LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021016\
Data File : BF084999.D
Acq On : 10 Feb 2016 18:08
Operator : SJ/IZ
Sample : H1386-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B018(10-12)

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-BF020116.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	1.632	3	4	8	rBV	279737	376903	8.33%	0.890%
2	1.701	8	10	12	rVV	150837	203494	4.50%	0.480%
3	1.747	12	14	50	rVB	1547531	3428372	75.80%	8.094%
4	4.764	275	278	291	rVB	716637	1191571	26.35%	2.813%
5	5.210	315	317	320	rBV	3328098	3788309	83.76%	8.943%
6	6.284	408	411	413	rBV	3834093	4522764	100.00%	10.677%
7	6.399	418	421	423	rBV	3033609	4169061	92.18%	9.842%
8	6.616	438	440	443	rBV	662793	865142	19.13%	2.042%
9	6.776	452	454	457	rBV	2889192	2874564	63.56%	6.786%
10	7.199	488	491	493	rBV	2505648	2853772	63.10%	6.737%
11	7.313	499	501	508	rVB	34289	47938	1.06%	0.113%
12	7.907	551	553	556	rBV	1169556	1138038	25.16%	2.687%
13	8.993	645	648	650	rBV	4569782	4204899	92.97%	9.927%
14	9.085	653	656	658	rVV	53640	54712	1.21%	0.129%
15	9.393	681	683	685	rBV	886745	788640	17.44%	1.862%
16	9.610	700	702	704	rBV	211383	172825	3.82%	0.408%
17	9.656	704	706	708	rBV2	1030784	1131919	25.03%	2.672%
18	9.862	718	724	726	rBV2	41493	96517	2.13%	0.228%
19	10.102	743	745	747	rVB	144395	198955	4.40%	0.470%
20	10.319	761	764	766	rBV	57604	97696	2.16%	0.231%
21	10.445	773	775	778	rBV	2154382	2189943	48.42%	5.170%
22	10.582	785	787	791	rBV	176038	238625	5.28%	0.563%
23	10.776	802	804	808	rVB2	23613	49010	1.08%	0.116%
24	11.028	824	826	827	rBV	93088	85955	1.90%	0.203%
25	11.142	833	836	839	rVV	736542	1208460	26.72%	2.853%
26	11.211	839	842	844	rVB	50441	59400	1.31%	0.140%
27	12.342	939	941	943	rBV	267584	220445	4.87%	0.520%
28	12.559	958	960	963	rBV2	323695	433309	9.58%	1.023%
29	12.719	972	974	977	rVB	2094222	2829699	62.57%	6.680%
30	13.268	1020	1022	1023	rBV	165824	154047	3.41%	0.364%
31	13.314	1023	1026	1030	rVB2	25377	58589	1.30%	0.138%
32	13.634	1051	1054	1057	rBV	173879	262627	5.81%	0.620%
33	13.759	1063	1065	1067	rBV	710901	926848	20.49%	2.188%
34	13.954	1080	1082	1085	rBV2	42559	54784	1.21%	0.129%

LSC Area Percent Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B018(10-12)

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-BF020116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.262	1104	1109	1111	rBV2	49725	119052	2.63%	0.281%
36	14.559	1130	1135	1137	rBV3	38321	110592	2.45%	0.261%
37	14.754	1150	1152	1157	rBV	54435	113306	2.51%	0.267%
38	14.845	1158	1160	1162	rVV2	40571	47657	1.05%	0.113%
39	15.017	1173	1175	1178	rBV	43663	52755	1.17%	0.125%
40	15.074	1178	1180	1182	rVV	55283	62817	1.39%	0.148%
41	15.131	1182	1185	1187	rVV	557811	764369	16.90%	1.804%
42	15.165	1187	1188	1191	rVB	39445	54628	1.21%	0.129%
43	15.542	1219	1221	1223	rBV	35124	56324	1.25%	0.133%

