LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083167.D
Acq On : 22 Nov 2015 19:13
Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 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-BF112115.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	4.810	244	247	262	rVB	2216680	3588246	53.91%	5.836%
2	5.256	284	286	289	rBV	4283204	5987764	89.97%	9.739%
3	6.319	376	379	381	rBV	5851760	6655380	100.00%	10.825%
4	6.422	386	388	391	rBV	5365309	5836181	87.69%	9.493%
5	6.650	406	408	410	rBV	1241075	1183231	17.78%	1.925%
6	6.810	419	422	424	rBV	3952063	4781832	71.85%	7.778%
7	7.222	455	458	460	rBV	3940466	4195682	63.04%	6.825%
8	7.942	518	521	523	rBV	1121898	1504743	22.61%	2.448%
9	9.016	612	615	618	rBV	5808295	6367748	95.68%	10.358%
10	9.107	621	623	626	rVB	75581	73018	1.10%	0.119%
11	9.416	648	650	655	rBV	1238126	1164714	17.50%	1.894%
12	9.633	667	669	671	rBV	228790	214745	3.23%	0.349%
13	9.679	671	673	676	rBV	1313663	1713330	25.74%	2.787%
14	10.136	709	713	714	rBV	277814	273880	4.12%	0.445%
15	10.353	729	732	735	rBV	92863	149512	2.25%	0.243%
16	10.468	740	742	745	rBV2	2743222	4046865	60.81%	6.582%
17	10.605	751	754	761	rVB	275478	352773	5.30%	0.574%
18	11.051	789	793	794	rBV	133468	138132	2.08%	0.225%
19	11.165	800	803	805	rBV	1259127	1722747	25.89%	2.802%
20	11.222	805	808	813	rVB2	40798	97419	1.46%	0.158%
21	11.713	849	851	855	rBV	473107	466904	7.02%	0.759%
22	12.399	907	911	917	rBV4	30910	88333	1.33%	0.144%
23	12.491	917	919	925	rBV	460826	555244	8.34%	0.903%
24	12.582	925	927	930	rVB	173044	169907	2.55%	0.276%
25	12.662	930	934	936	rVB2	66716	73661	1.11%	0.120%
26	12.754	939	942	944	rBV	4698638	6541685	98.29%	10.640%
27	13.291	987	989	990	rBV	89899	102406	1.54%	0.167%
28	13.657	1018	1021	1028	rBV	222672	294907	4.43%	0.480%
29	13.782	1030	1032	1035	rBV	1776619	1625164	24.42%	2.643%
30	14.274	1073	1075	1078	rBV	42363	78020	1.17%	0.127%
31	14.571	1097	1101	1103	rBV2	53228	72225	1.09%	0.117%
32	15.142	1149	1151	1154	rBV	825341	1217087	18.29%	1.980%
33	15.565	1186	1188	1191	rBV	38432	67080	1.01%	0.109%
34	16.000	1222	1226	1233	rBV4	31385	78985	1.19%	0.128%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083167.D
Acq On : 22 Nov 2015 19:13
Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 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-BF112115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

