LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098823.D
Acq On : 26 Sep 2017 10:51
Operator : SJ/JU
Sample : I5384-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092017-SIDI-F-U-S

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	2.204	15	20	25	rVB	306325	375964	8.29%	1.398%
2	5.128	514	517	529	rVB	237889	248102	5.47%	0.923%
3	5.528	580	585	588	rBV	1424477	1366668	30.15%	5.083%
4	6.528	751	755	758	rBV	962717	847792	18.70%	3.153%
5	6.681	776	781	784	rBV	2584488	2397844	52.90%	8.919%
6	6.910	817	820	824	rBV	966667	793289	17.50%	2.951%
7	7.069	843	847	851	rBV	3330478	3102421	68.44%	11.540%
8	7.475	911	916	919	rBV	2494606	2568779	56.67%	9.555%
9	8.192	1034	1038	1042	rBV	1305884	1072634	23.66%	3.990%
10	9.269	1215	1221	1224	rBV	4496569	4532916	100.00%	16.861%
11	9.657	1283	1287	1290	rVB	149262	108730	2.40%	0.404%
12	9.951	1333	1337	1340	rBV	1321610	1133607	25.01%	4.217%
13	10.733	1466	1470	1474	rBV	1698159	1647657	36.35%	6.129%
14	10.845	1485	1489	1495	rBV2	42863	54386	1.20%	0.202%
15	11.433	1585	1589	1593	rBV	1246293	1070456	23.62%	3.982%
16	13.021	1854	1859	1862	rBV	3617834	3508281	77.40%	13.049%
17	13.904	2006	2009	2017	rBV	58612	65034	1.43%	0.242%
18	14.074	2034	2038	2041	rBV	750285	710918	15.68%	2.644%
19	15.562	2285	2291	2299	rBV	541299	739899	16.32%	2.752%
20	16.027	2364	2370	2376	rBV	59431	92355	2.04%	0.344%
21	16.545	2453	2458	2464	rVB2	66126	114358	2.52%	0.425%
22	17.156	2556	2562	2571	rVB3	59287	118763	2.62%	0.442%
23	17.880	2678	2685	2695	rVB4	48905	129232	2.85%	0.481%
24	18.745	2824	2832	2840	rVB5	31318	84710	1.87%	0.315%