Sum of corrected areas: 42359332

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Instrument :
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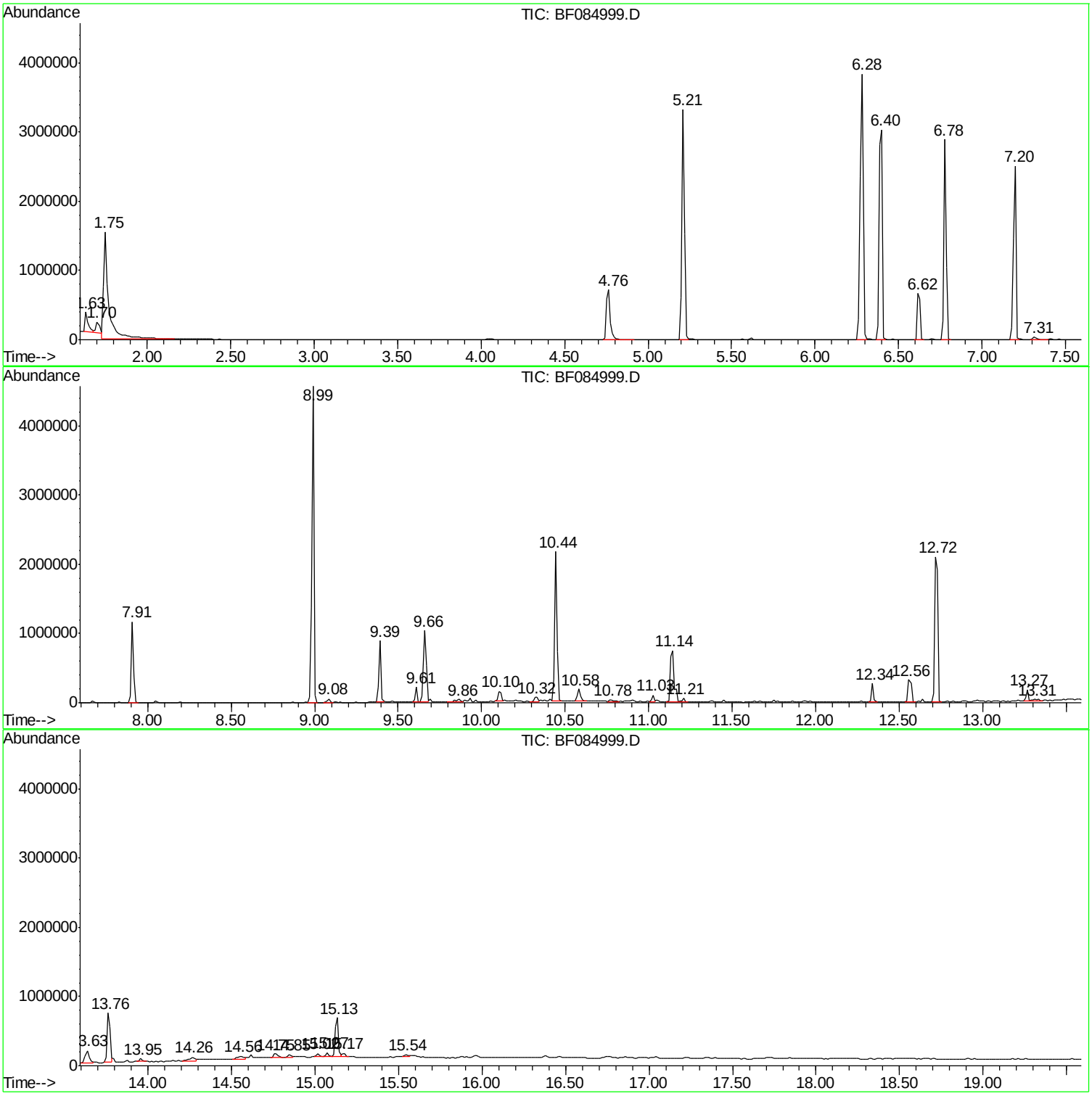
ClientSampleId :
S4-B018(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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

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Operator : SJ/IZ
Sample : H1386-05
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Instrument :
BNA_F
ClientSampleId :
S4-B018(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

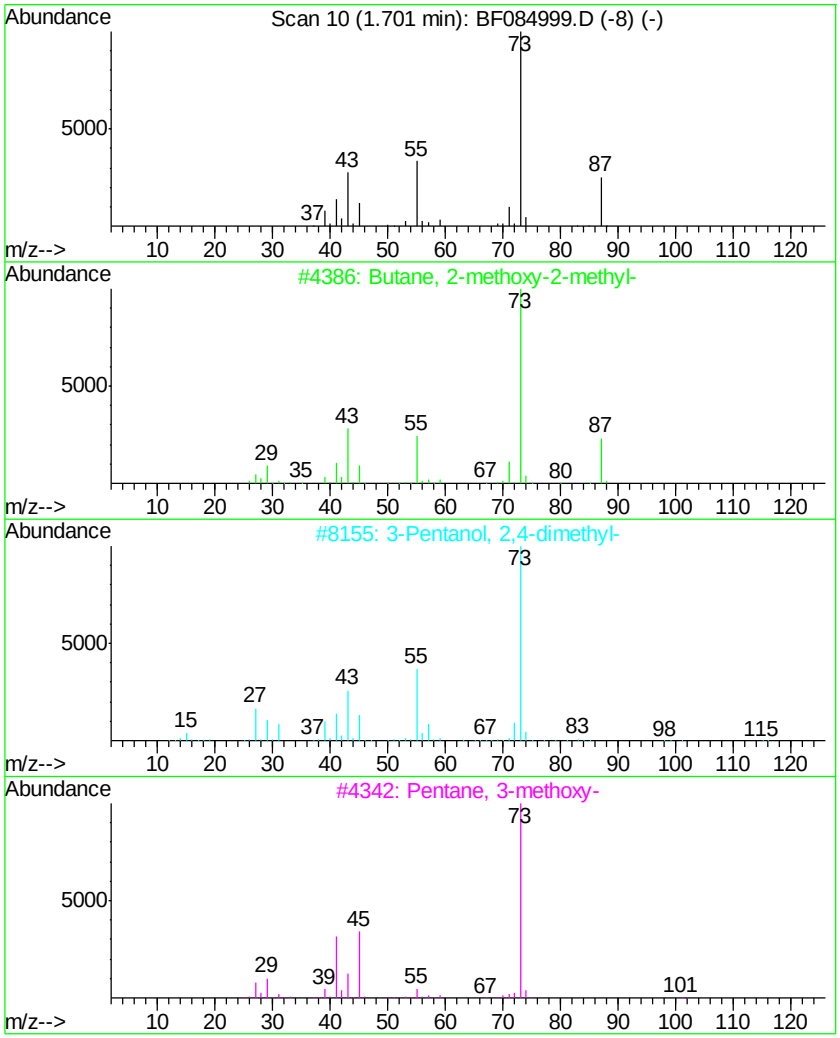
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

