LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

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-BF063016.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	1.667	5	7	16	rVV	186978	312309	10.61%	1.655%
2	1.781	16	17	40	rVB	1362663	2942332	100.00%	15.588%
3	2.844	107	110	121	rBV	21837	49460	1.68%	0.262%
4	4.844	282	285	291	rBV	154072	222470	7.56%	1.179%
5	5.290	321	324	326	rBV	1520654	1541276	52.38%	8.166%
6	6.341	413	416	419	rVB	1208957	1670858	56.79%	8.852%
7	6.467	424	427	429	rBV	1869093	1876638	63.78%	9.942%
8	6.696	444	447	449	rBV	424898	387415	13.17%	2.052%
9	6.856	458	461	463	rVB	1163589	1404520	47.73%	7.441%
10	7.267	493	497	499	rBV	919919	1216629	41.35%	6.446%
11	7.976	557	559	562	rVB	481421	481841	16.38%	2.553%
12	9.062	651	654	656	rVB	2234085	1963620	66.74%	10.403%
13	9.450	686	688	691	rBV	209671	236533	8.04%	1.253%
14	9.725	710	712	715	rBV	401353	516189	17.54%	2.735%
15	10.513	779	781	784	rBV	1023167	1058990	35.99%	5.610%
16	10.650	790	793	796	rBV	37398	60103	2.04%	0.318%
17	11.096	830	832	833	rBV	73045	66600	2.26%	0.353%
18	11.199	839	841	844	rBV	324445	436737	14.84%	2.314%
19	11.451	862	863	867	rVB	30012	33599	1.14%	0.178%
20	11.519	867	869	872	rVB	37432	33516	1.14%	0.178%
21	11.748	886	889	893	rBV	49291	75034	2.55%	0.398%
22	12.788	978	980	983	rBV	1216425	1196879	40.68%	6.341%
23	13.702	1057	1060	1069	rBV	98027	151815	5.16%	0.804%
24	13.828	1069	1071	1073	rBV	407979	359985	12.23%	1.907%
25	14.331	1112	1115	1121	rBV	72416	110257	3.75%	0.584%
26	14.617	1136	1140	1142	rBV4	12912	31245	1.06%	0.166%
27	15.200	1188	1191	1194	rVV	332666	368463	12.52%	1.952%
28	17.428	1382	1386	1391	rVB2	33434	70098	2.38%	0.371%

Sum of corrected areas: 18875411

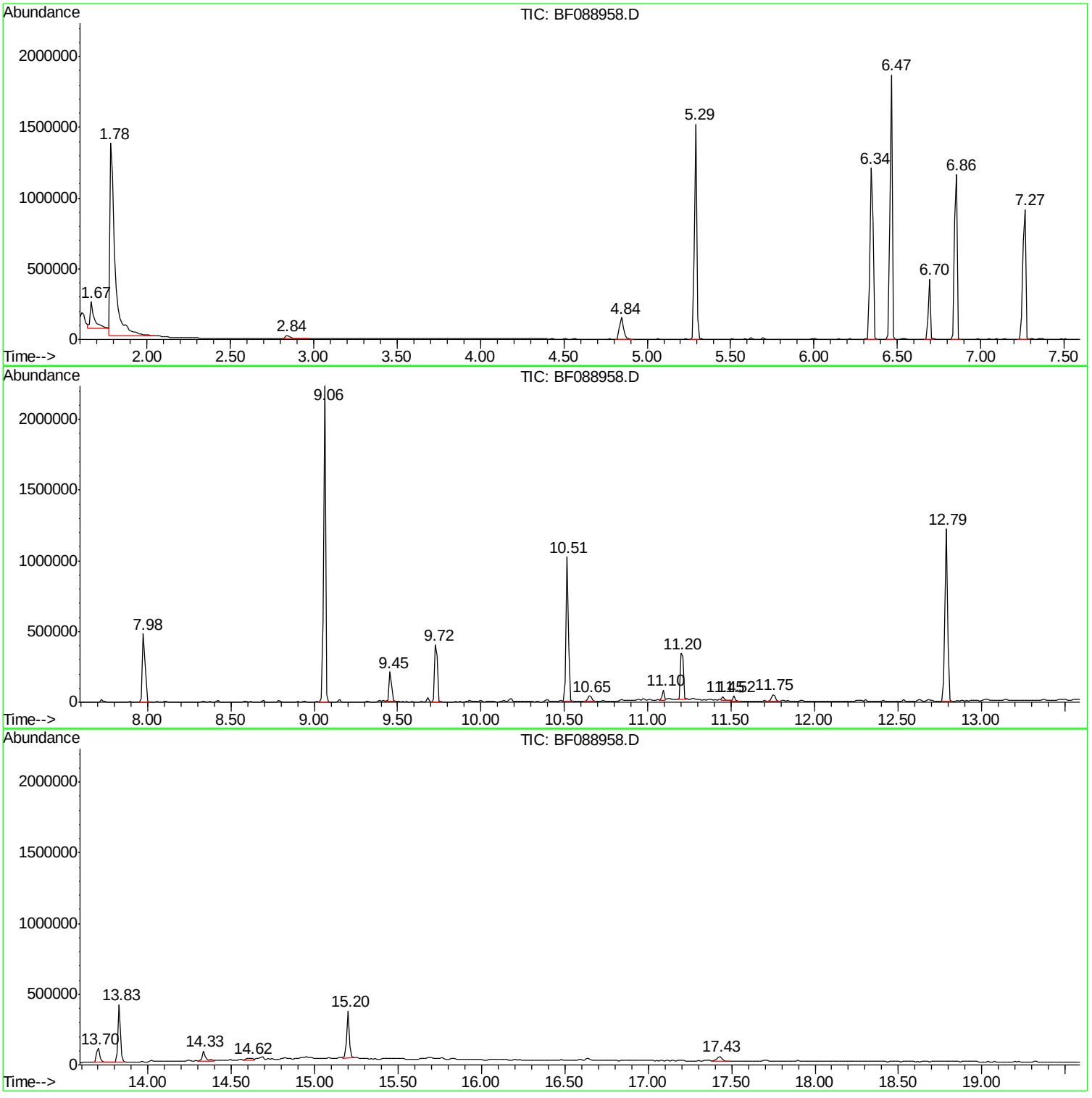
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

