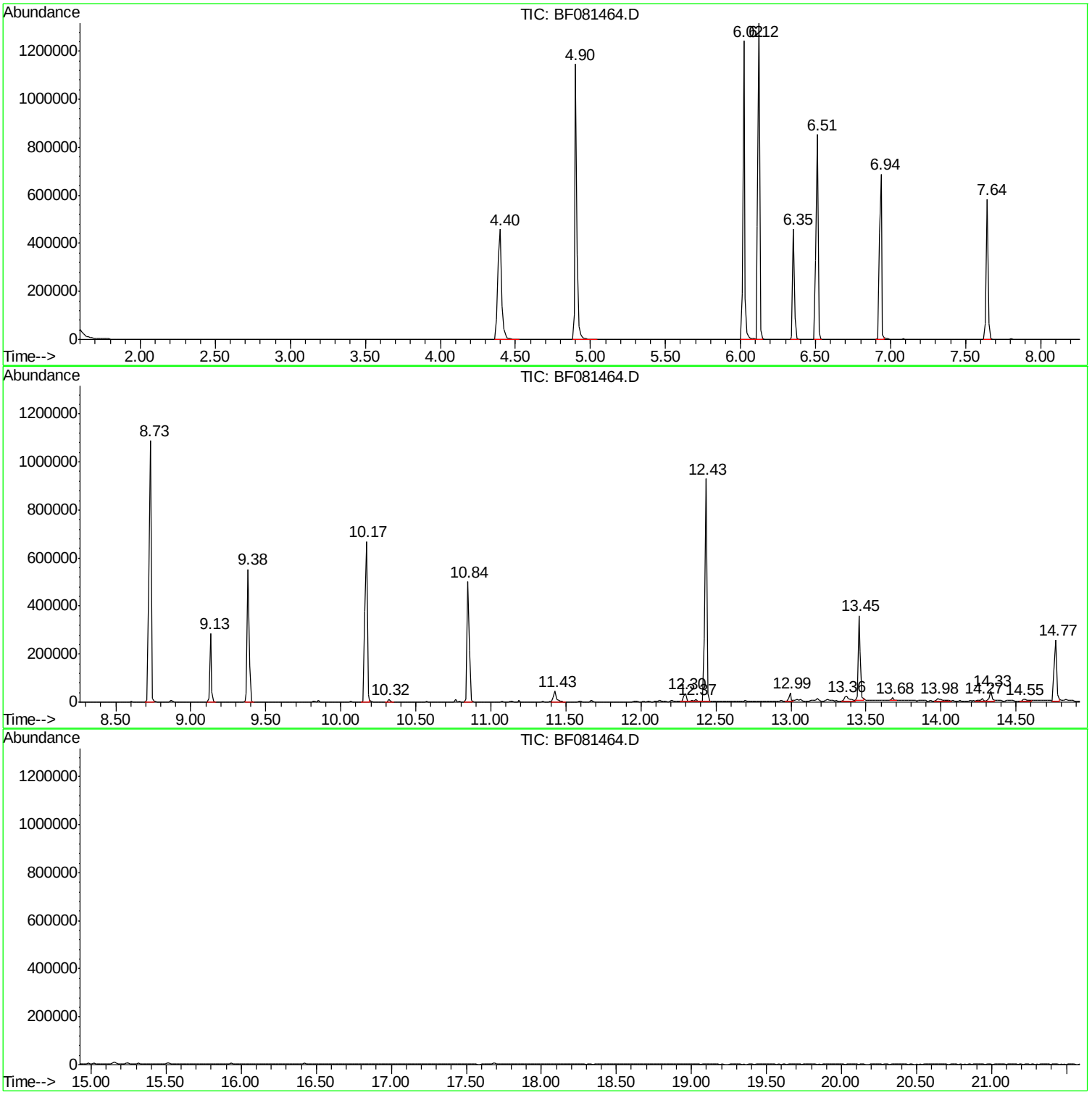
Sum of corrected areas: 11730057

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081464.D
Acq On : 5 Sep 2015 14:47
Operator : UM/IZ
Sample : G3526-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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\BF090415\
Data File : BF081464.D
Acq On : 5 Sep 2015 14:47
Operator : UM/IZ
Sample : G3526-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-16(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