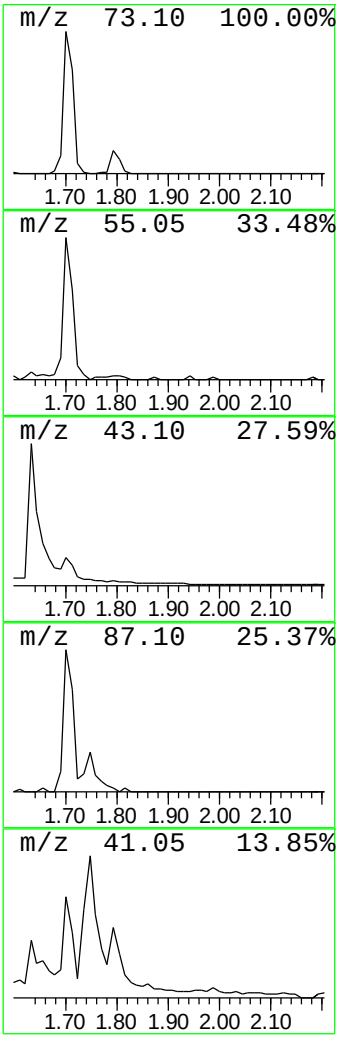
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.70	4.70 ng	203494	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16





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Sample : H1386-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B018(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

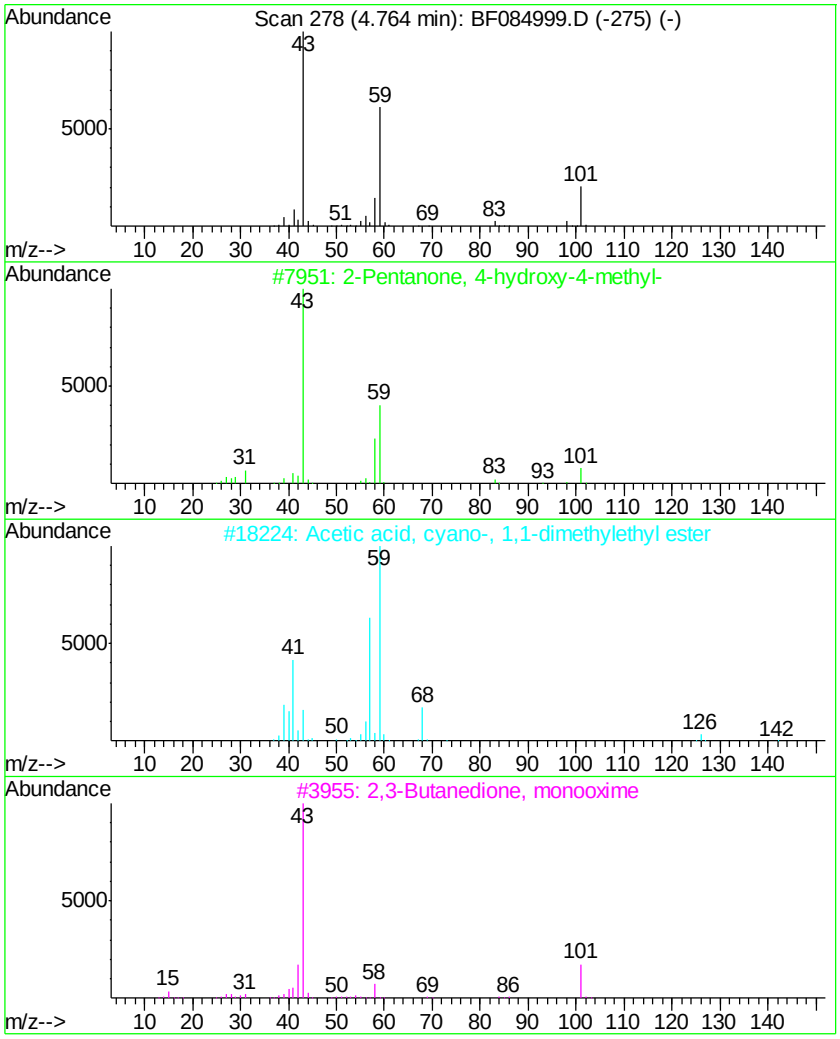
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

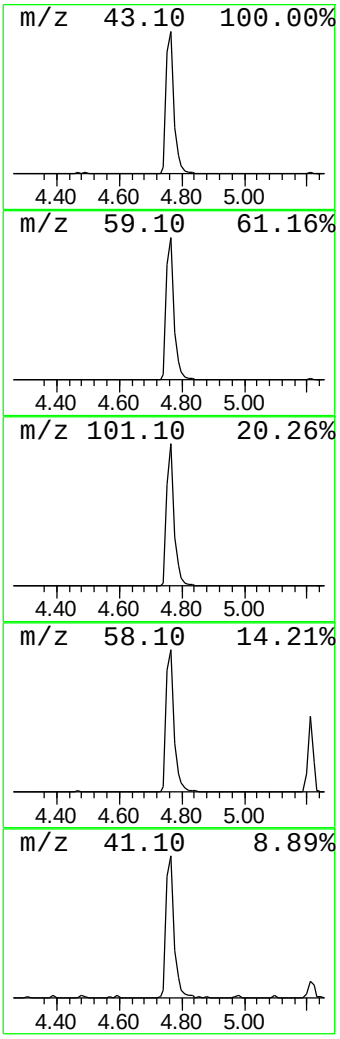
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	27.55 ng	1191570	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Library Search Compound Report