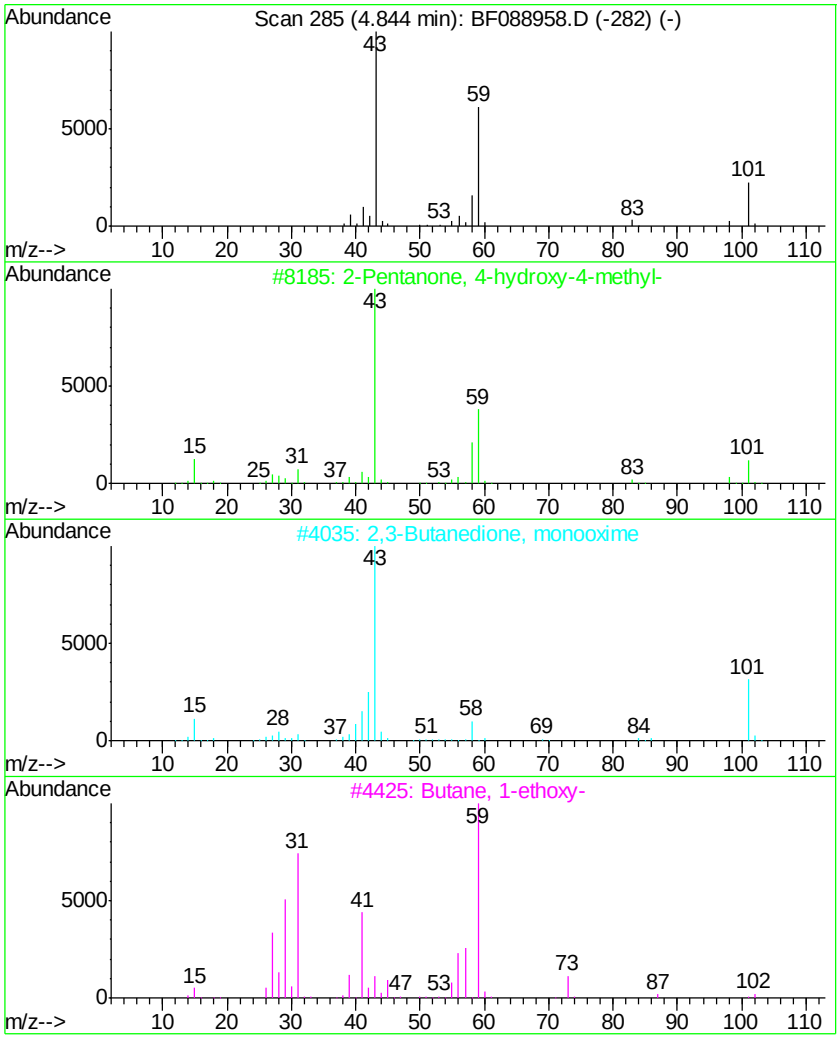
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

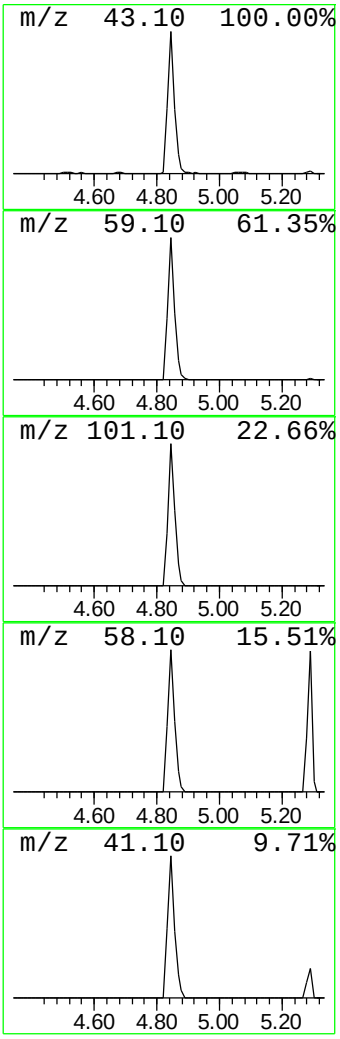
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	11.48 ng	222470	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