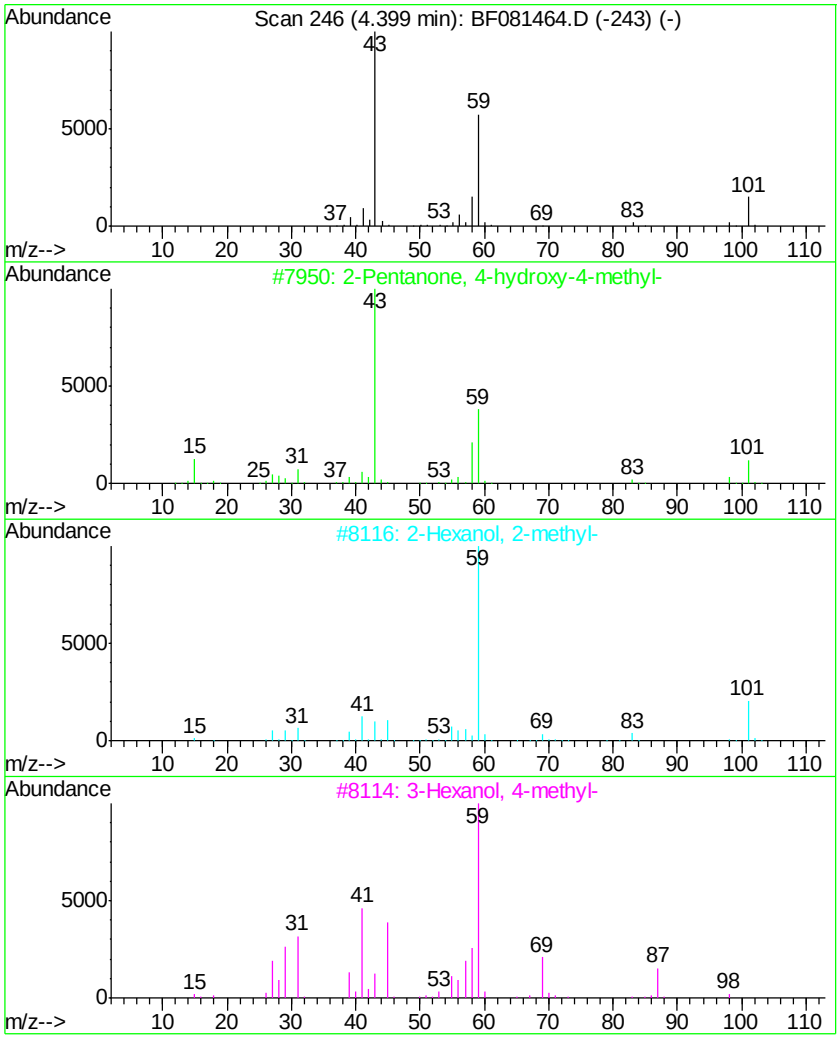
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

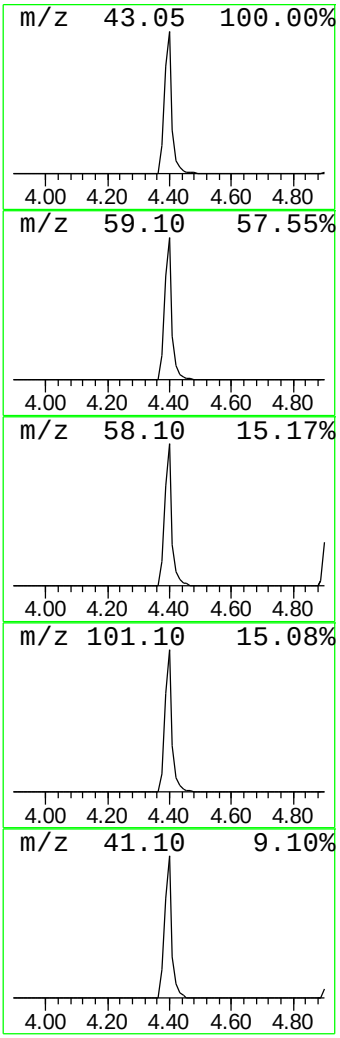
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	38.82 ng	749002	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081464.D
Acq On : 5 Sep 2015 14:47
Operator : UM/IZ
Sample : G3526-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-16(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