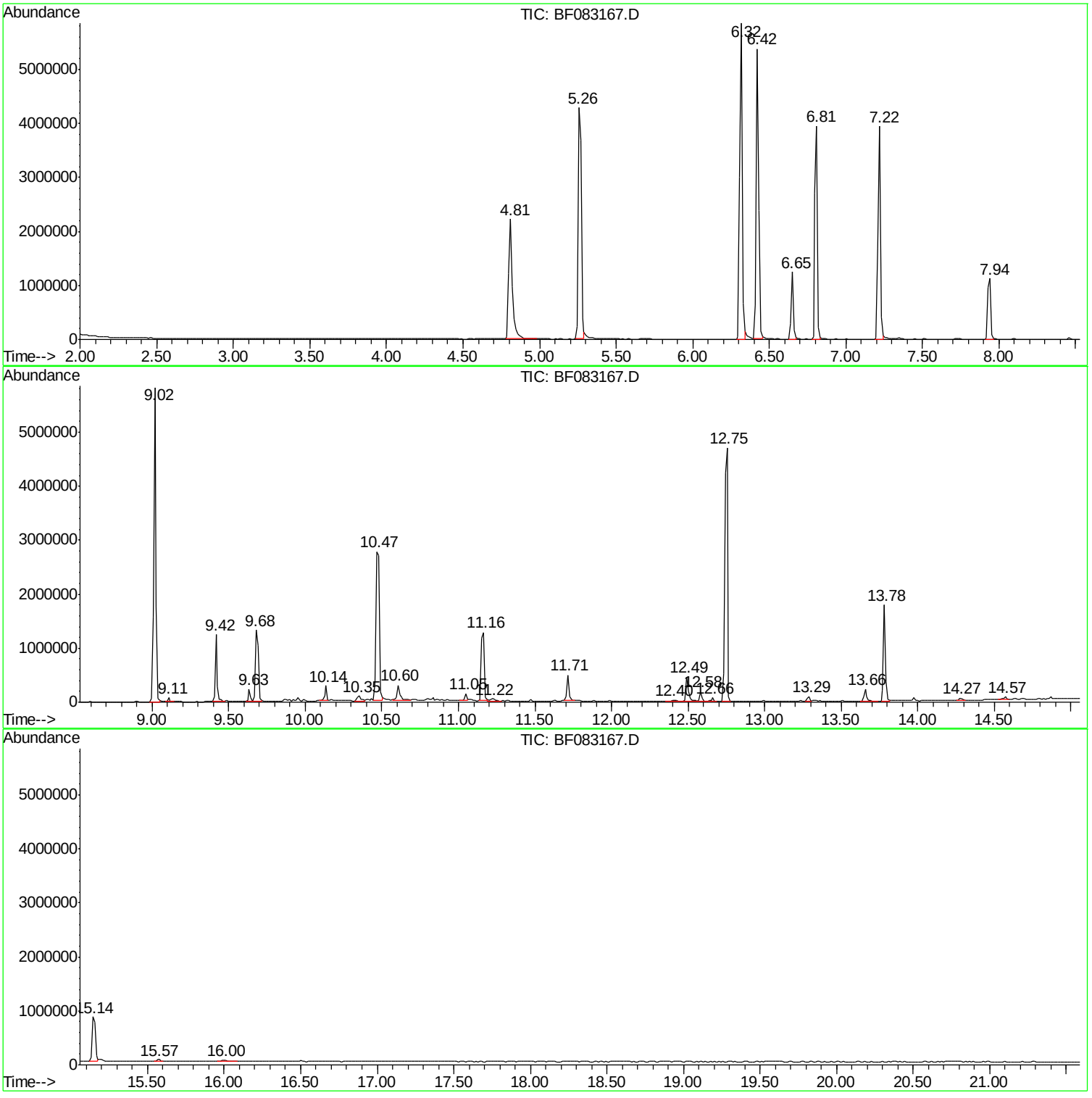
Sum of corrected areas: 61479550

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083167.D
Acq On : 22 Nov 2015 19:13
Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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\BF112215\
Data File : BF083167.D
Acq On : 22 Nov 2015 19:13
Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

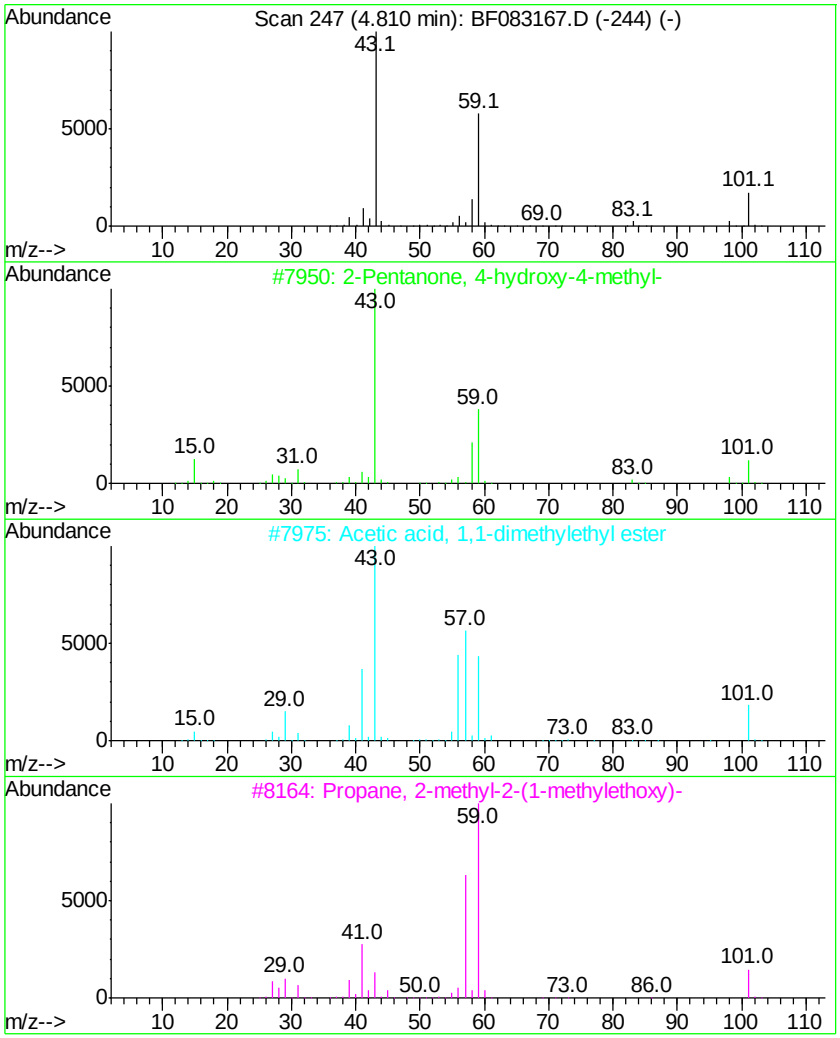
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