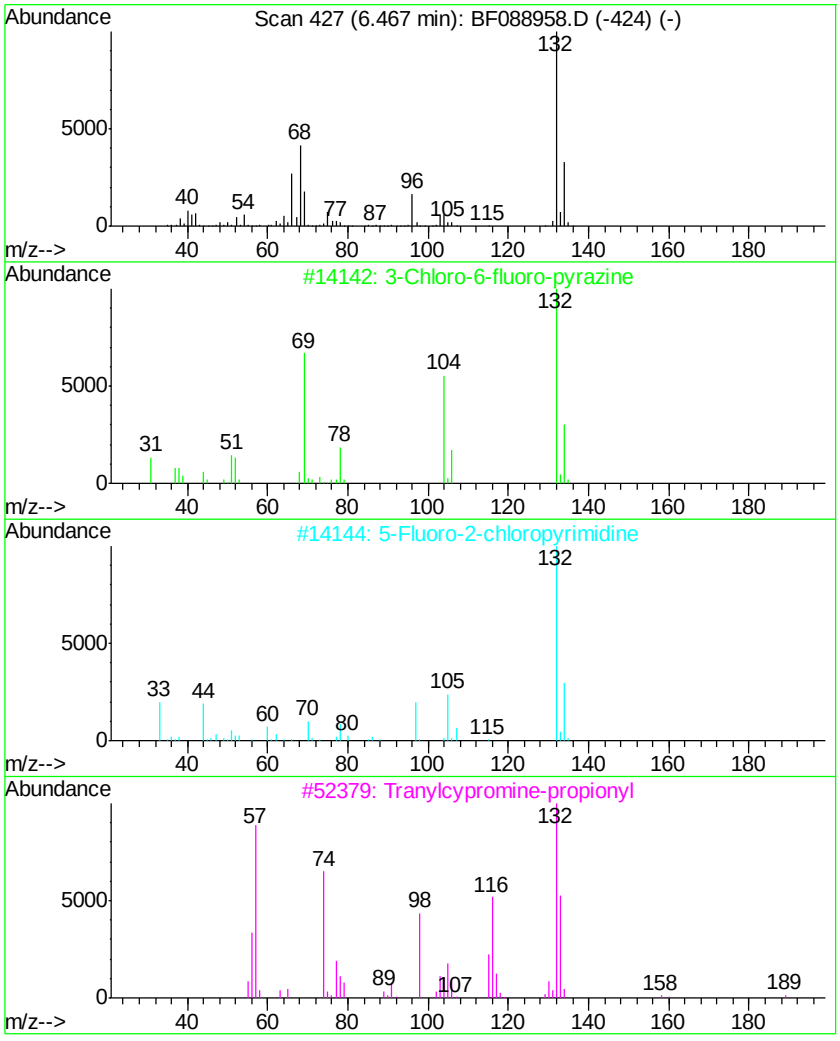
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

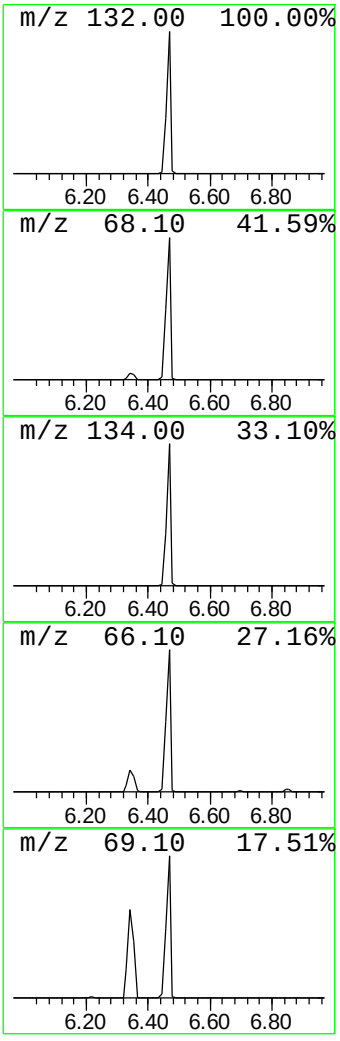
****

Peak Number 5 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	96.88 ng	1876640	1,4-Dichlorobenzene-d4	6.70

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	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