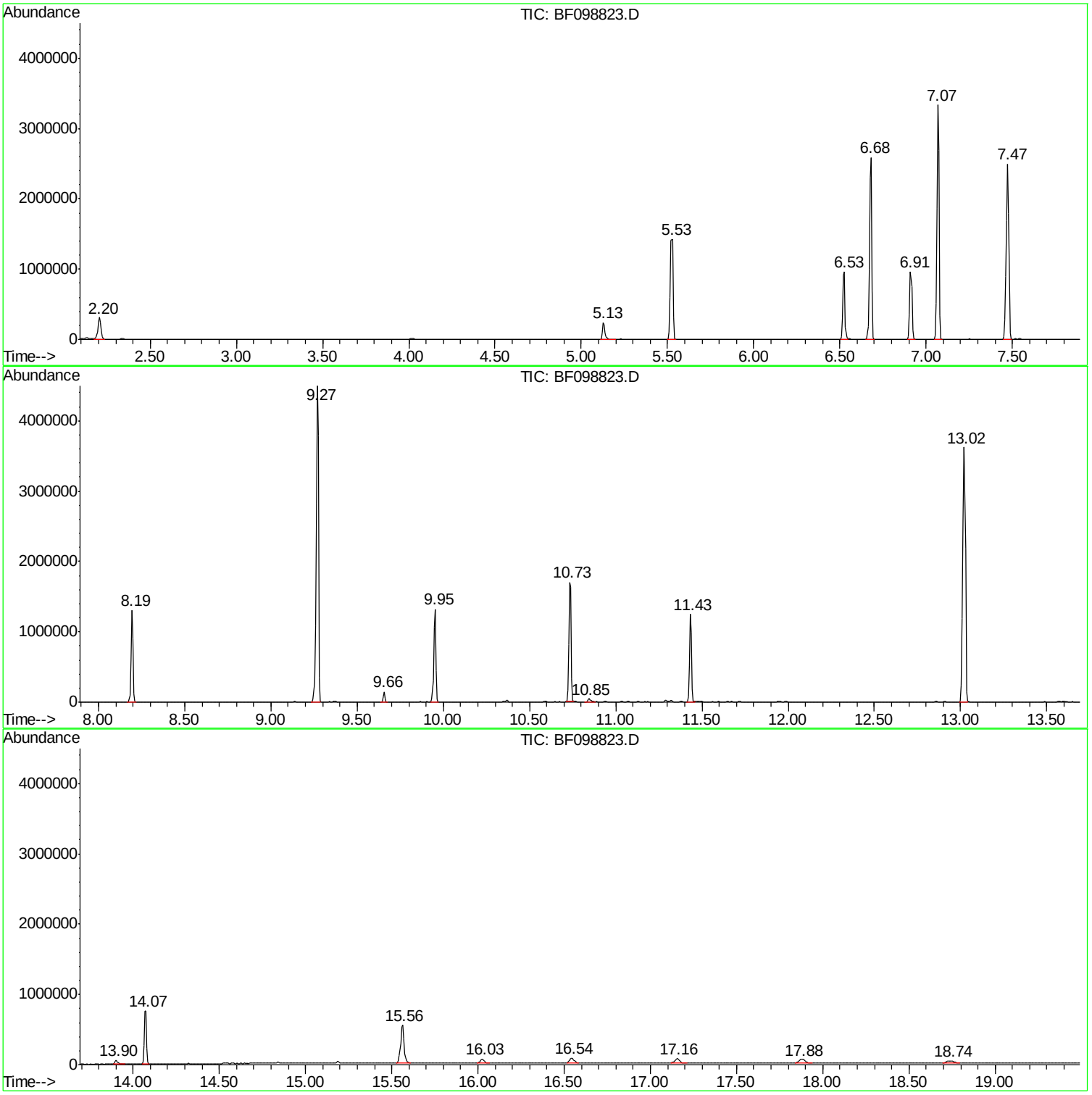
Sum of corrected areas: 26884795

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098823.D
Acq On : 26 Sep 2017 10:51
Operator : SJ/JU
Sample : I5384-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092017-SIDI-F-U-S

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098823.D
Acq On : 26 Sep 2017 10:51
Operator : SJ/JU
Sample : I5384-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092017-SIDI-F-U-S

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

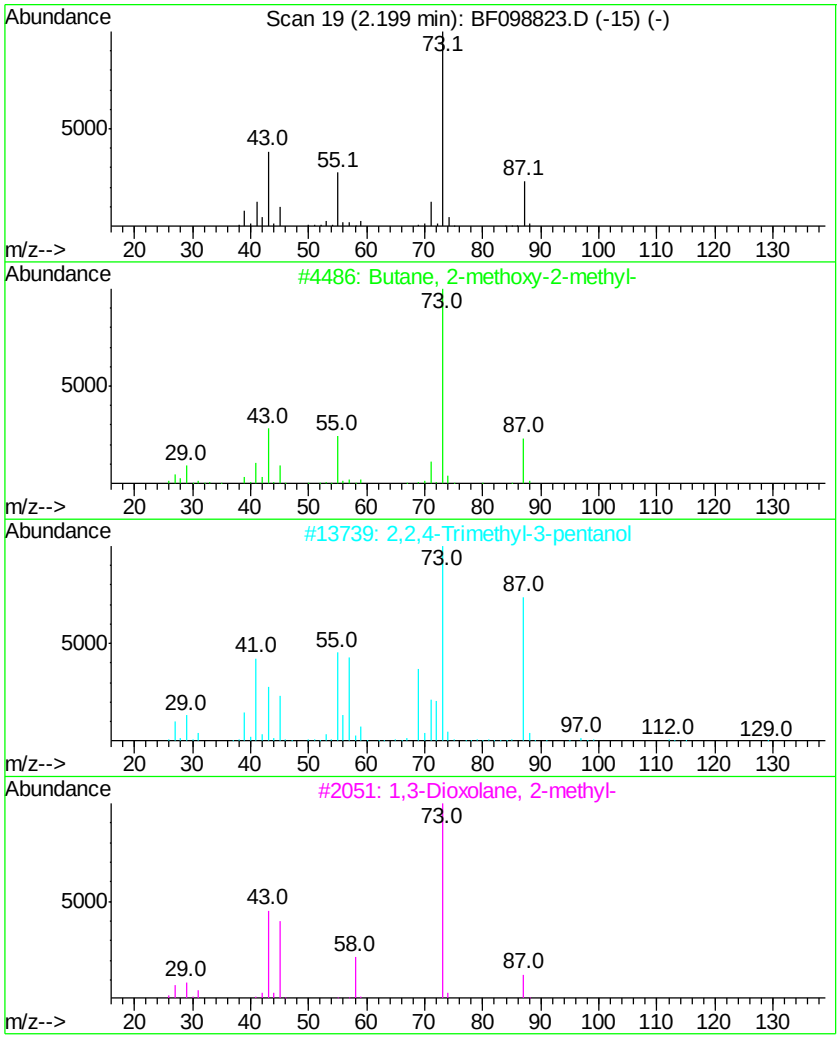
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

