LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
Data File : BF098940.D
Acq On : 29 Sep 2017 10:45
Operator : SJ/JU
Sample : I5488-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

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-BF092317.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	2.263	24	30	39	rVB	171780	240733	6.75%	0.789%
2	4.046	328	333	340	rBV	42943	53999	1.51%	0.177%
3	4.546	414	418	425	rBV	64098	70670	1.98%	0.232%
4	5.157	517	522	535	rVB	615789	853166	23.91%	2.796%
5	5.546	582	588	591	rBV	3315850	3509336	98.33%	11.501%
6	6.545	752	758	770	rVB	3158115	3529335	98.89%	11.567%
7	6.687	777	782	785	rBV	3459093	3568903	100.00%	11.697%
8	6.740	788	791	800	rVB	55120	48889	1.37%	0.160%
9	6.916	817	821	824	rBV	1012821	822490	23.05%	2.696%
10	7.075	843	848	851	rBV	2960625	2659014	74.51%	8.715%
11	7.481	911	917	920	rBV	2099016	2219994	62.20%	7.276%
12	7.575	930	933	939	rVB	54216	47056	1.32%	0.154%
13	8.198	1034	1039	1042	rBV	1263042	1085495	30.42%	3.558%
14	9.275	1216	1222	1225	rBV	3504129	3456354	96.85%	11.328%
15	9.663	1283	1288	1291	rBV	831674	686191	19.23%	2.249%
16	9.951	1332	1337	1341	rBV	1131580	1093280	30.63%	3.583%
17	10.375	1406	1409	1412	rVB2	54727	49432	1.39%	0.162%
18	10.745	1467	1472	1475	rBV	1927437	1788839	50.12%	5.863%
19	10.845	1486	1489	1498	rVB	122308	128577	3.60%	0.421%
20	11.292	1559	1565	1567	rBV	42726	35770	1.00%	0.117%
21	11.439	1586	1590	1593	rBV	1074472	948069	26.56%	3.107%
22	12.651	1793	1796	1800	rBV	70513	59706	1.67%	0.196%
23	12.880	1830	1835	1838	rBV	53742	55718	1.56%	0.183%
24	13.022	1855	1859	1863	rBV	2191918	2042694	57.24%	6.695%
25	13.904	2006	2009	2014	rBV	99476	115511	3.24%	0.379%
26	14.080	2035	2039	2042	rBV	713465	644270	18.05%	2.112%
27	15.574	2288	2293	2301	rVB	516075	698623	19.58%	2.290%