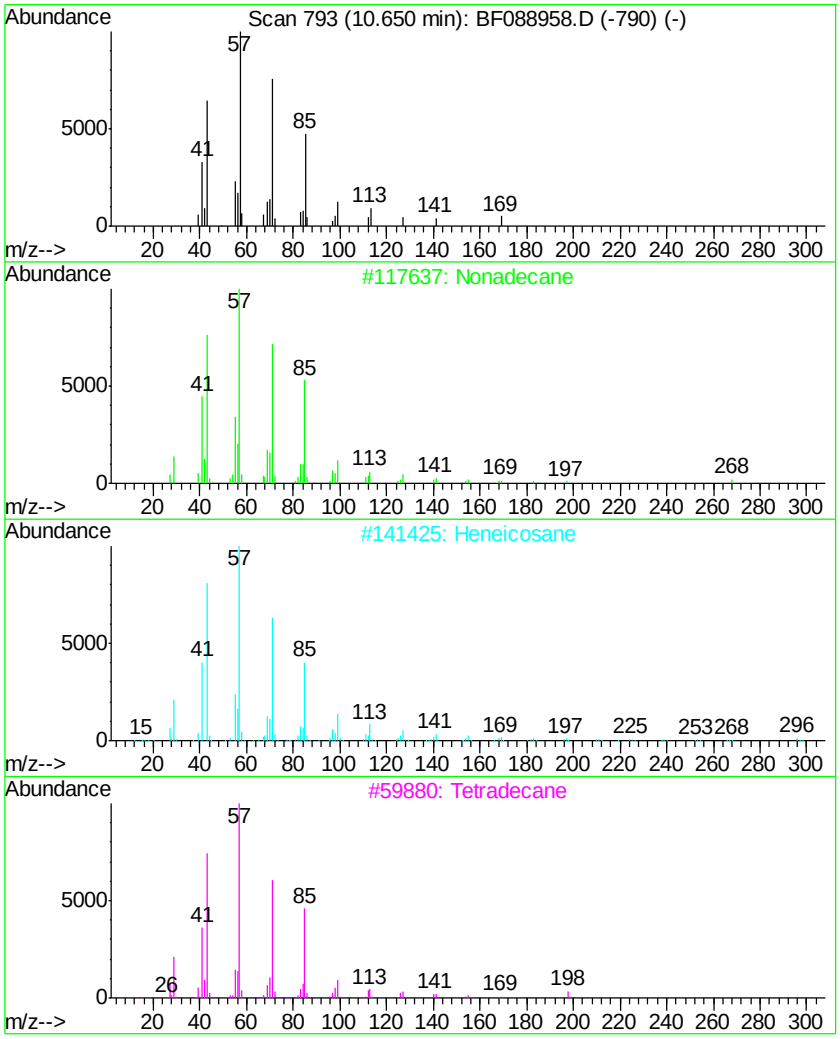
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

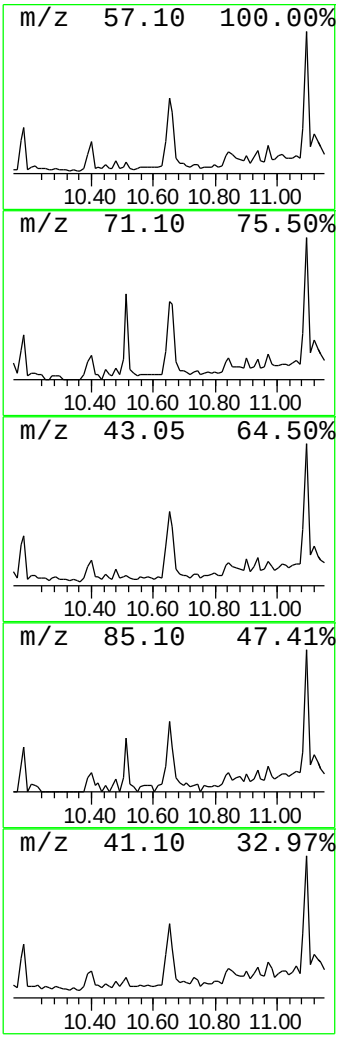
****

Peak Number 7 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	2.75 ng	60103	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetradecane	198	C14H30	000629-59-4	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Tritetracontane	605	C43H88	007098-21-7	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

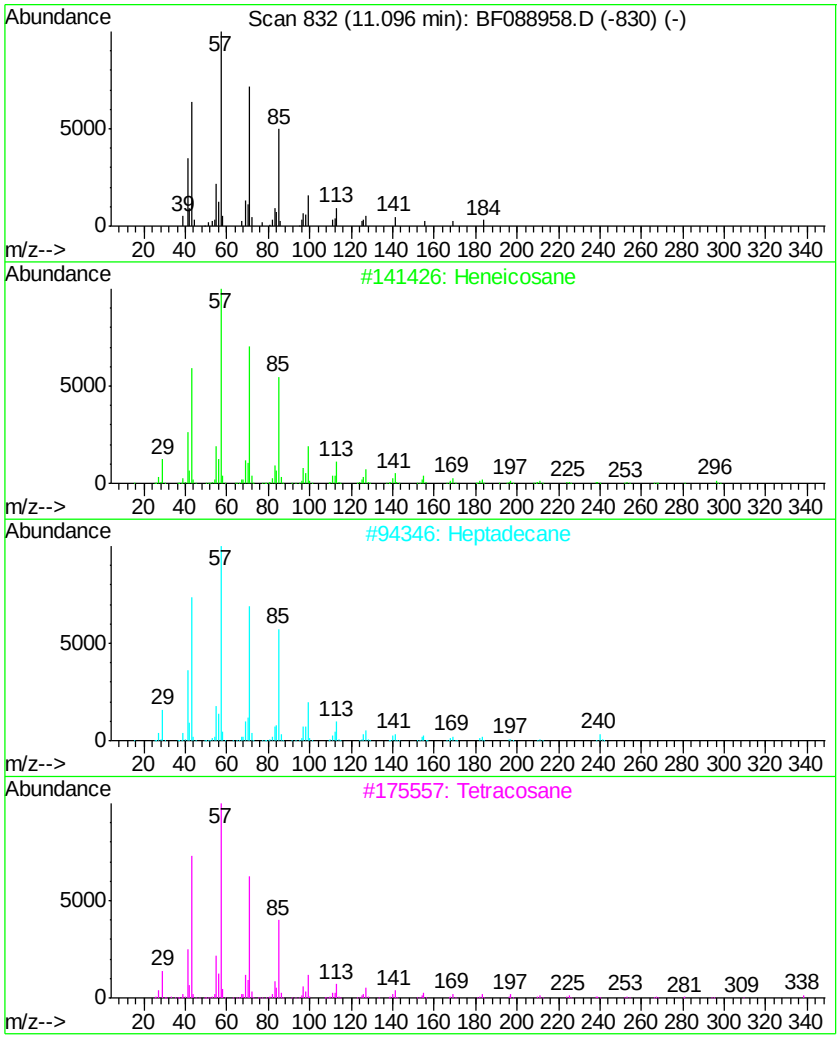
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