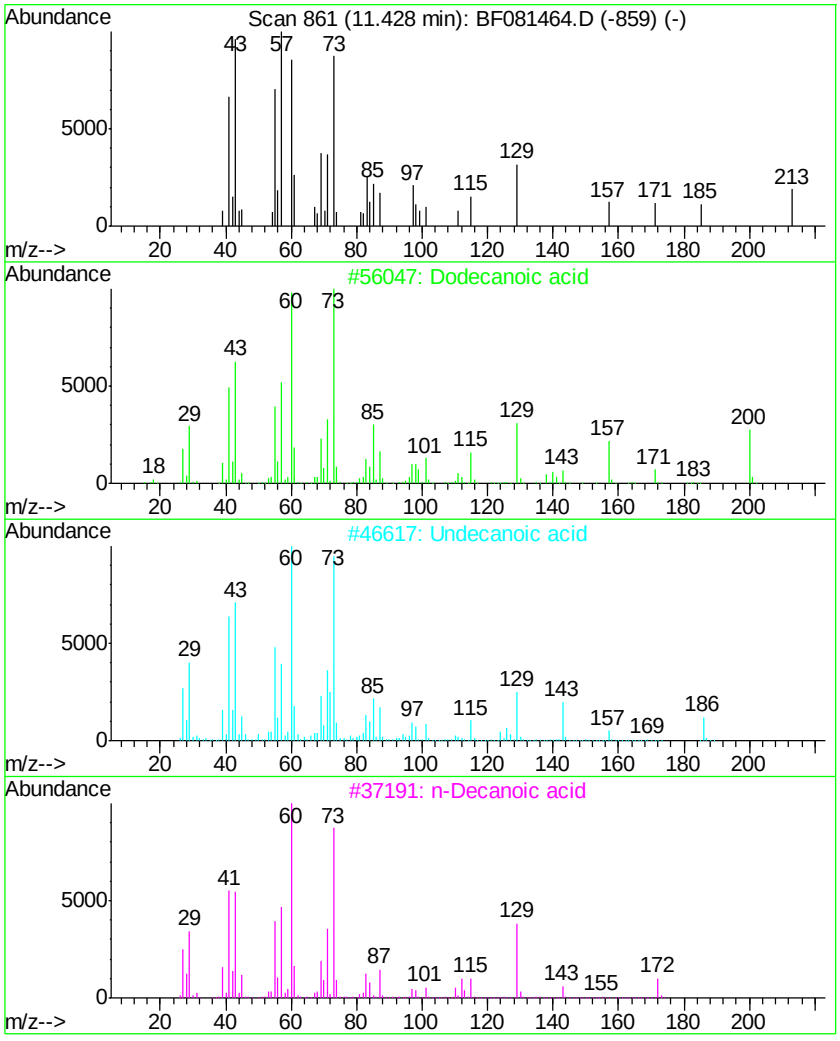
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

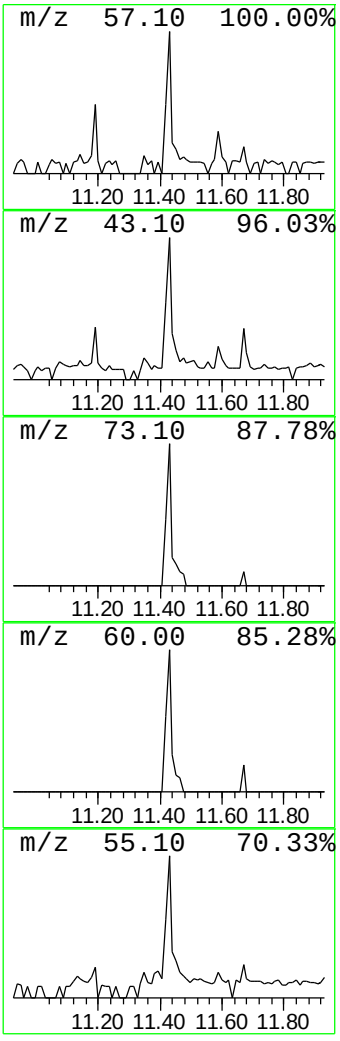
****

Peak Number 4 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	2.30 ng	58241	Phenanthrene-d10	10.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	59
2	Undecanoic acid	186	C11H22O2	000112-37-8	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	47
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081464.D
Acq On : 5 Sep 2015 14:47
Operator : UM/IZ
Sample : G3526-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-16(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