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Sample : H1386-05
Misc :
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Instrument :
BNA_F
ClientSampleId :
S4-B018(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

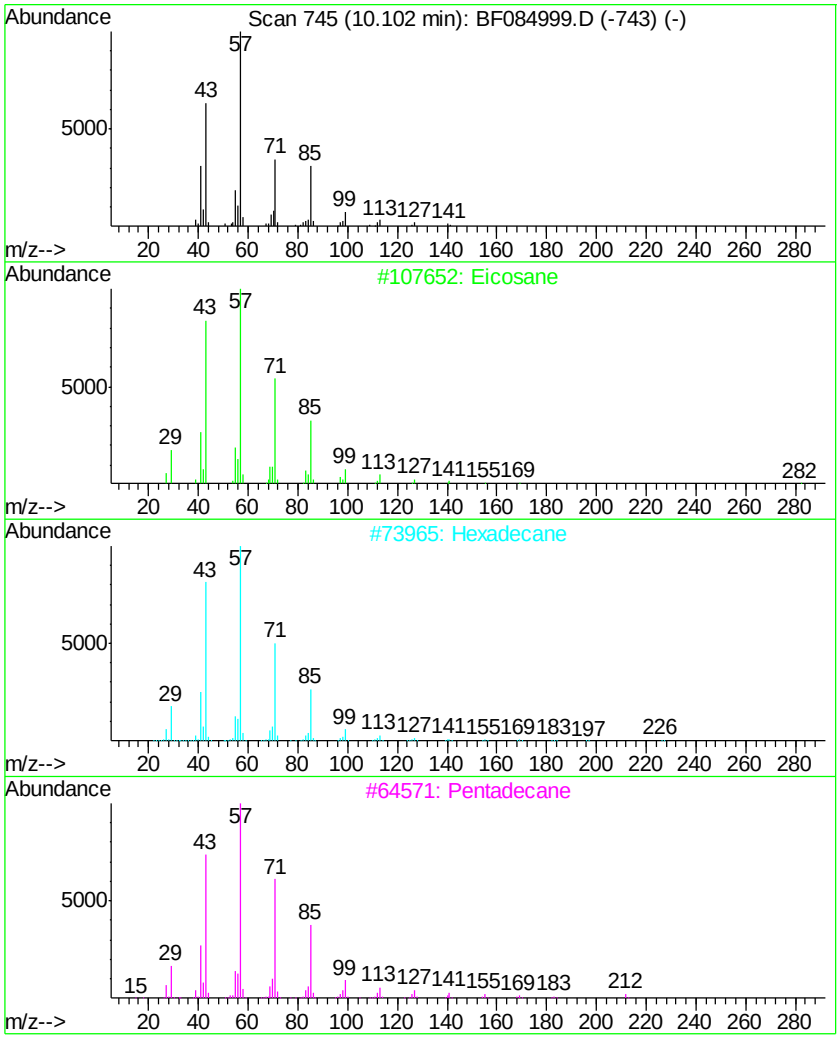
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

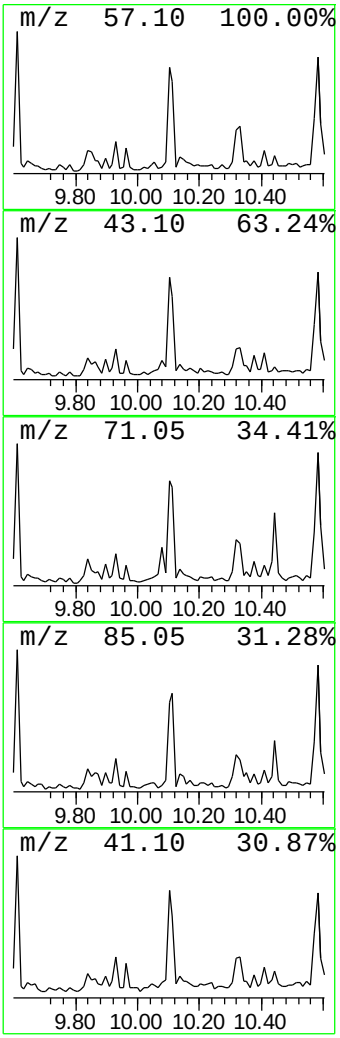
****

Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	3.52 ng	198955	Acenaphthene-d10	9.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	72
2	Hexadecane	226	C16H34	000544-76-3	72
3	Pentadecane	212	C15H32	000629-62-9	72
4	Octadecane	254	C18H38	000593-45-3	72
5	Tetradecane	198	C14H30	000629-59-4	64