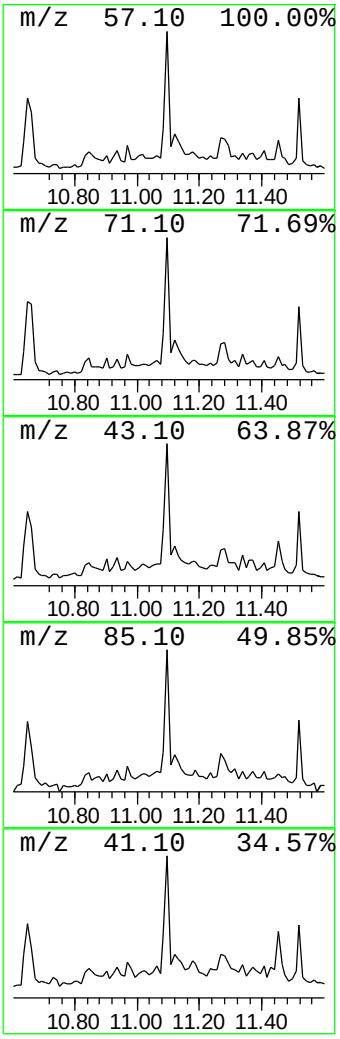
****

Peak Number 8 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	3.05 ng	66600	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Octadecane	254	C18H38	000593-45-3	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

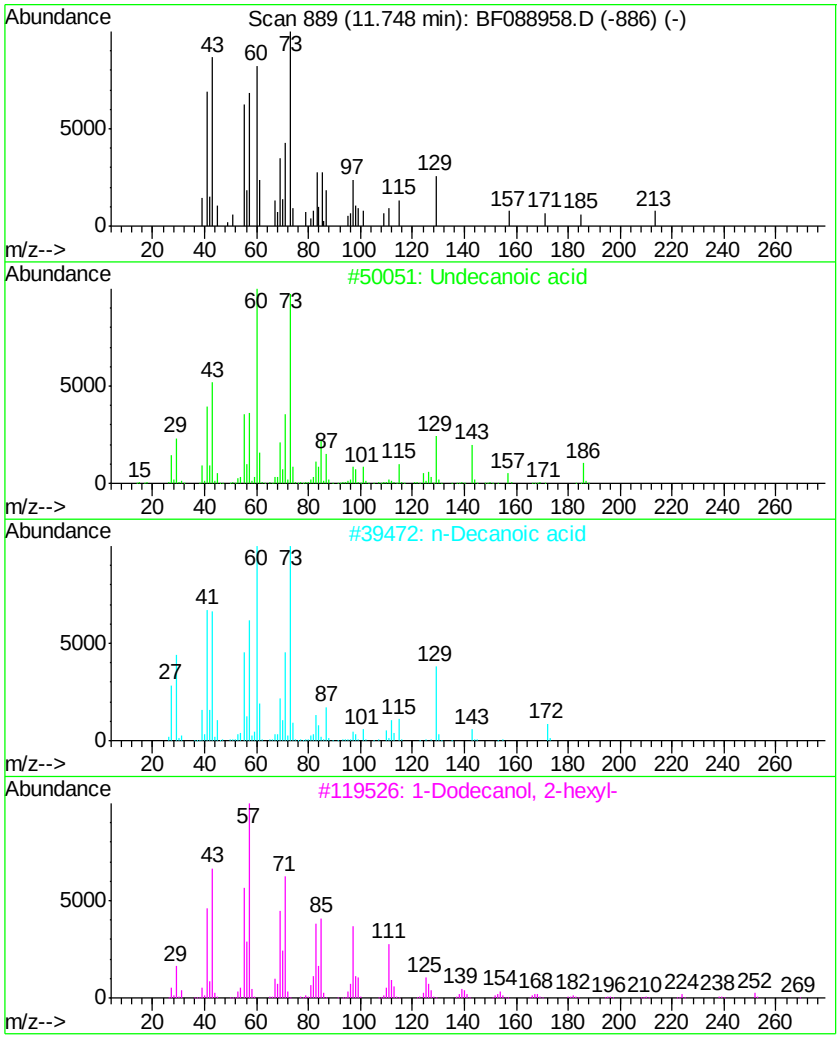
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