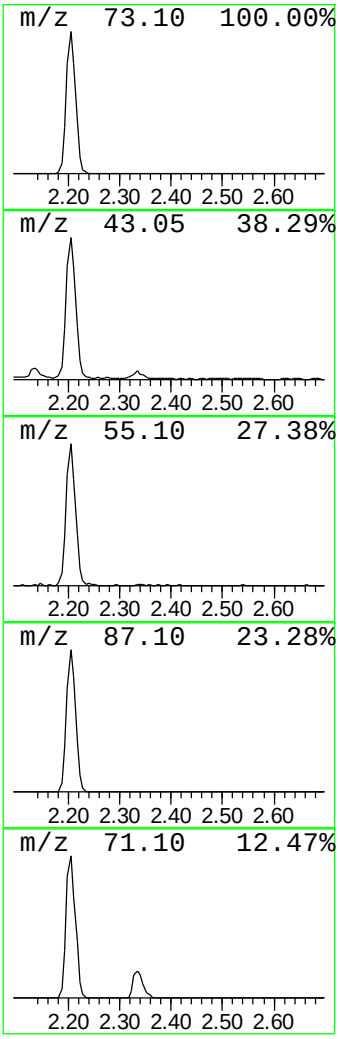
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	9.48 ng	375964	1,4-Dichlorobenzene-d4	6.91

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098823.D
Acq On : 26 Sep 2017 10:51
Operator : SJ/JU
Sample : I5384-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092017-SIDI-F-U-S

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

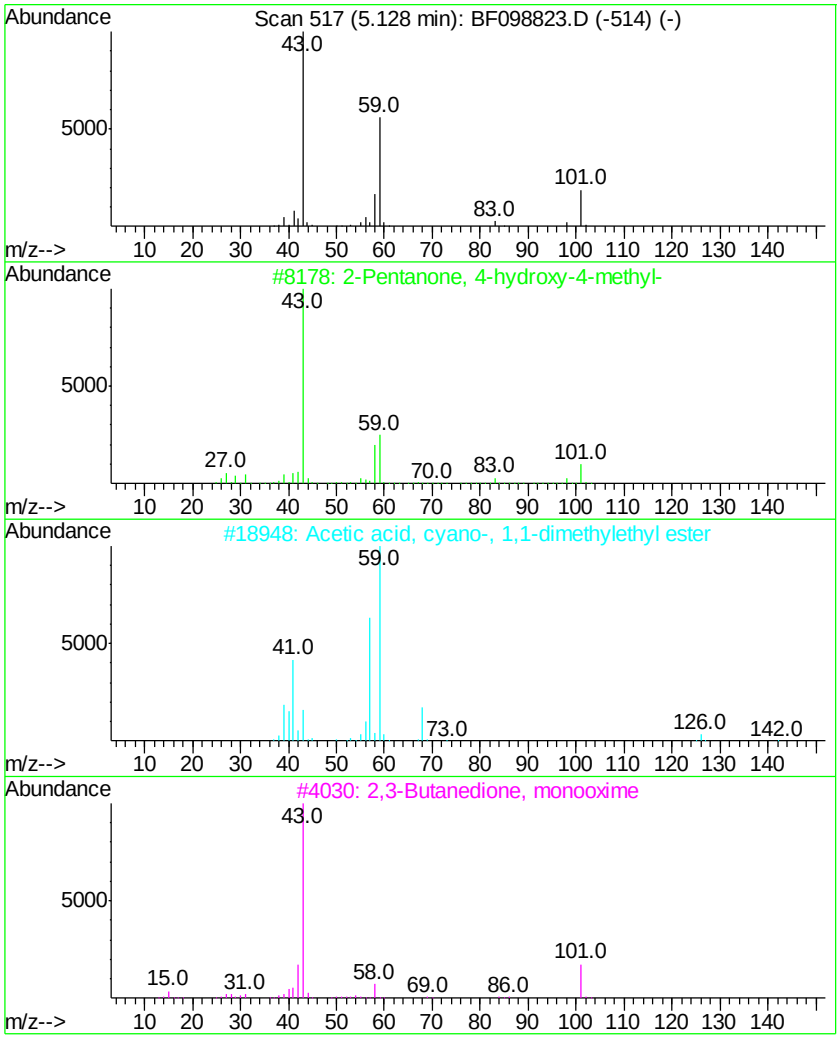
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