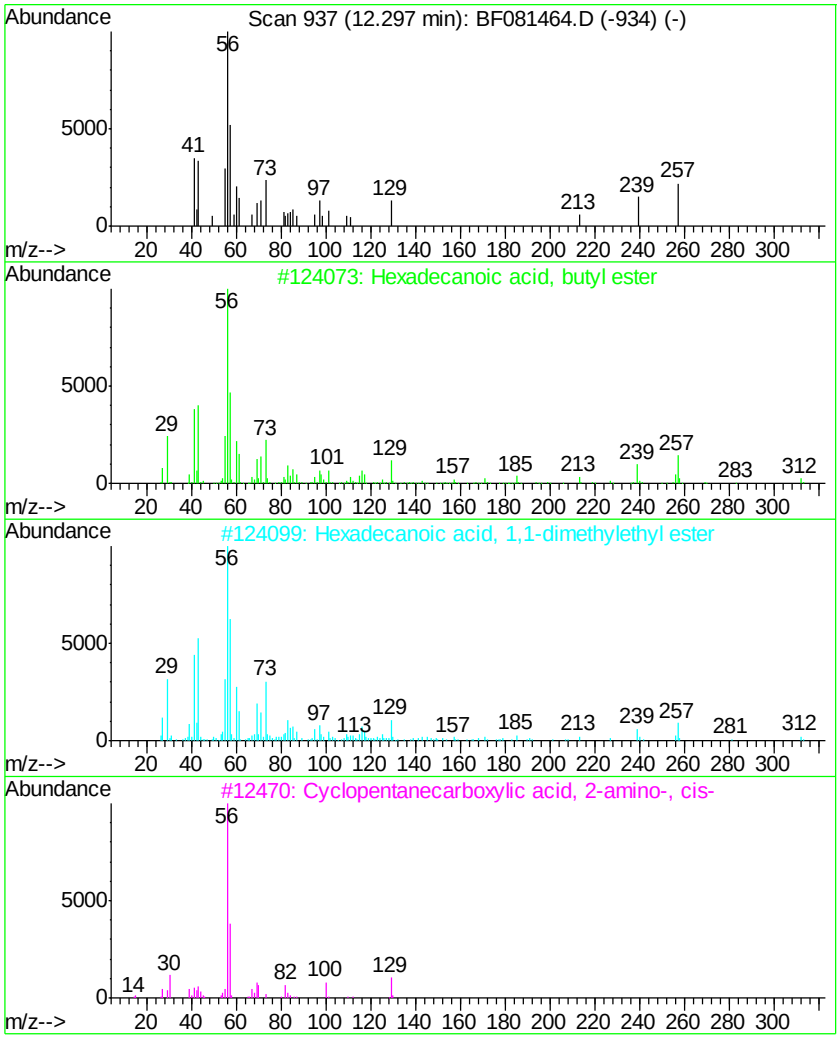
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

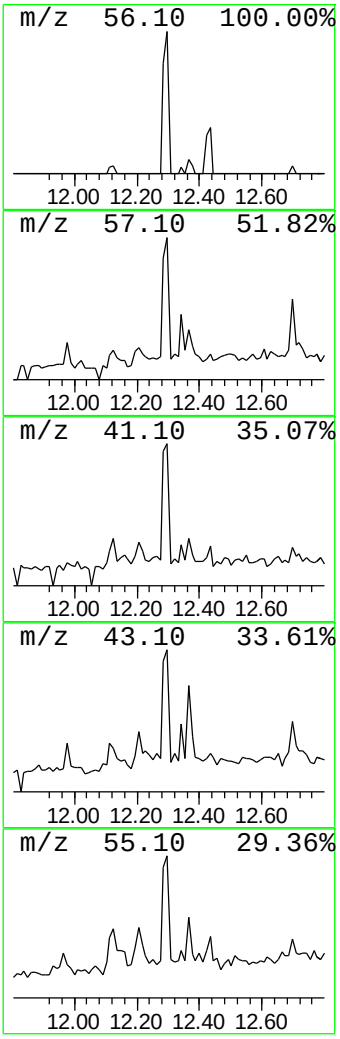
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.04 ng	41599	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	86
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	35
4	2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	35
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081464.D
Acq On : 5 Sep 2015 14:47
Operator : UM/IZ
Sample : G3526-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-16(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