Sum of corrected areas: 30512114

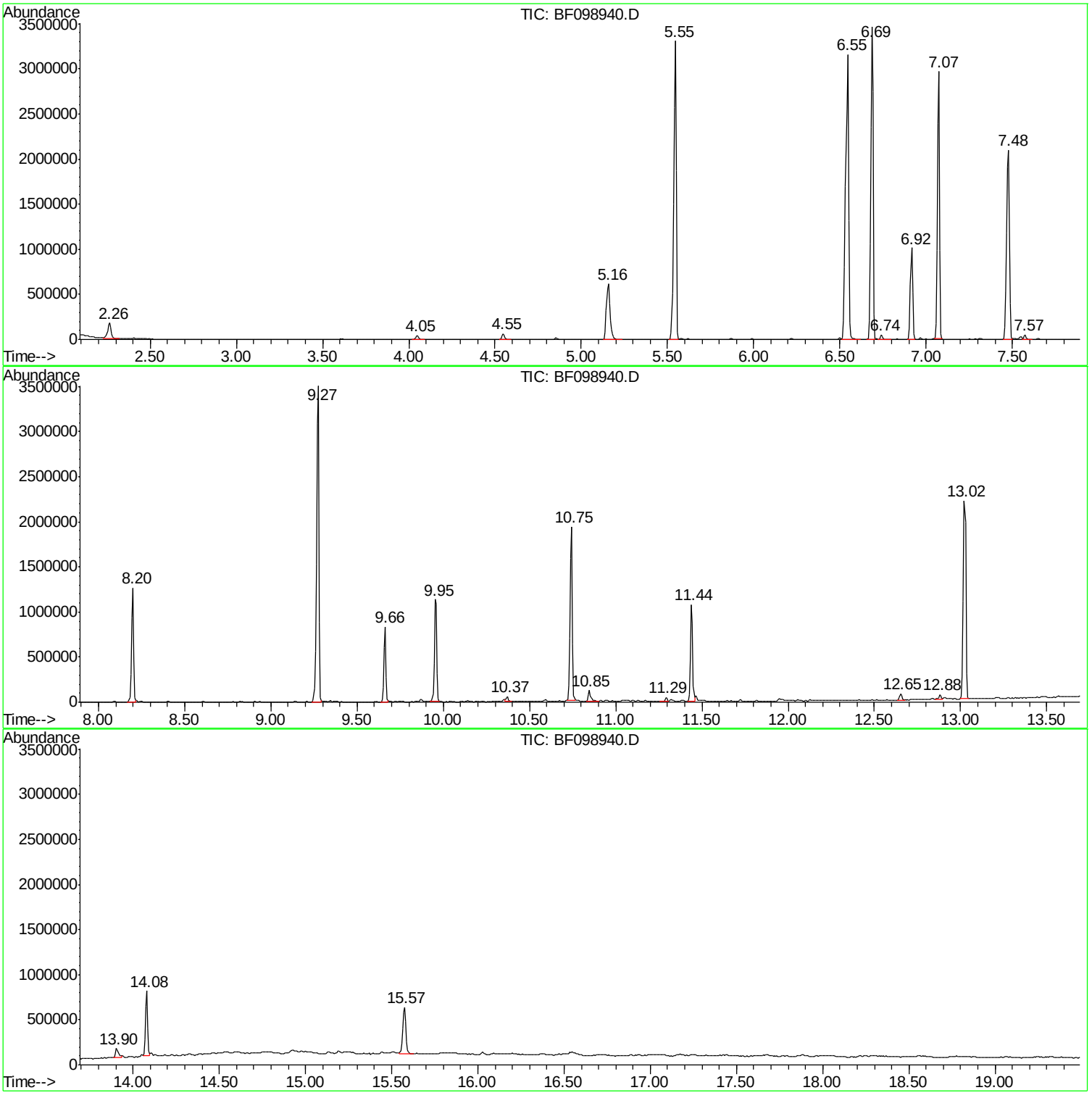
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
Data File : BF098940.D
Acq On : 29 Sep 2017 10:45
Operator : SJ/JU
Sample : I5488-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
Data File : BF098940.D
Acq On : 29 Sep 2017 10:45
Operator : SJ/JU
Sample : I5488-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

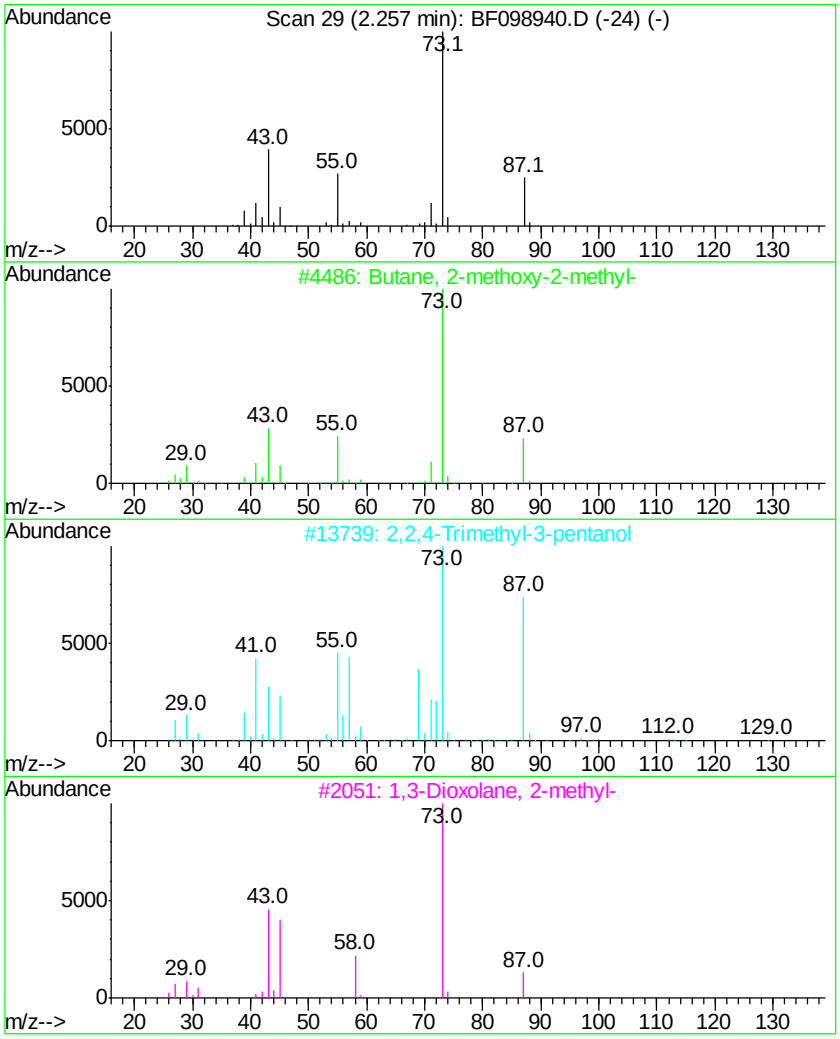
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