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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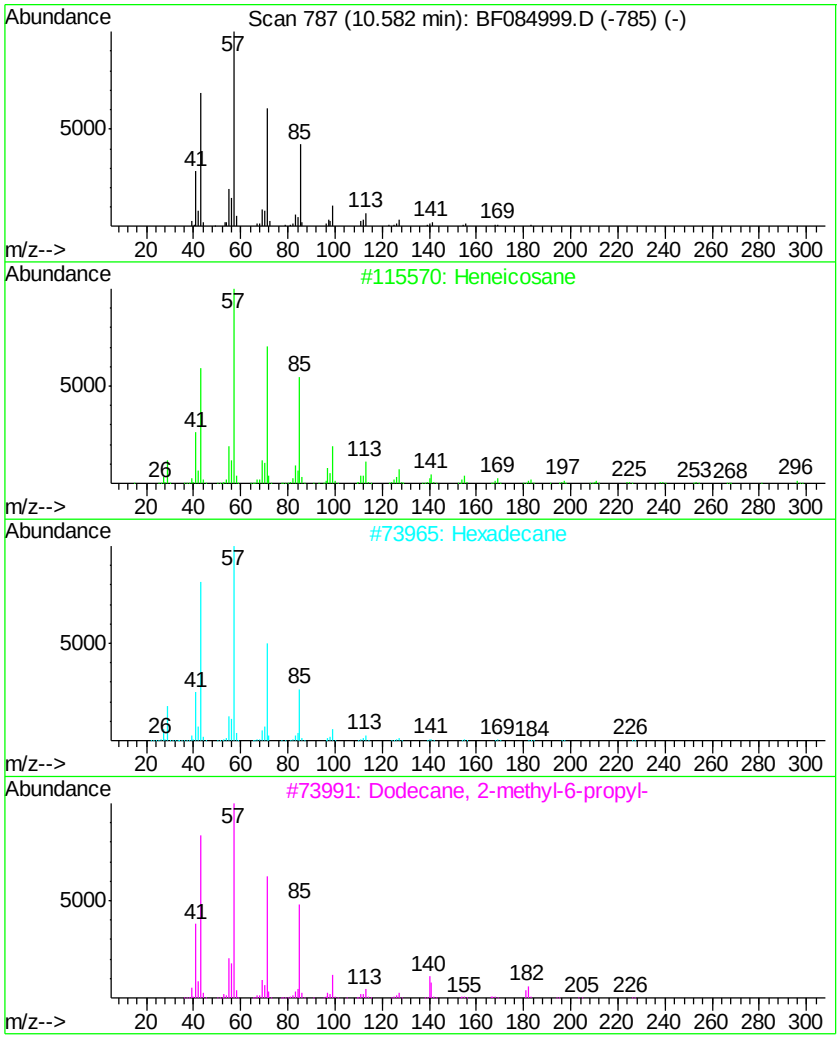
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

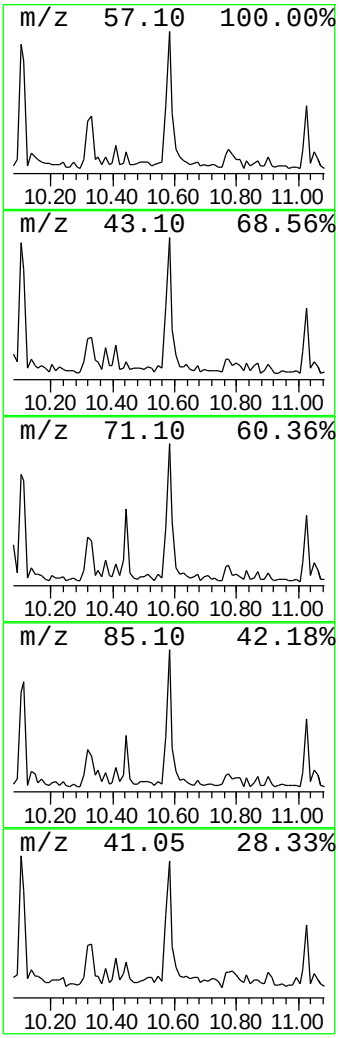
****

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	3.95 ng	238625	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	86
5	Eicosane	282	C20H42	000112-95-8	83





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ClientSampleId :
S4-B018(10-12)

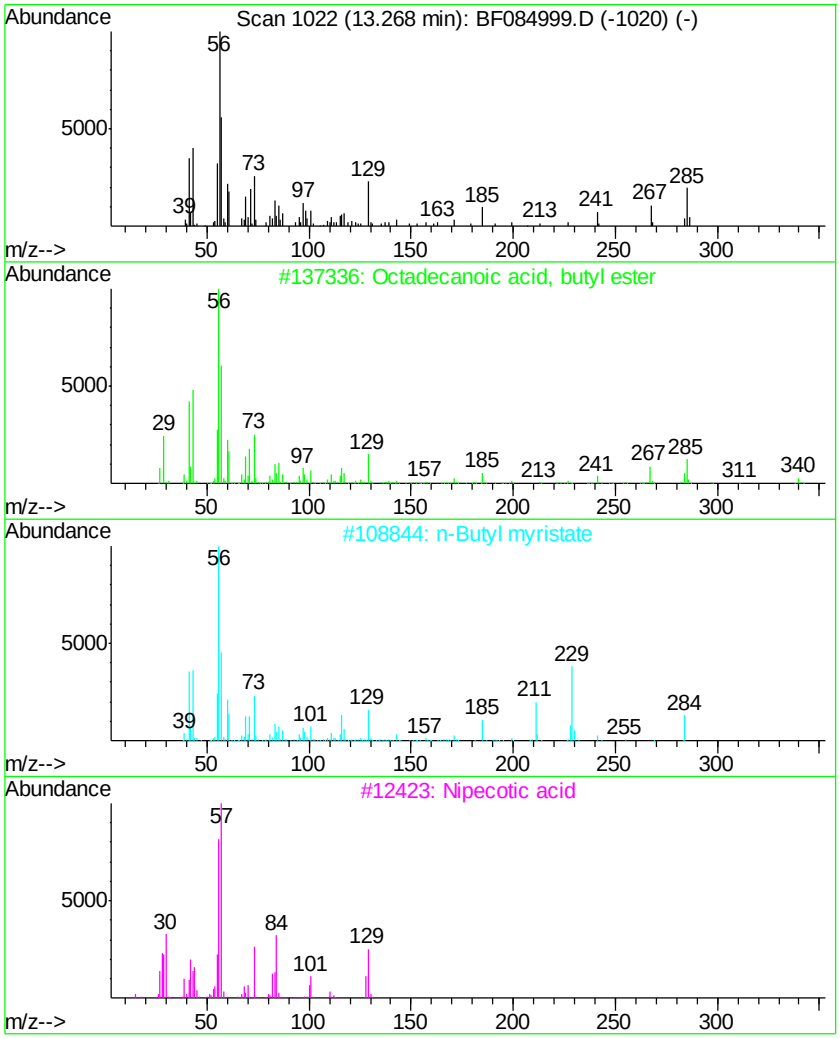
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