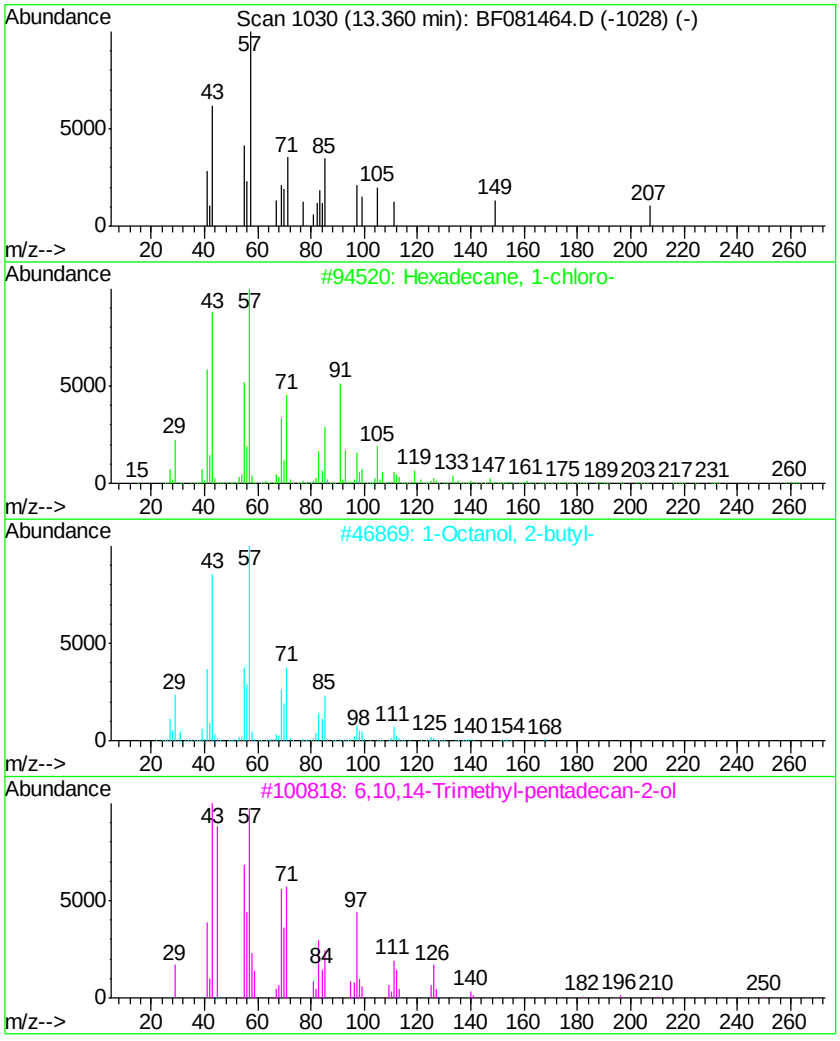
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

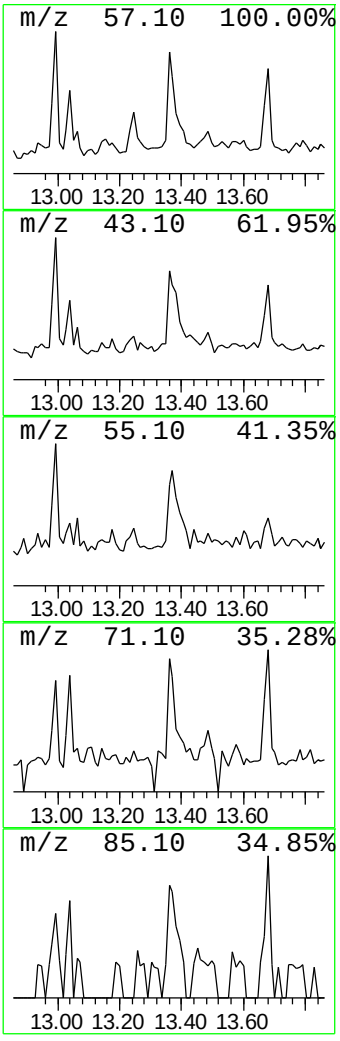
****

Peak Number 6 Hexadecane, 1-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	2.07 ng	42295	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	50
2	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	43
3	6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	1000143-49-8	43
4	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	43
5	Decane	142	C10H22	000124-18-5	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081464.D
Acq On : 5 Sep 2015 14:47
Operator : UM/IZ
Sample : G3526-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-16(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