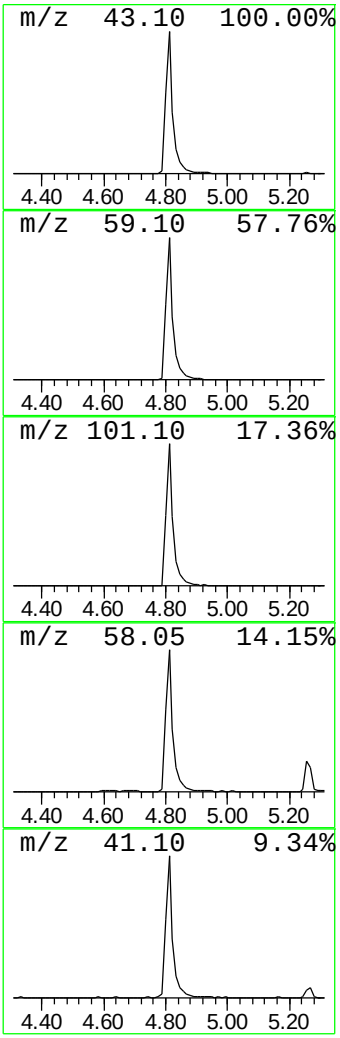
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	60.65 ng	3588250	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083167.D
Acq On : 22 Nov 2015 19:13
Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

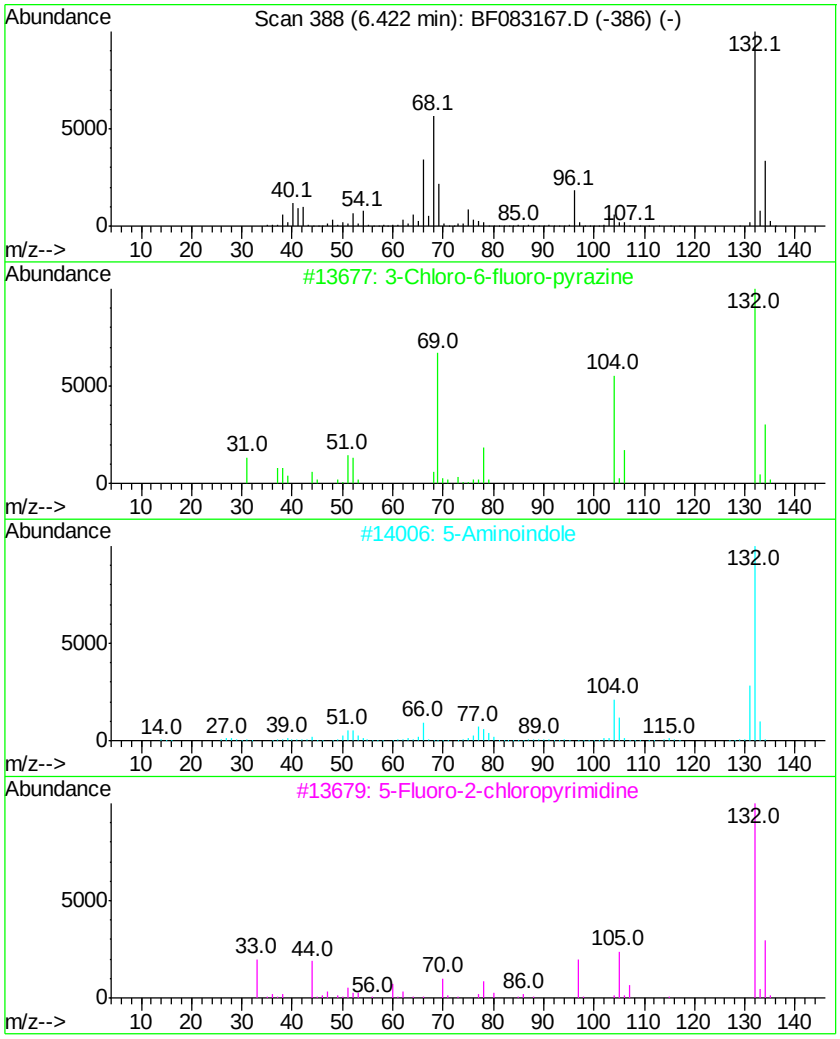
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

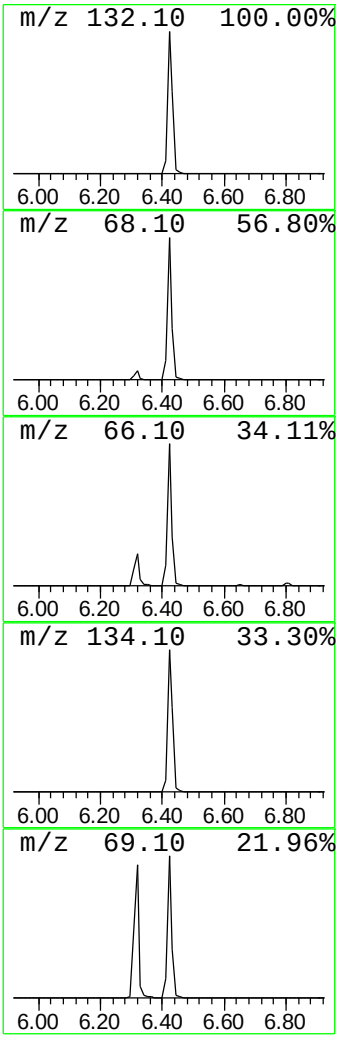
****

Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	98.65 ng	5836180	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083167.D
Acq On : 22 Nov 2015 19:13
Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