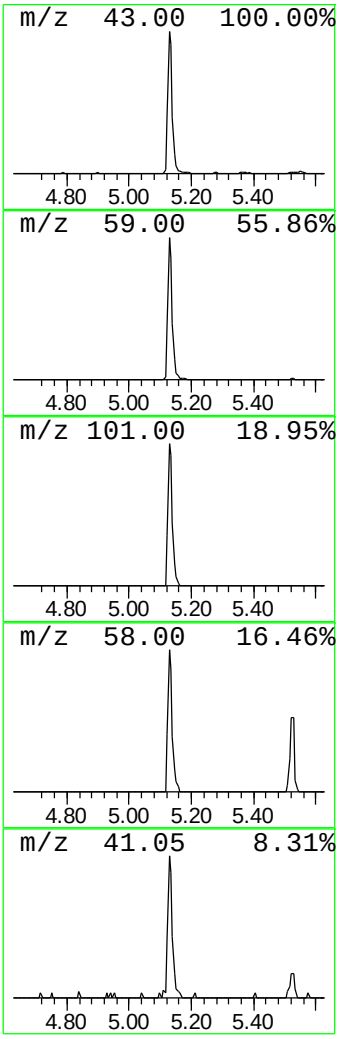
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	6.26 ng	248102	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098823.D
Acq On : 26 Sep 2017 10:51
Operator : SJ/JU
Sample : I5384-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092017-SIDI-F-U-S