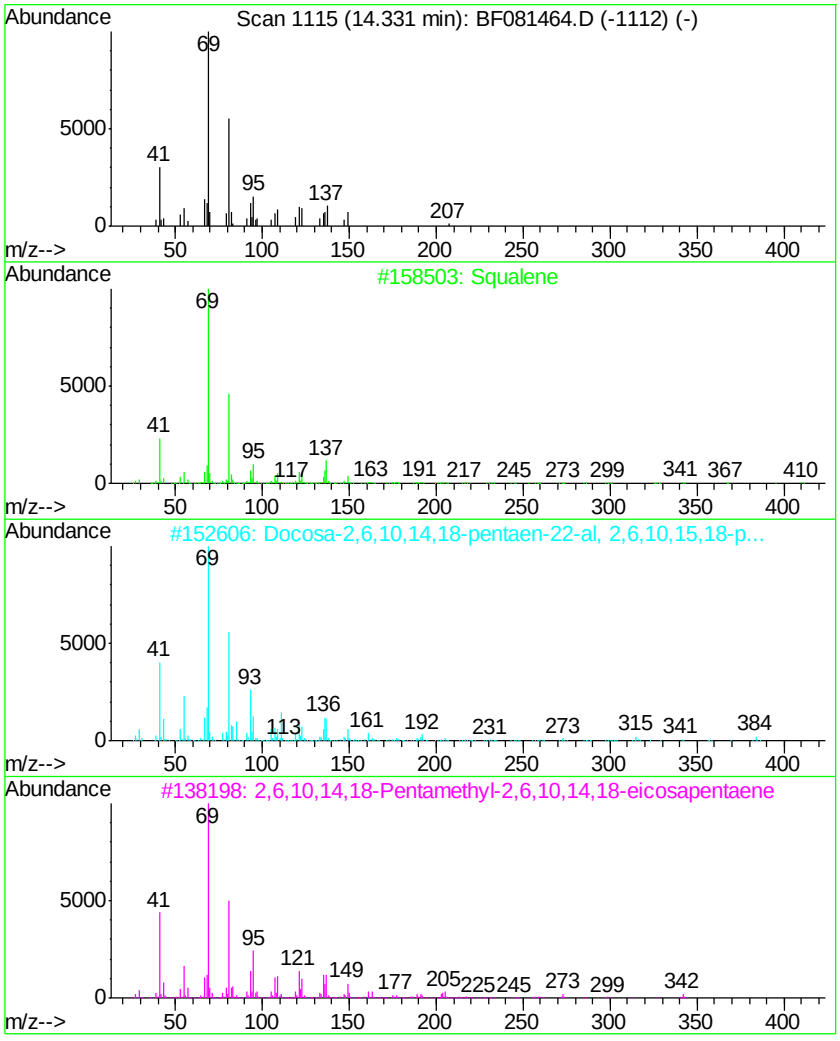
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

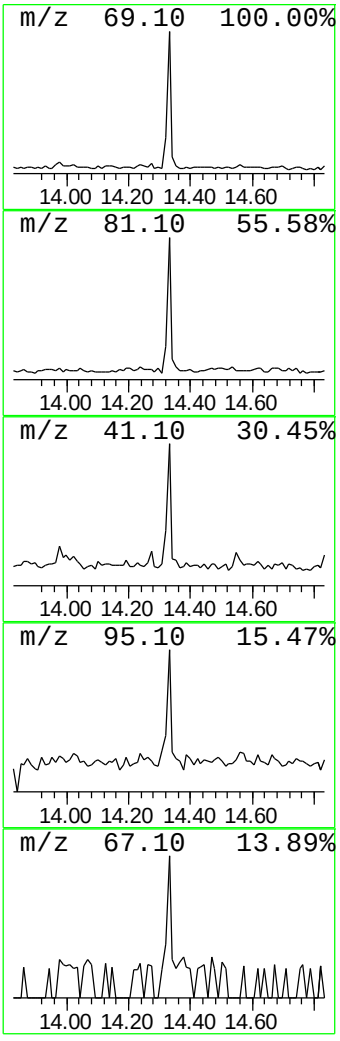
****

Peak Number 7 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	2.77 ng	39380	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	86
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	86
4	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	78
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081464.D
Acq On : 5 Sep 2015 14:47
Operator : UM/IZ
Sample : G3526-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-16(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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
2-Pentanone, 4-hy...	4.40	38.8	ng	749002	1	6.35	385840	20.0
Dodecanoic acid	11.43	2.3	ng	58241	4	10.85	507402	20.0
Hexadecanoic acid...	12.30	2.0	ng	41599	5	13.45	407730	20.0
Hexadecane, 1-chl...	13.36	2.1	ng	42295	5	13.45	407730	20.0
Squalene	14.33	2.8	ng	39380	6	14.77	284632	20.0