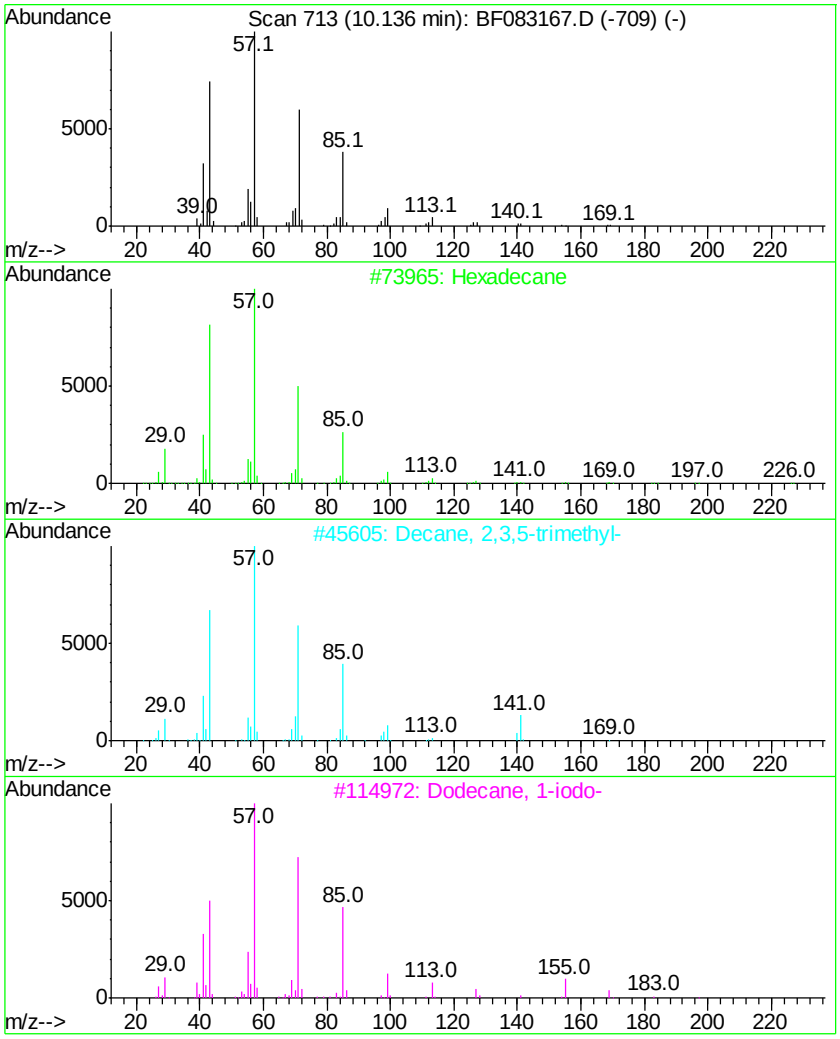
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