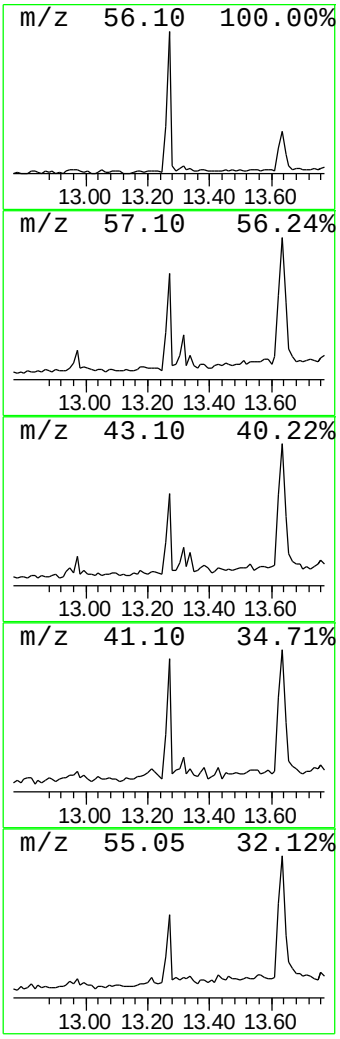
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	3.32 ng	154047	Chrysene-d12	13.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	83
2	n-Butyl myristate	284	C18H36O2	000110-36-1	59
3	Nipecotic acid	129	C6H11NO2	000498-95-3	38
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	35
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35





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S4-B018(10-12)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

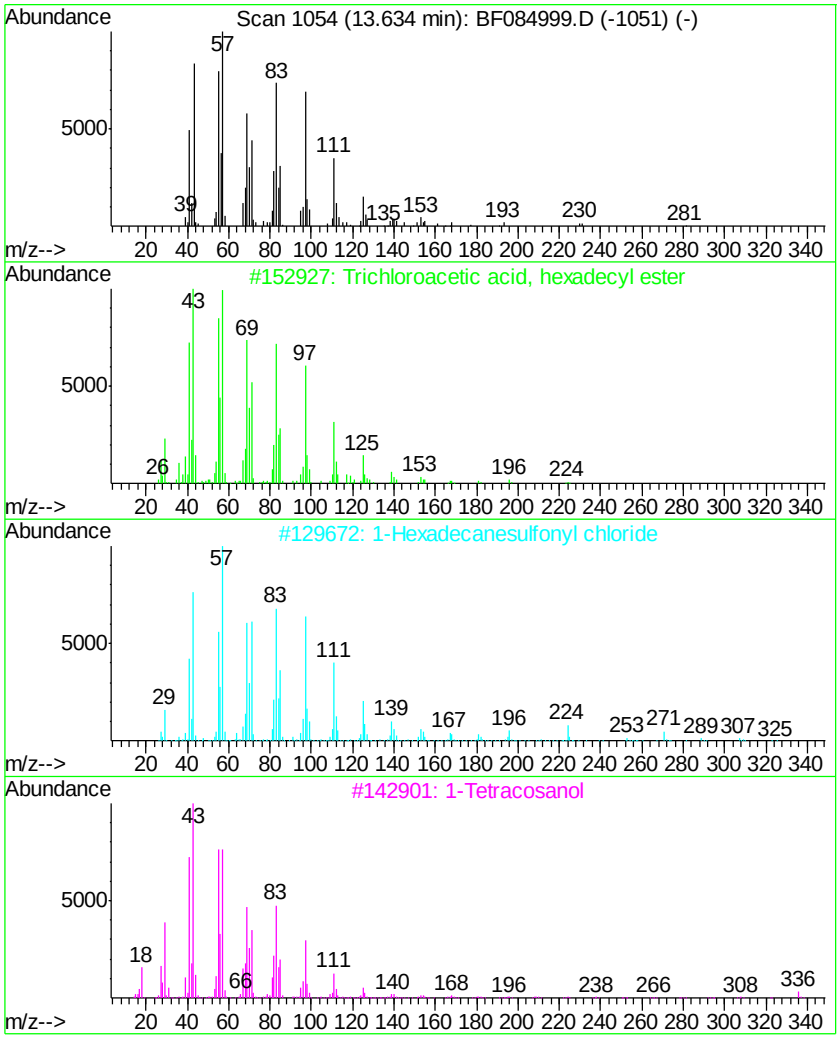
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