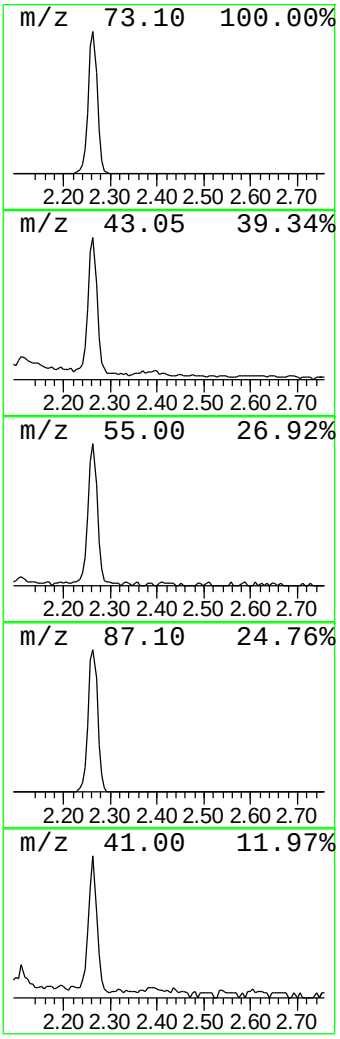
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	5.85 ng	240733	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
Data File : BF098940.D
Acq On : 29 Sep 2017 10:45
Operator : SJ/JU
Sample : I5488-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