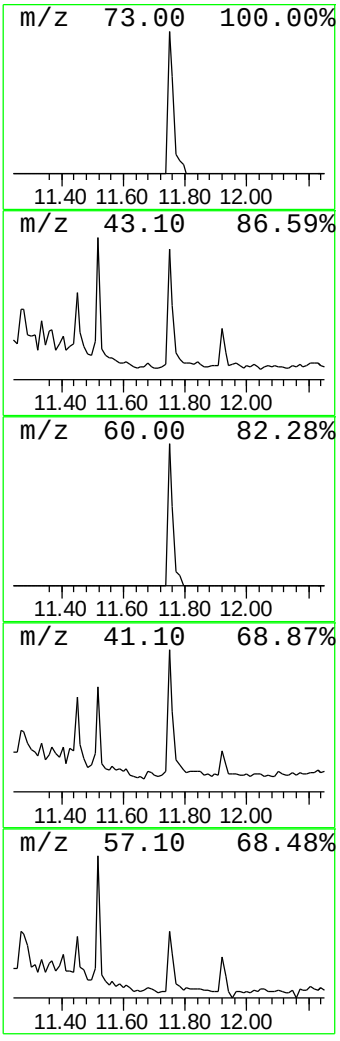
****

Peak Number 9 Undecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	3.44 ng	75034	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	59
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53
3	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	30
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	30
5	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

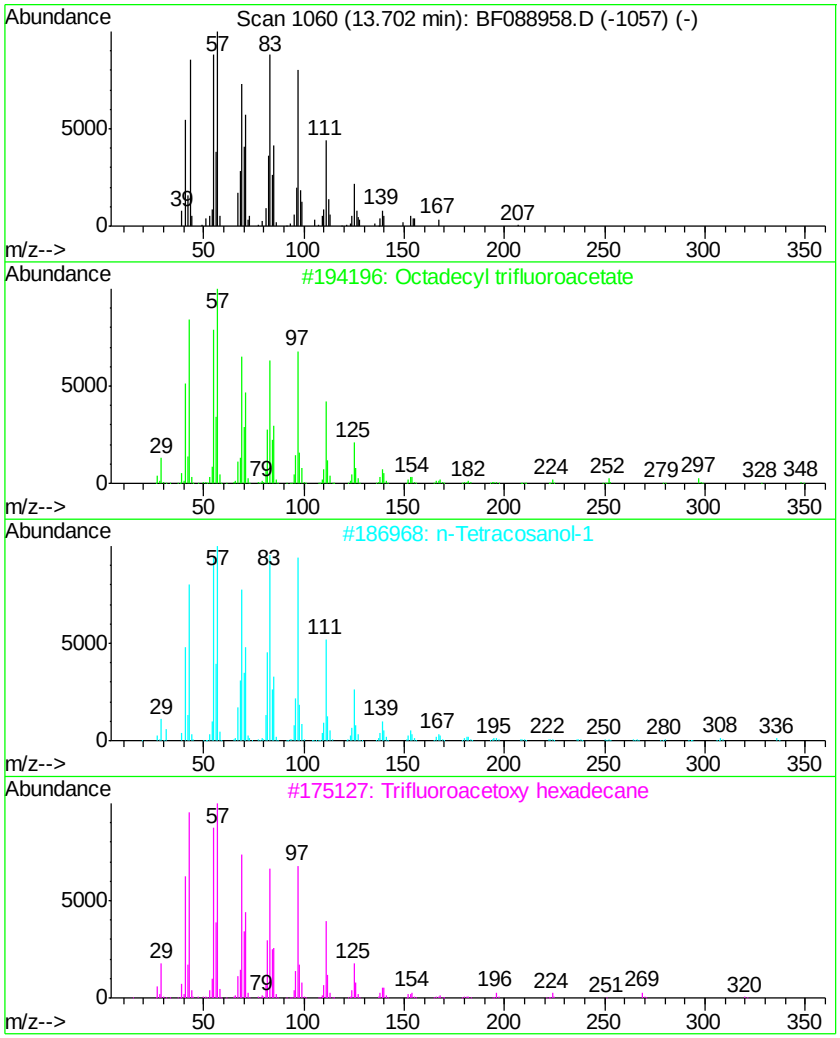
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

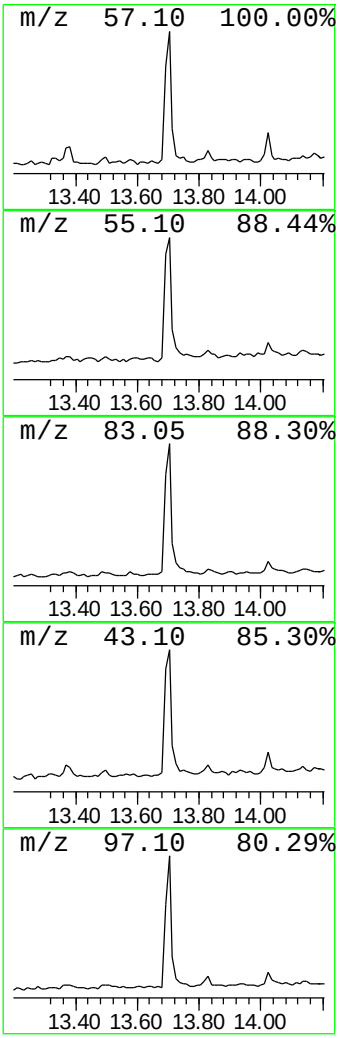
****

Peak Number 10 Octadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	8.43 ng	151815	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