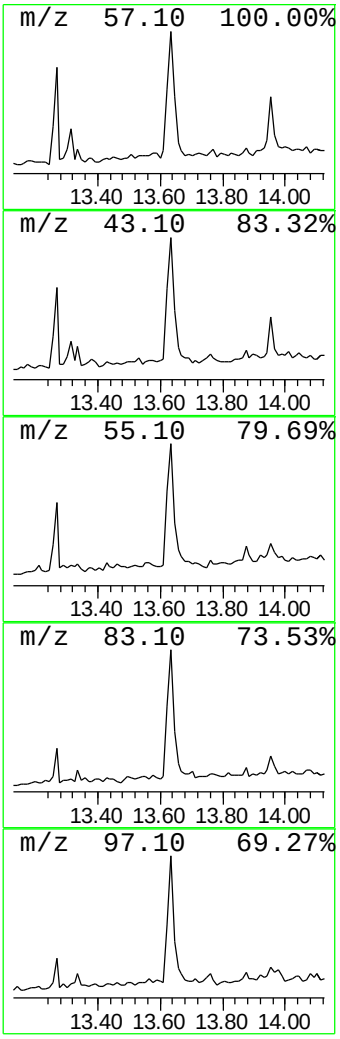
****

Peak Number 10 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	5.67 ng	262627	Chrysene-d12	13.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
3	1-Tetracosanol	354	C24H50O	000506-51-4	90
4	1-Octadecanol	270	C18H38O	000112-92-5	87
5	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	83





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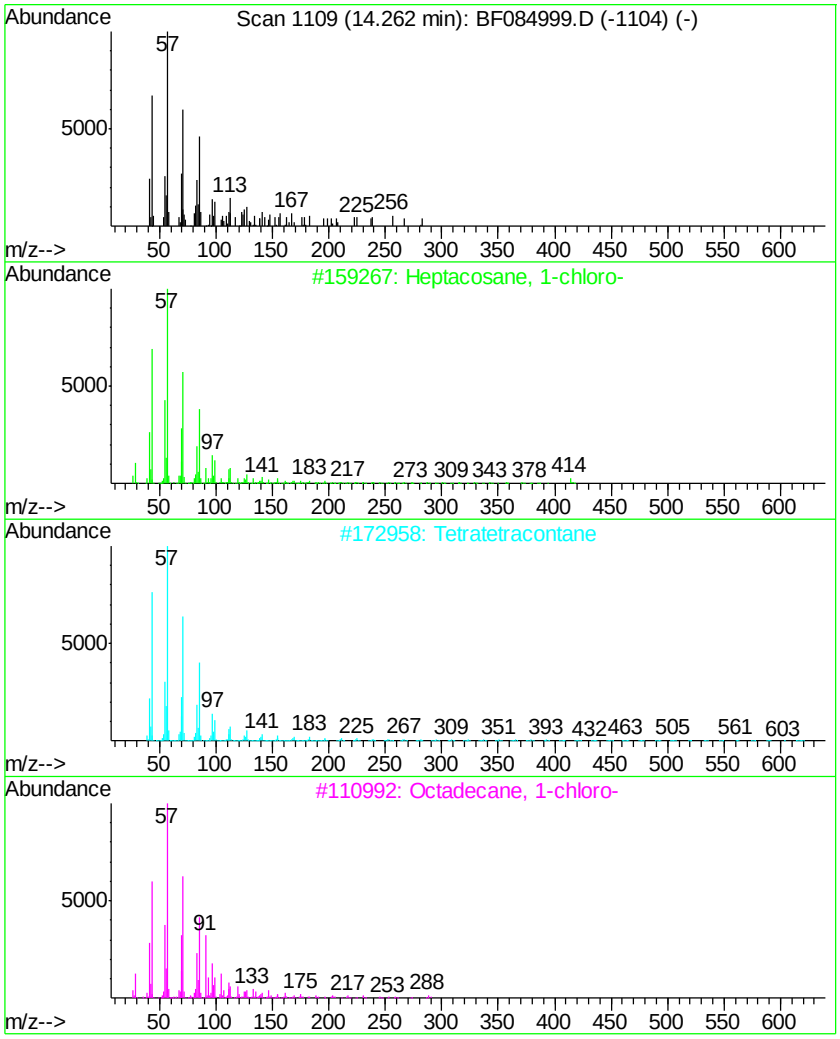
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

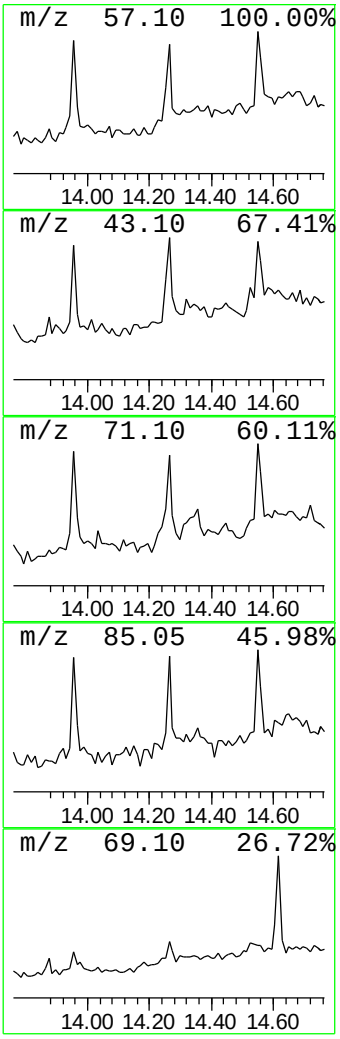
****

Peak Number 11 Heptacosane, 1-chloro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	2.57 ng	119052	Chrysene-d12	13.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	86
4	Tritetracontane	605	C43H88	007098-21-7	86
5	Hexacosane	366	C26H54	000630-01-3	83