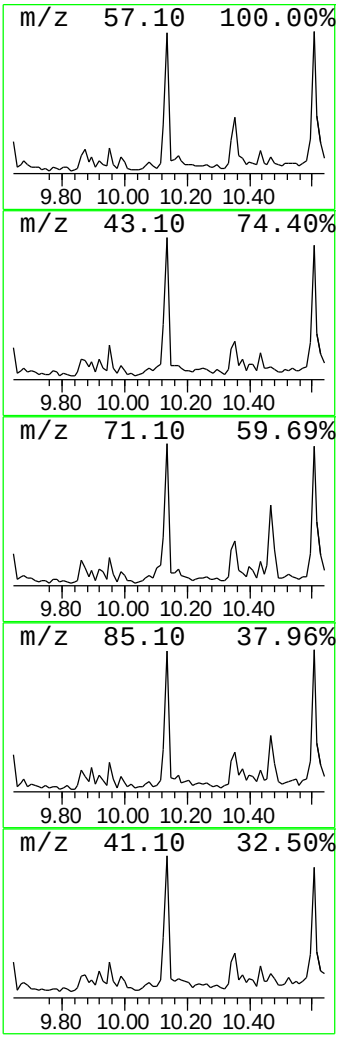
****

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.14	3.20 ng	273880	Acenaphthene-d10	9.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
4	Tridecane	184	C13H28	000629-50-5	53
5	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083167.D
Acq On : 22 Nov 2015 19:13
Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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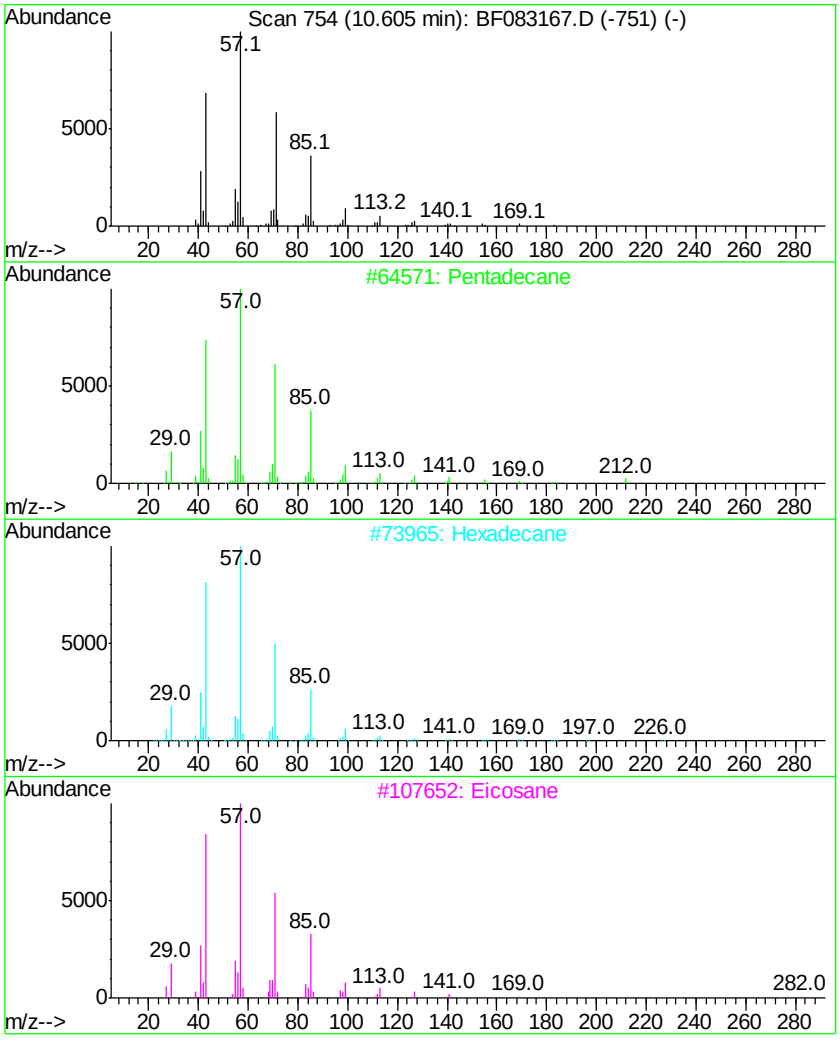
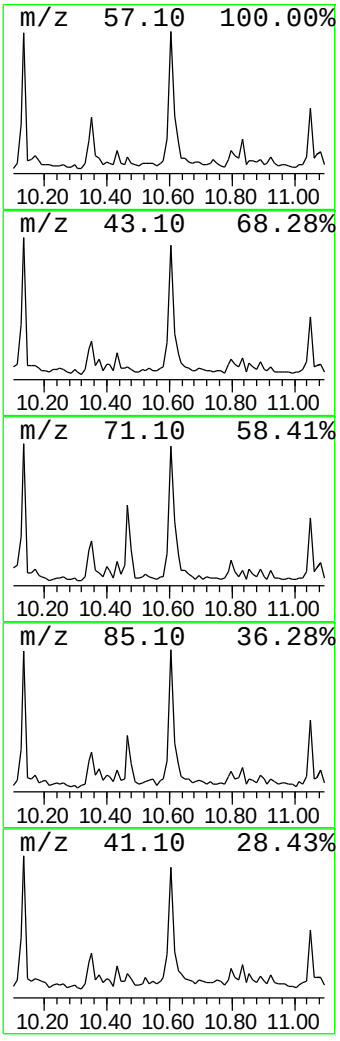
Peak Number 5 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	4.10 ng	352773	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hexadecane	226	C16H34	000544-76-3	87
3	Eicosane	282	C20H42	000112-95-8	87
4	Heptadecane	240	C17H36	000629-78-7	83
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
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Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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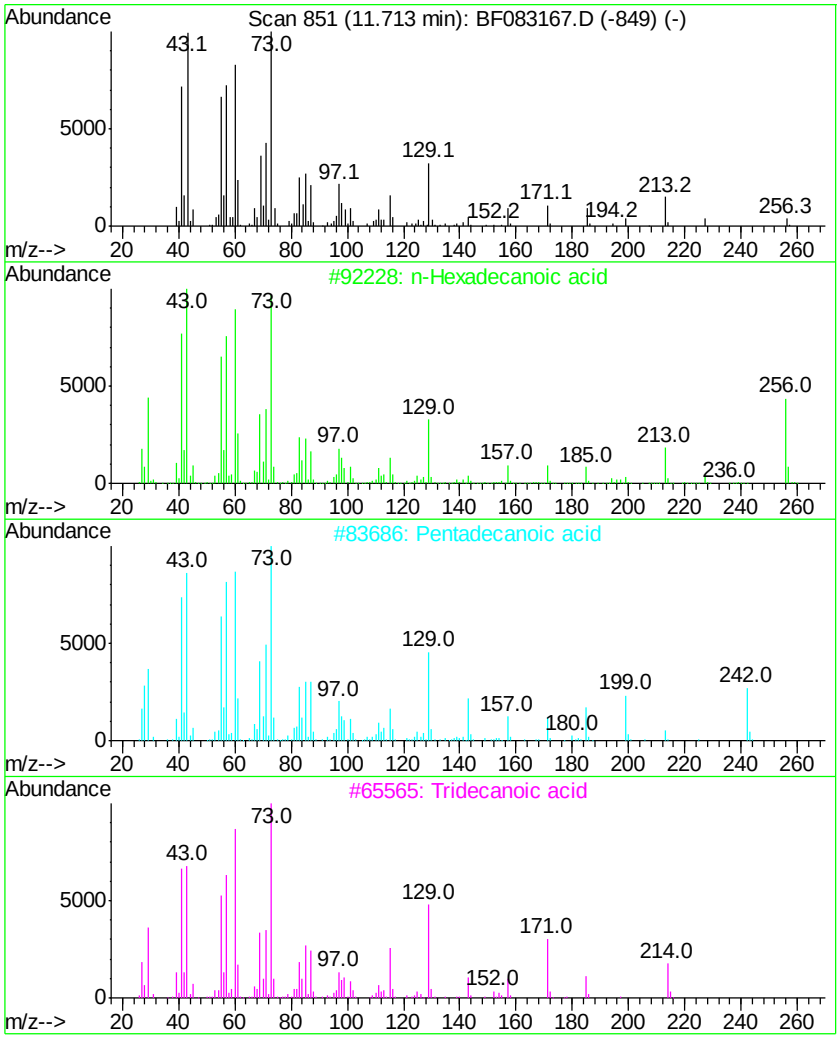
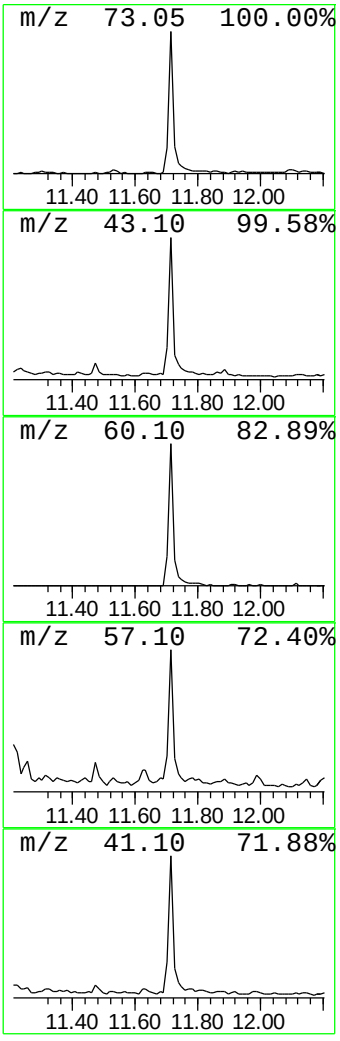
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	5.42 ng	466904	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	58
4	N-Acetylisoxazolidine	115	C5H9NO2	115615-36-6	30
5	Amyl Nitrite	117	C5H11NO2	000110-46-3	22