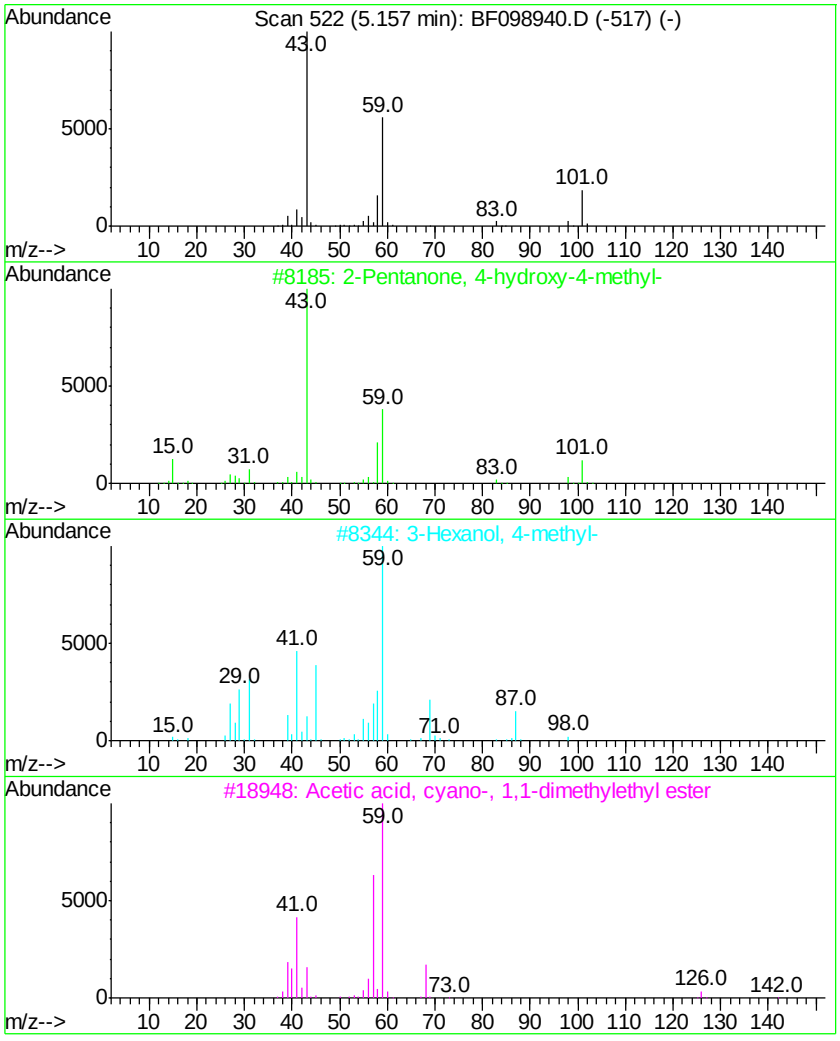
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

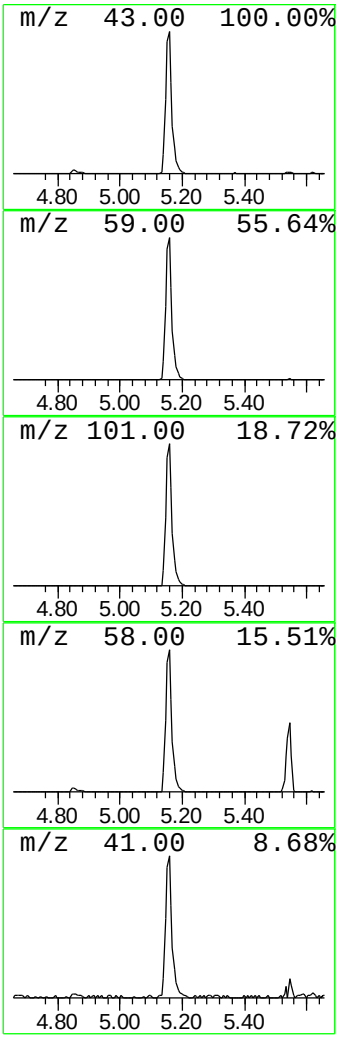
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	20.75 ng	853166	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	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
Data File : BF098940.D
Acq On : 29 Sep 2017 10:45
Operator : SJ/JU
Sample : I5488-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