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

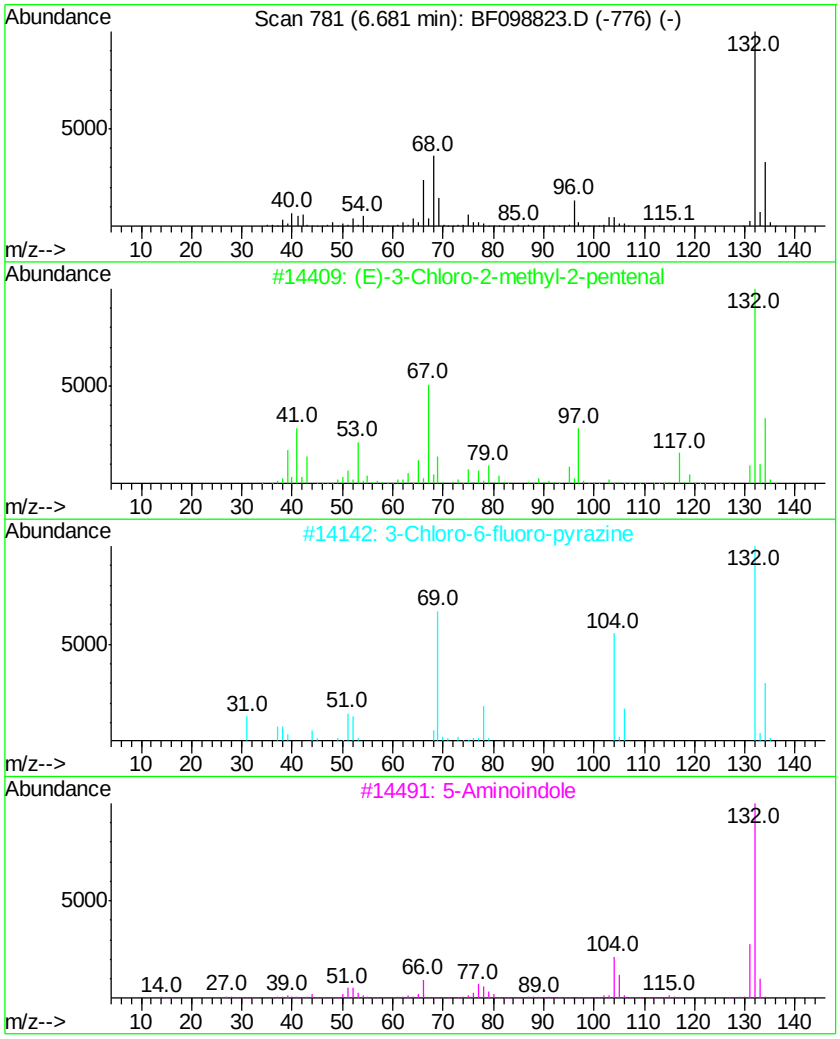
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

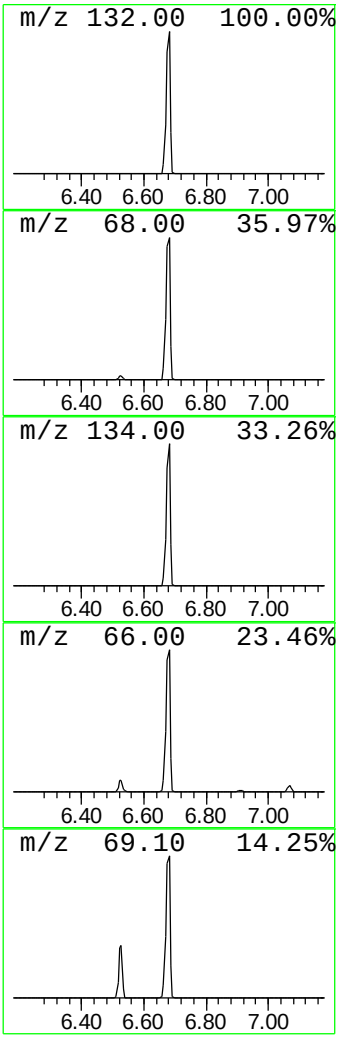
****

Peak Number 3 unknown6.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	60.45 ng	2397840	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098823.D
Acq On : 26 Sep 2017 10:51
Operator : SJ/JU
Sample : I5384-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092017-SIDI-F-U-S