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Acq On : 22 Nov 2015 19:13
Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

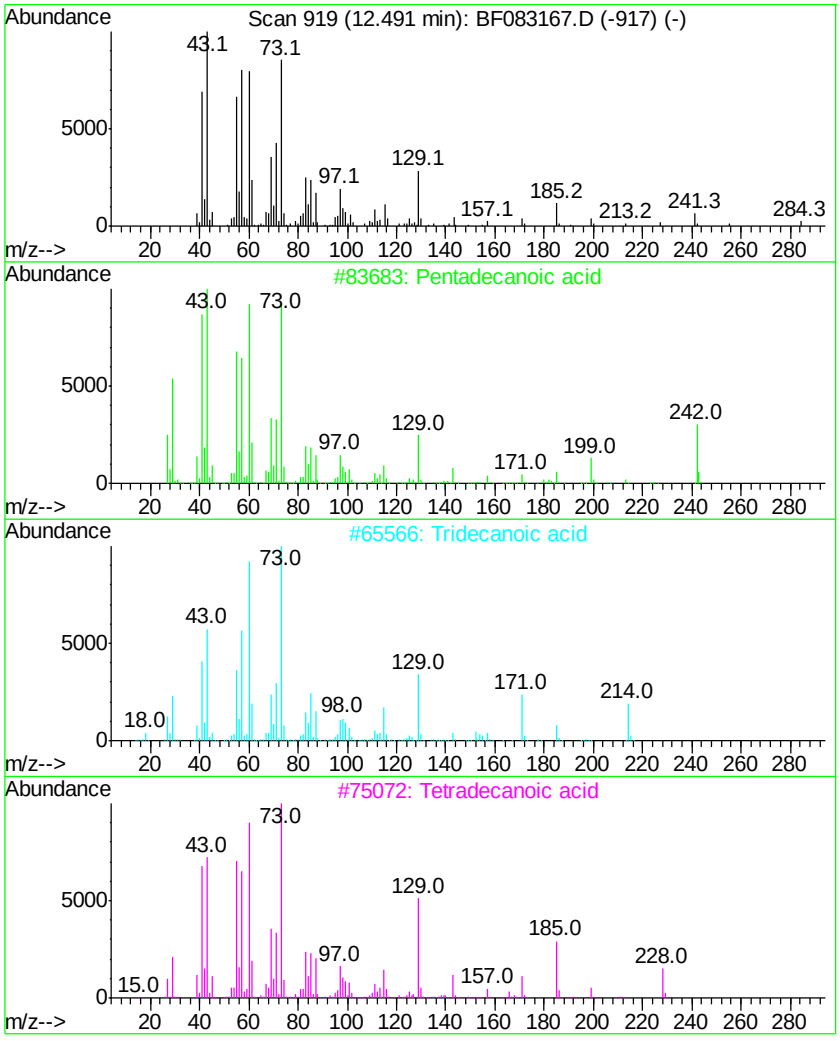
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