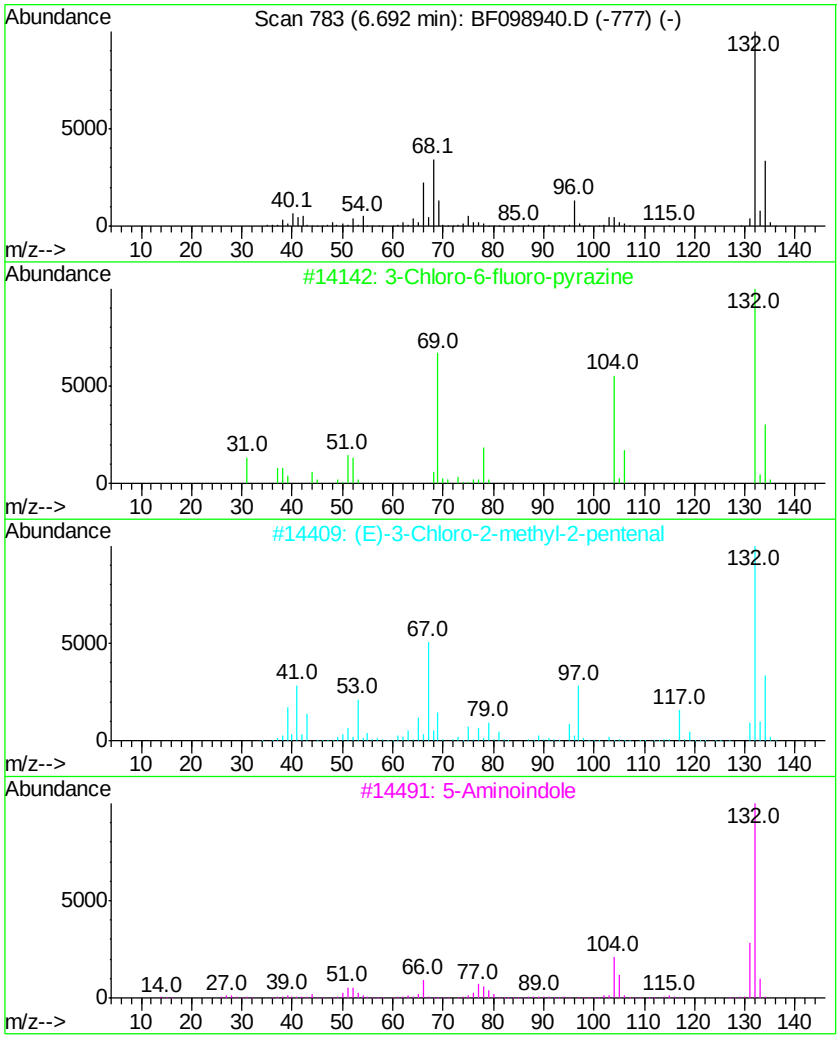
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

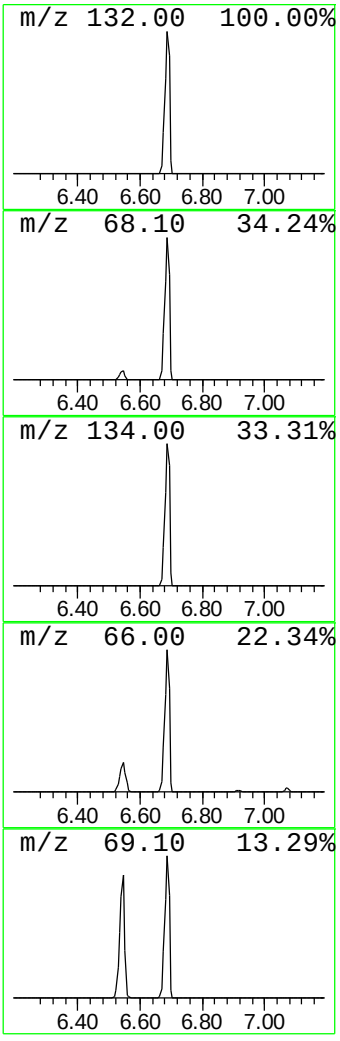
****

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	86.78 ng	3568900	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
Data File : BF098940.D
Acq On : 29 Sep 2017 10:45
Operator : SJ/JU
Sample : I5488-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