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

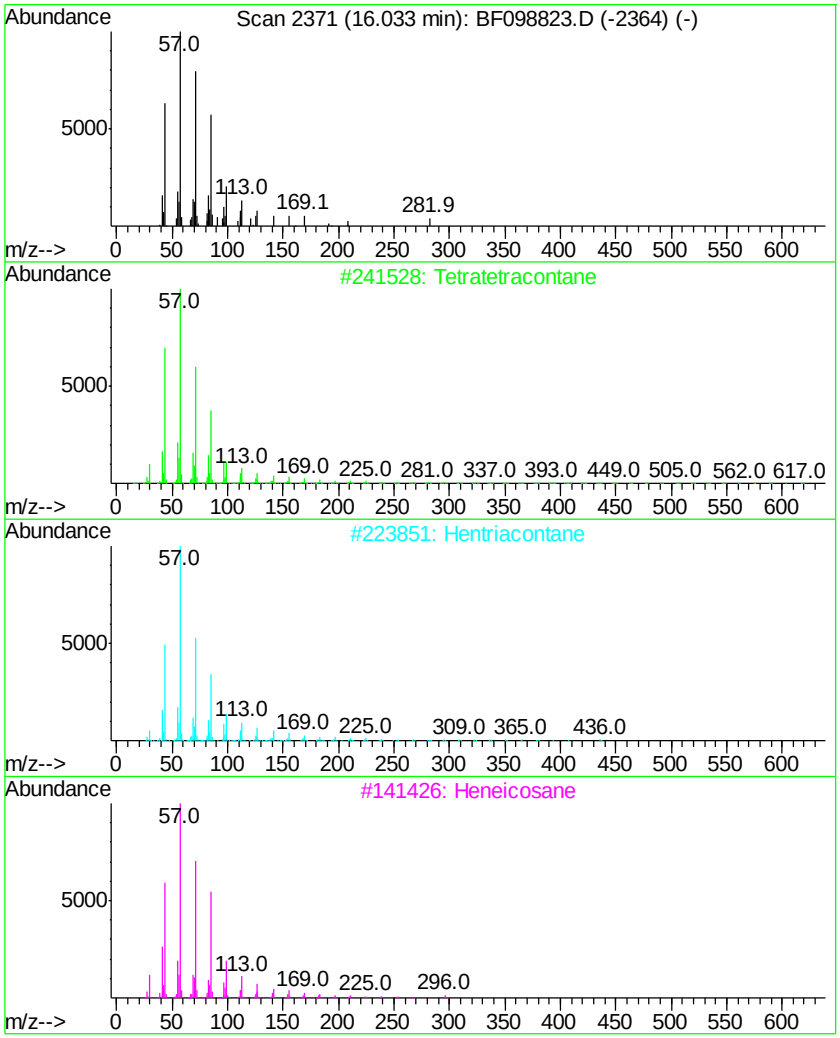
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

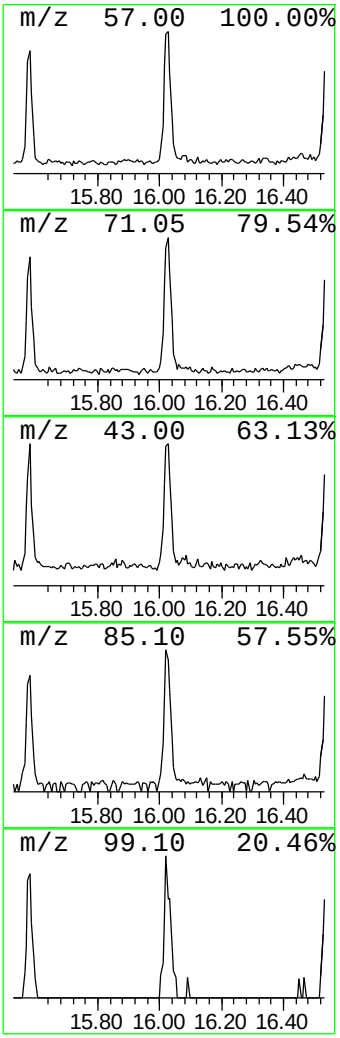
****

Peak Number 5 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.50 ng	92355	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098823.D
Acq On : 26 Sep 2017 10:51
Operator : SJ/JU
Sample : I5384-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092017-SIDI-F-U-S