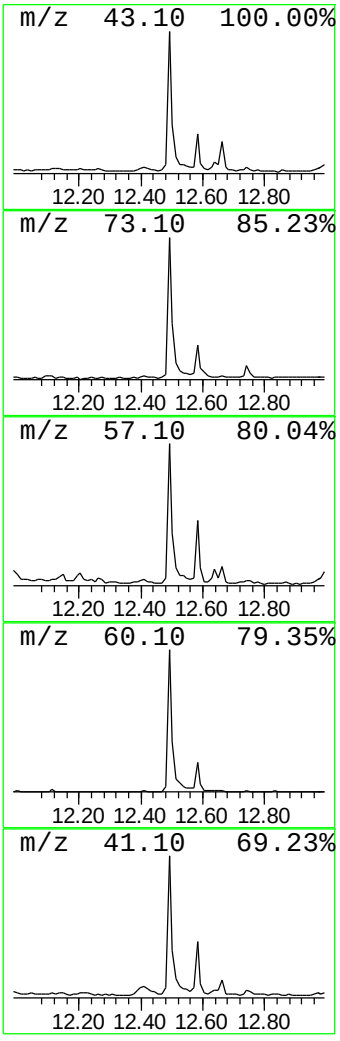
****

Peak Number 7 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	6.83 ng	555244	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Amyl Nitrite	117	C5H11NO2	000110-46-3	27
5	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083167.D
Acq On : 22 Nov 2015 19:13
Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

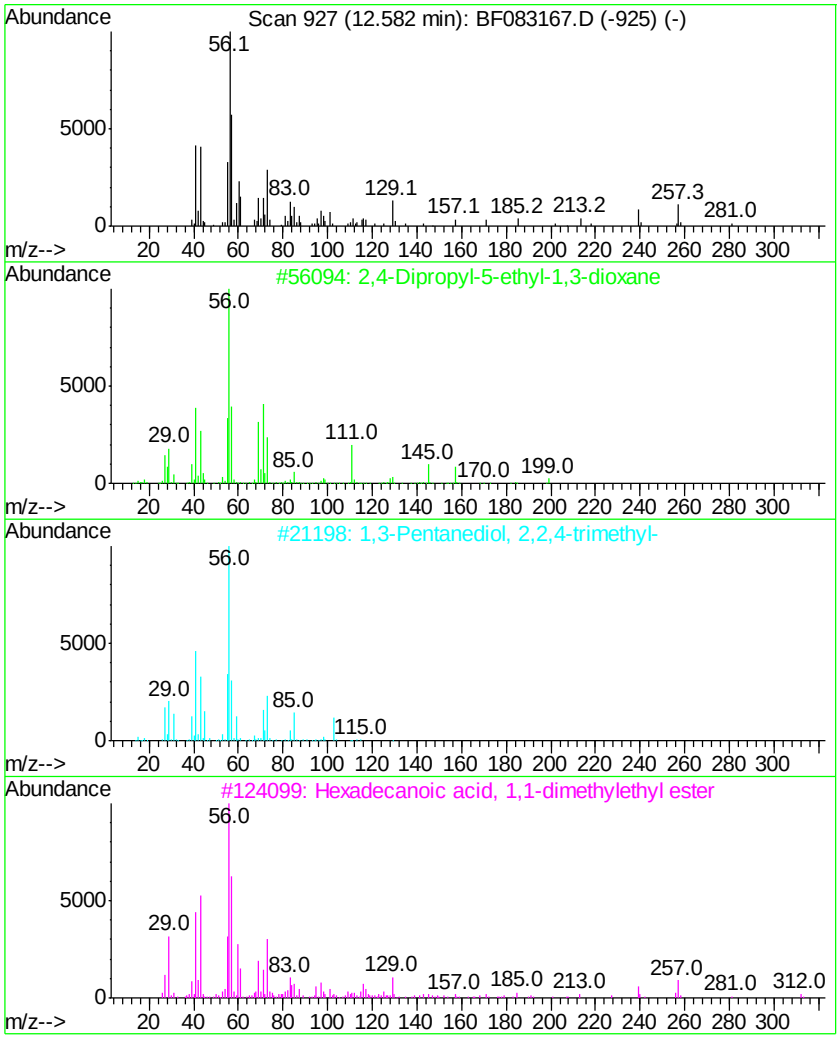
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

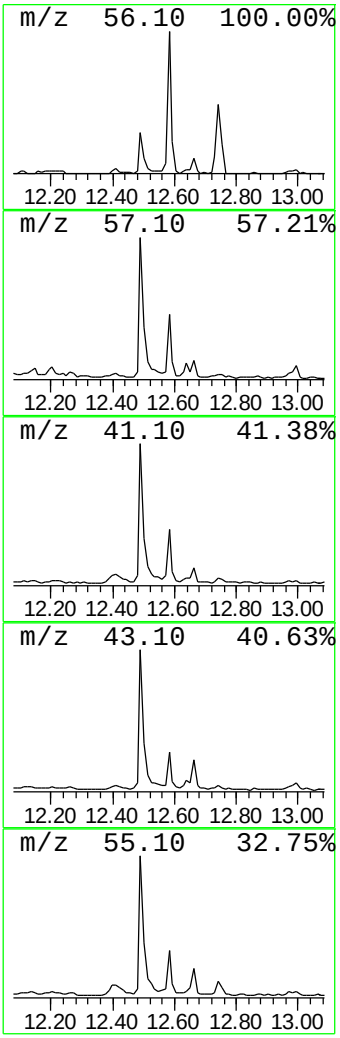
****

Peak Number 8 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	2.09 ng	169907	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	50
2	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	50
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
4	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	46
5	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	45