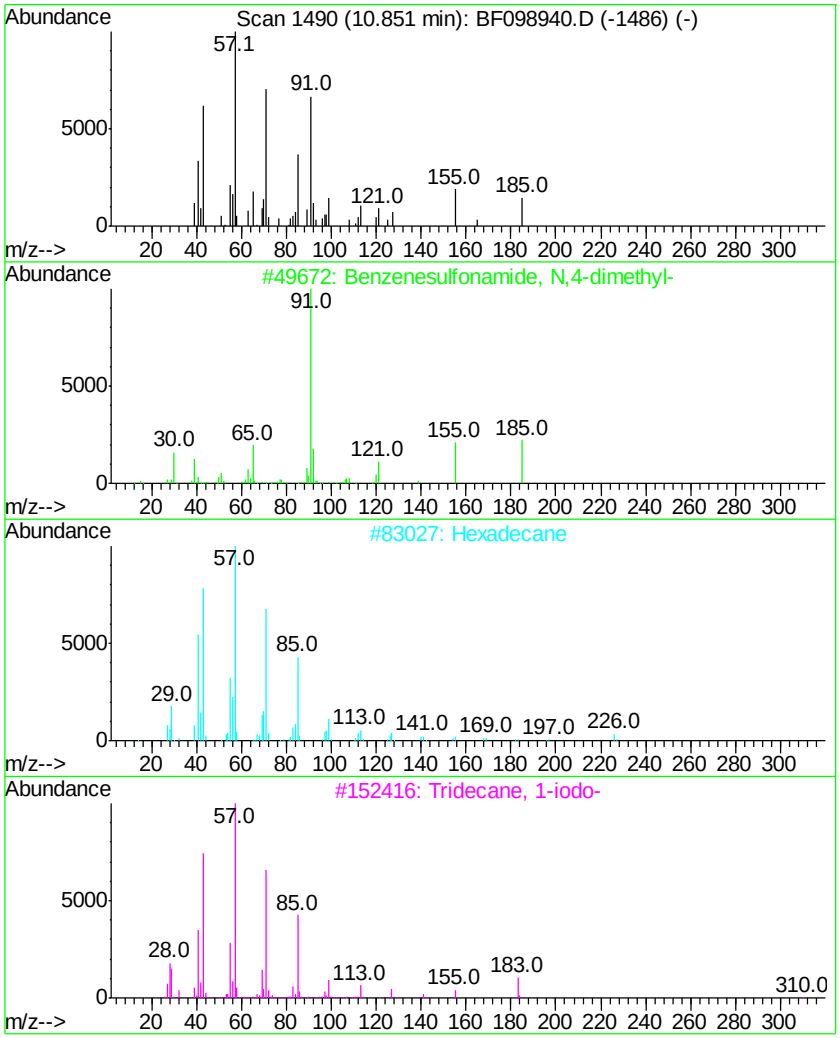
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

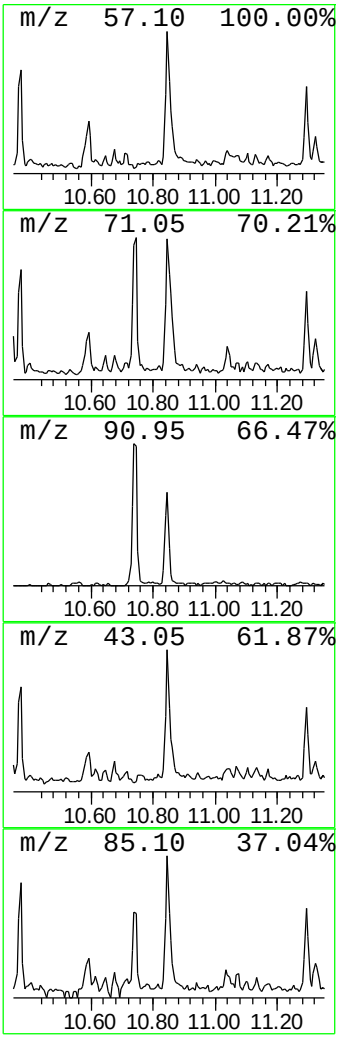
****

Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	2.71 ng	128577	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	50
2	Hexadecane	226	C16H34	000544-76-3	41
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	38
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	38
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
Data File : BF098940.D
Acq On : 29 Sep 2017 10:45
Operator : SJ/JU
Sample : I5488-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