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

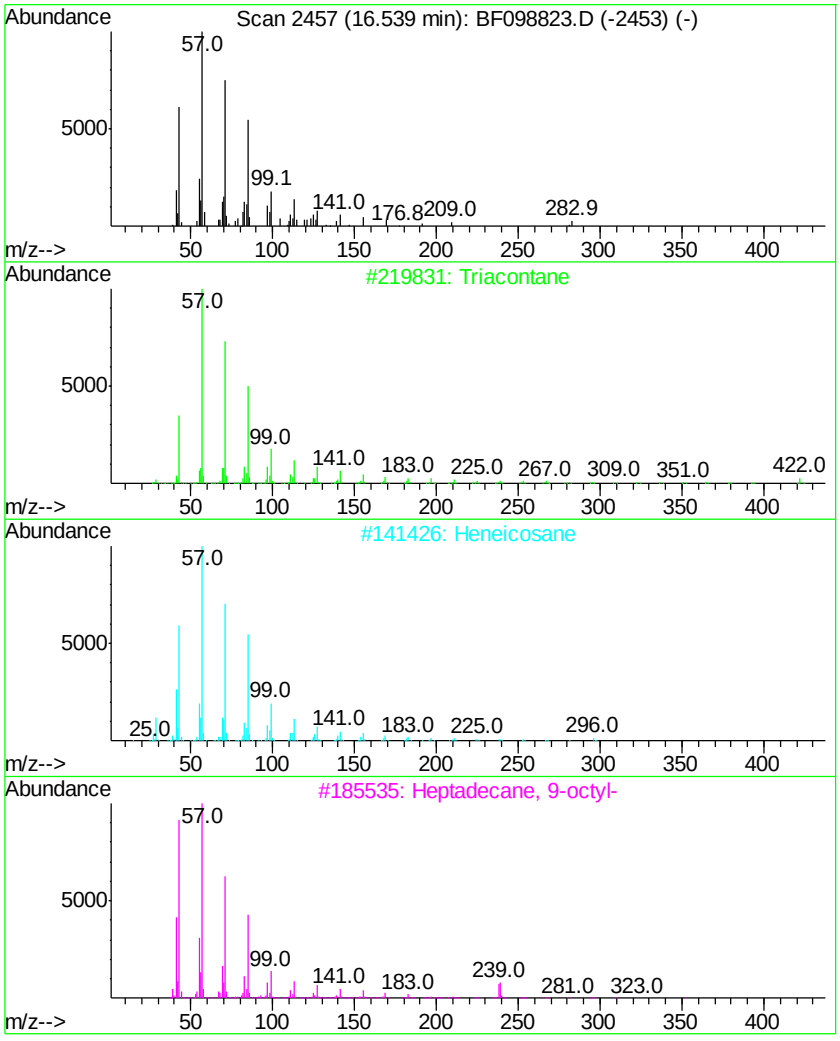
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

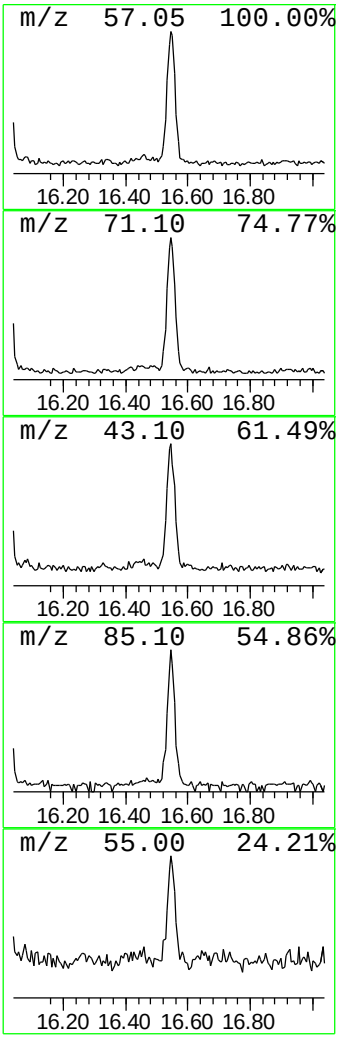
****

Peak Number 6 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	3.09 ng	114358	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Octacosane	394	C28H58	000630-02-4	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098823.D
Acq On : 26 Sep 2017 10:51
Operator : SJ/JU
Sample : I5384-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092017-SIDI-F-U-S