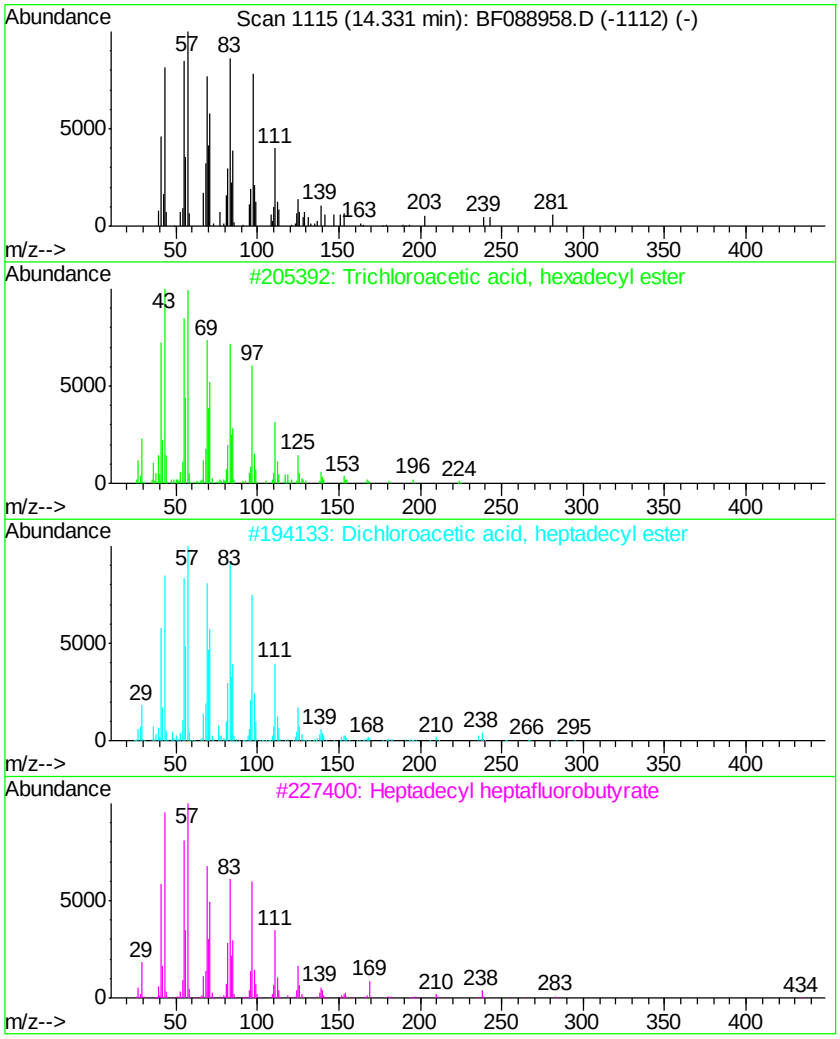
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

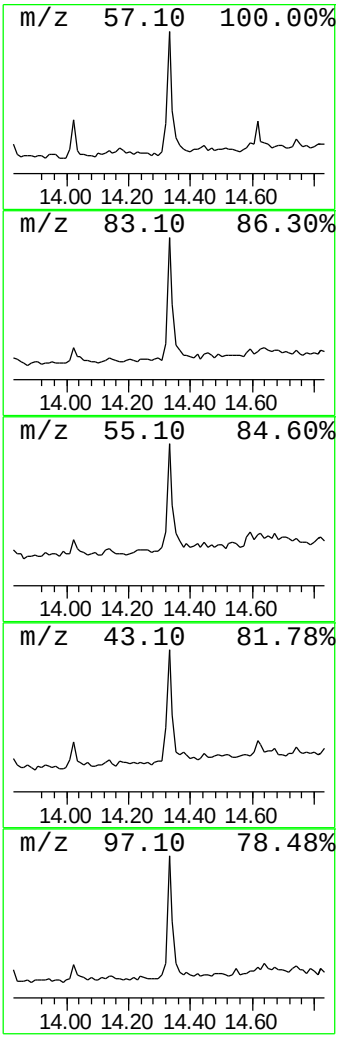
****

Peak Number 11 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	6.13 ng	110257	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