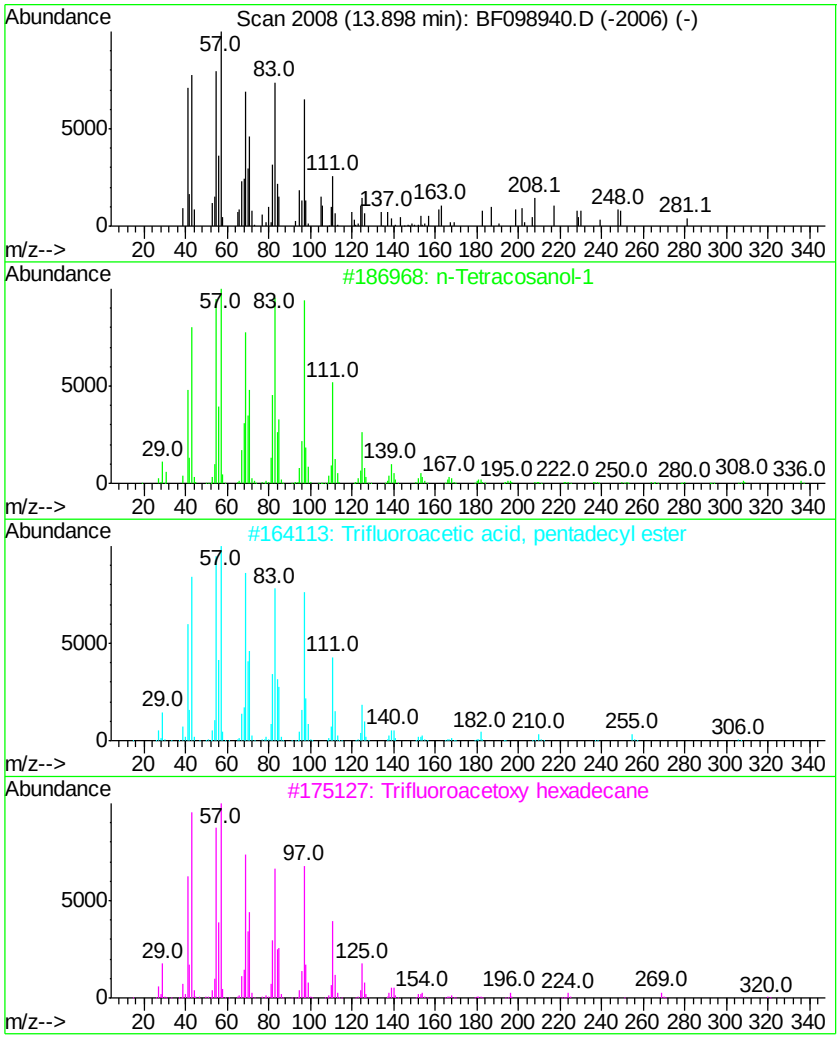
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

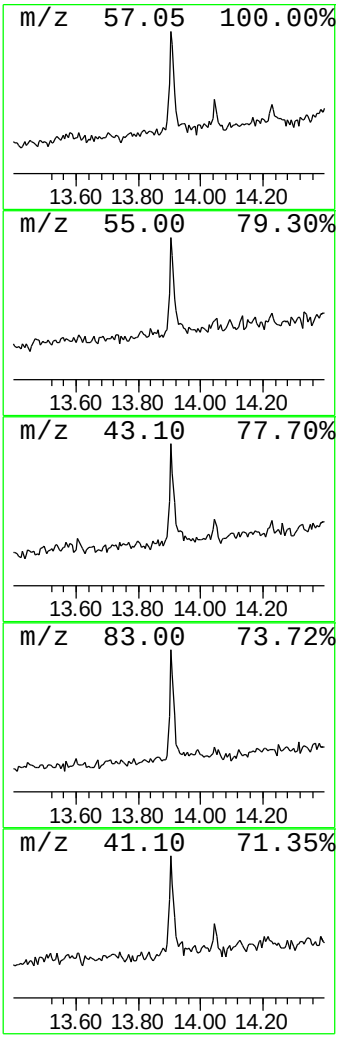
****

Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	3.59 ng	115511	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Cyclopentadecane	210	C15H30	000295-48-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092917\
Data File : BF098940.D
Acq On : 29 Sep 2017 10:45
Operator : SJ/JU
Sample : I5488-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.26	5.8	ng	240733	1	6.92	822490	20.0
2-Pentanone, 4-hy...	5.16	20.8	ng	853166	1	6.92	822490	20.0
unknown6.69	6.69	86.8	ng	3568900	1	6.92	822490	20.0
Benzenesulfonamid...	10.85	2.7	ng	128577	4	11.44	948069	20.0
n-Tetracosanol-1	13.90	3.6	ng	115511	5	14.08	644270	20.0