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

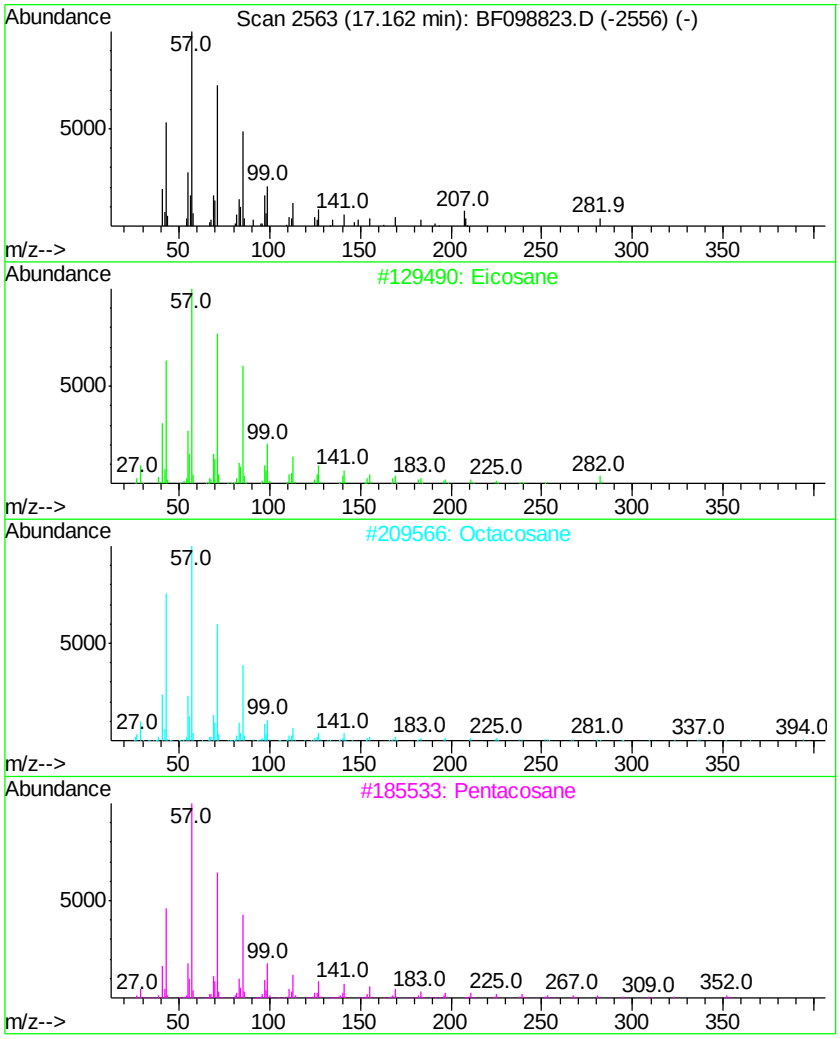
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

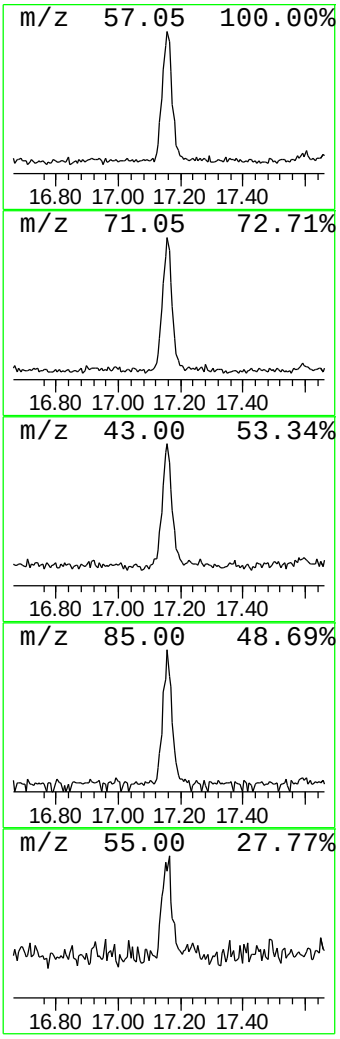
****

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	3.21 ng	118763	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Octacosane	394	C28H58	000630-02-4	90
3	Pentacosane	352	C25H52	000629-99-2	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heneicosane	296	C21H44	000629-94-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098823.D
Acq On : 26 Sep 2017 10:51
Operator : SJ/JU
Sample : I5384-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092017-SIDI-F-U-S

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...	2.20	9.5	ng	375964	1	6.91	793289	20.0
2-Pentanone, 4-hy...	5.13	6.3	ng	248102	1	6.91	793289	20.0
unknown6.68	6.68	60.5	ng	2397840	1	6.91	793289	20.0
Tetratetracontane	16.03	2.5	ng	92355	6	15.56	739899	20.0
Triacontane	16.54	3.1	ng	114358	6	15.56	739899	20.0
Eicosane	17.16	3.2	ng	118763	6	15.56	739899	20.0