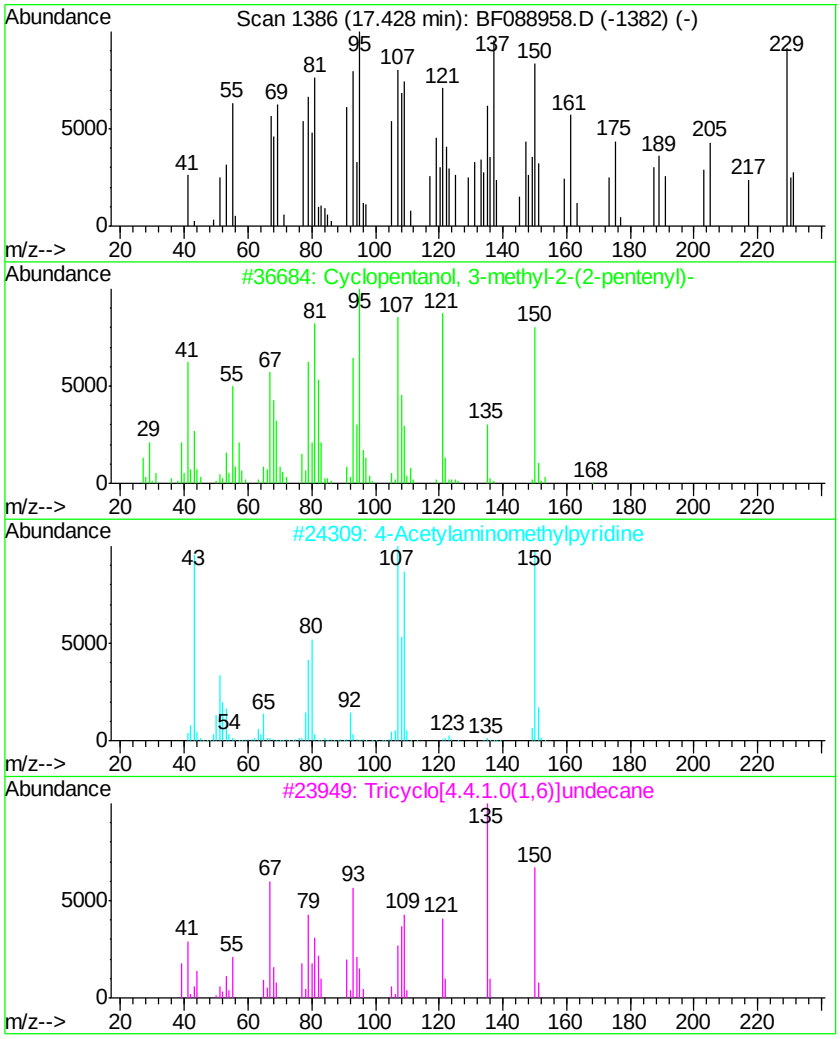
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

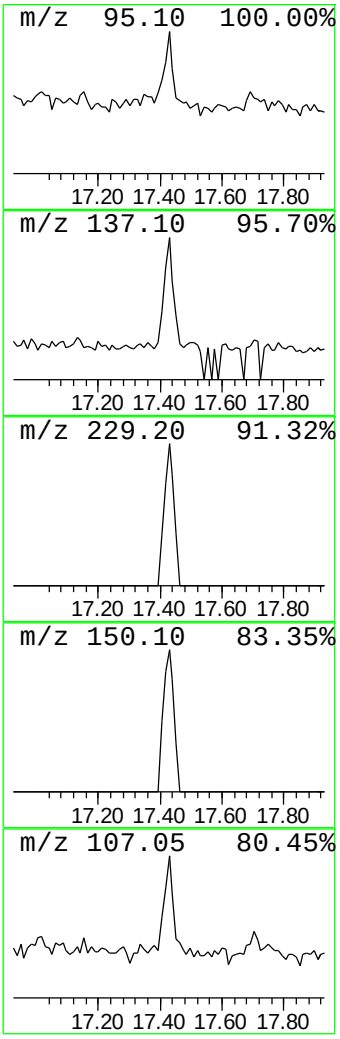
****

Peak Number 12 unknown17.43 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.43	3.80 ng	70098	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanol, 3-methyl-2-(2-pen...	168	C11H20O	137303-64-1	30
2	4-Acetylaminomethylpyridine	150	C8H10N2O	023974-15-4	25
3	Tricyclo[4.4.1.0(1,6)]undecane	150	C11H18	006571-73-9	20
4	Tricyclo[4.4.0.0(2,8)]dec-3-en-5-ol	150	C10H14O	1000193-38-7	20
5	Tricyclo[5.4.0.0(1,3)]undecane	150	C11H18	1000280-74-7	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071316\
Data File : BF088958.D
Acq On : 13 Jul 2016 15:17
Operator : UM/SJ
Sample : H3935-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.84	11.5	ng	222470	1	6.70	387415	20.0
unknown6.47	6.47	96.9	ng	1876640	1	6.70	387415	20.0
Nonadecane	10.65	2.8	ng	60103	4	11.21	436737	20.0
Heneicosane	11.10	3.0	ng	66600	4	11.21	436737	20.0
Undecanoic acid	11.75	3.4	ng	75034	4	11.21	436737	20.0
Octadecyl trifluo...	13.70	8.4	ng	151815	5	13.83	359985	20.0
Trichloroacetic a...	14.33	6.1	ng	110257	5	13.83	359985	20.0
unknown17.43	17.43	3.8	ng	70098	6	15.20	368463	20.0