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Instrument :
BNA_F
ClientSampleId :
S4-B018(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

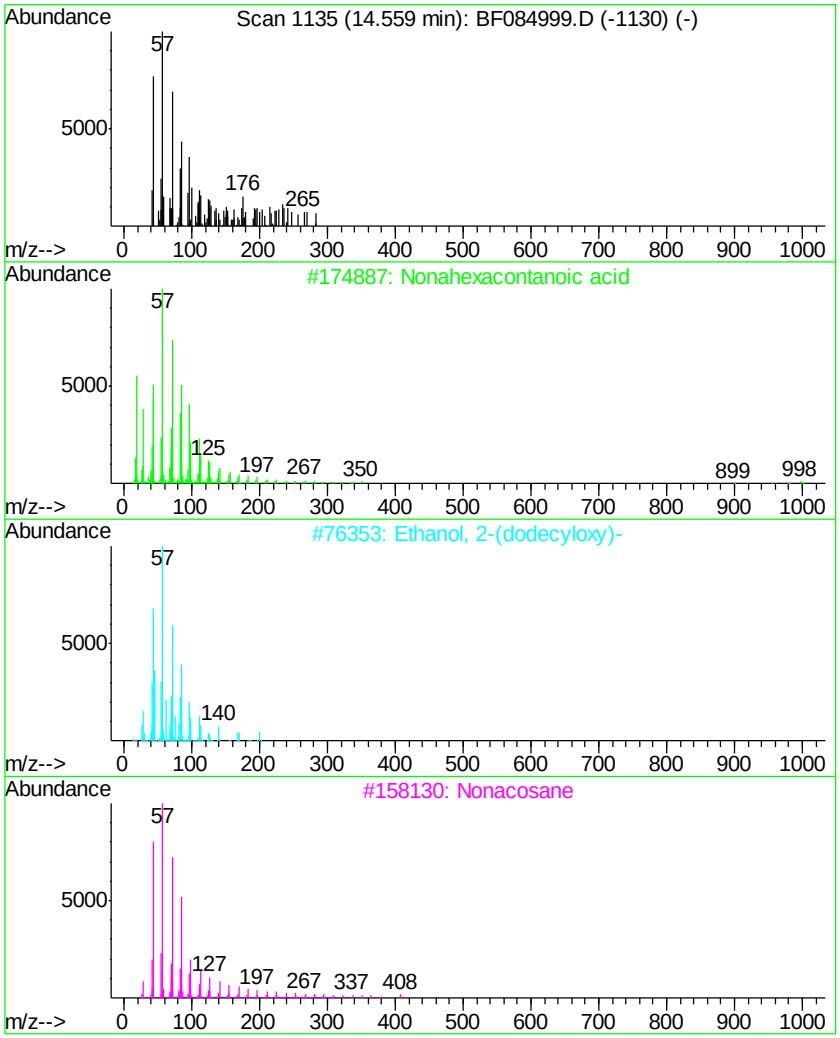
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

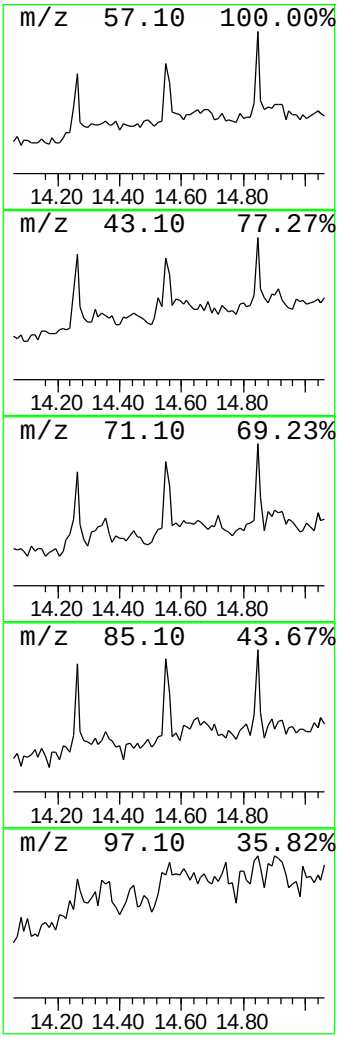
****

Peak Number 12 Nonahexacontanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.89 ng	110592	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	58
2	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	53
3	Nonacosane	408	C29H60	000630-03-5	47
4	Triacontane	422	C30H62	000638-68-6	47
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021016\
Data File : BF084999.D
Acq On : 10 Feb 2016 18:08
Operator : SJ/IZ
Sample : H1386-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B018(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-methoxy...	1.70	4.7	ng	203494	1	6.63	865142	20.0
2-Pentanone, 4-hy...	4.76	27.6	ng	1191570	1	6.63	865142	20.0
Eicosane	10.10	3.5	ng	198955	3	9.66	1131920	20.0
Heneicosane	10.58	4.0	ng	238625	4	11.14	1208460	20.0
Octadecanoic acid...	13.27	3.3	ng	154047	5	13.76	926848	20.0
Trichloroacetic a...	13.63	5.7	ng	262627	5	13.76	926848	20.0
Heptacosane, 1-ch...	14.26	2.6	ng	119052	5	13.76	926848	20.0
Nonahexacontanoic...	14.56	2.9	ng	110592	6	15.13	764369	20.0