Library Search Compound Report

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Sample : G4509-01
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

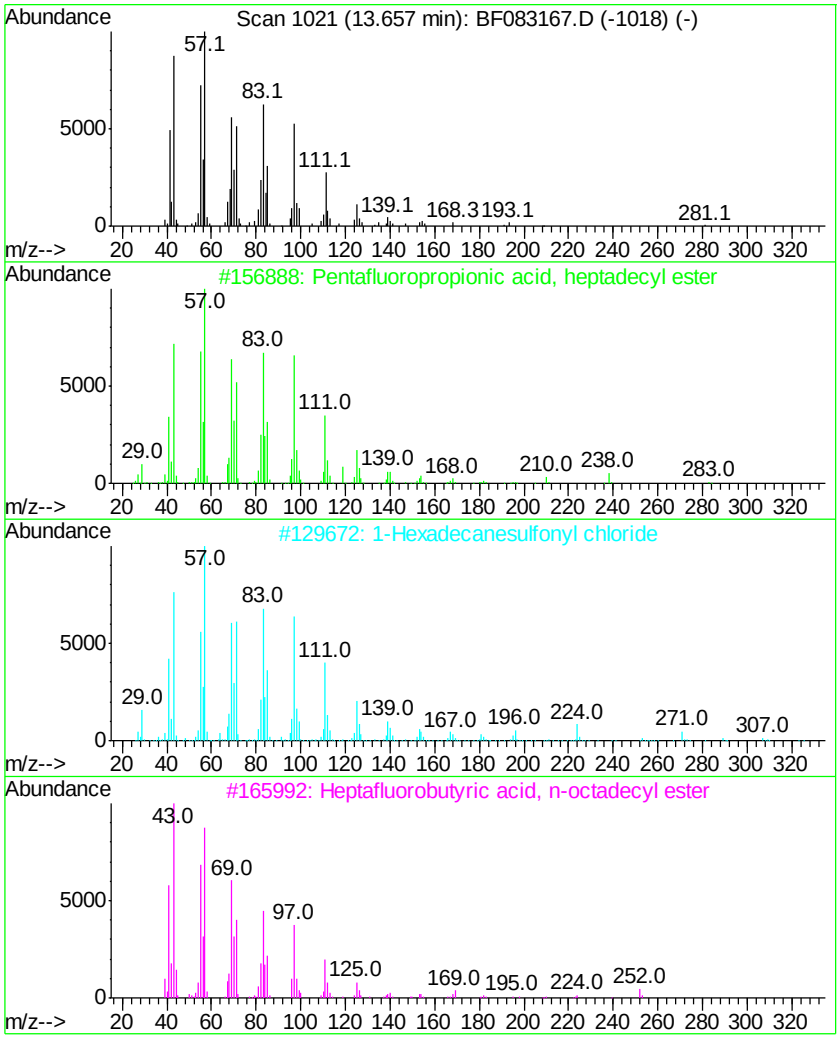
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

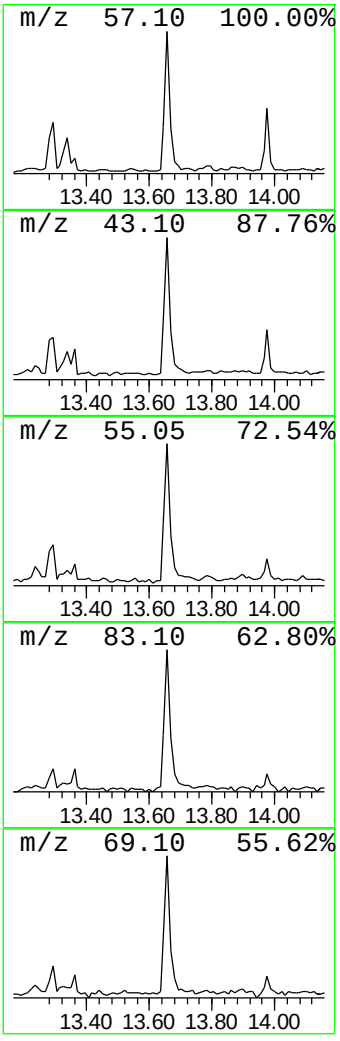
****

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	3.63 ng	294907	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112215\
Data File : BF083167.D
Acq On : 22 Nov 2015 19:13
Operator : UM/IZ
Sample : G4509-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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...	4.81	60.6	ng	3588250	1	6.65	1183230	20.0
unknown6.42	6.42	98.7	ng	5836180	1	6.65	1183230	20.0
Hexadecane	10.14	3.2	ng	273880	3	9.68	1713330	20.0
Pentadecane	10.60	4.1	ng	352773	4	11.16	1722750	20.0
n-Hexadecanoic acid	11.71	5.4	ng	466904	4	11.16	1722750	20.0
Pentadecanoic acid	12.49	6.8	ng	555244	5	13.78	1625160	20.0
2,4-Dipropyl-5-et...	12.58	2.1	ng	169907	5	13.78	1625160	20.0
Pentafluoropropio...	13.66	3.6	ng	294907	5	13.78	1625160	20.0