LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098857.D
Acq On : 27 Sep 2017 12:24
Operator : SJ/JU
Sample : I5403-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-66(7-7.5)

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	2.228	21	24	40	rVB	129902	241027	7.21%	0.798%
2	5.145	516	520	533	rVB	505852	652906	19.53%	2.162%
3	5.539	581	587	590	rBV	3187414	3237221	96.85%	10.721%
4	6.539	751	757	760	rBV	3094424	3290642	98.45%	10.898%
5	6.686	777	782	785	rBV	3263226	3342469	100.00%	11.069%
6	6.916	817	821	824	rVB	963014	823014	24.62%	2.726%
7	7.069	843	847	851	rBV	2577604	2272273	67.98%	7.525%
8	7.475	911	916	919	rBV	2143436	2048988	61.30%	6.786%
9	7.545	924	928	933	rVB	38604	37590	1.12%	0.124%
10	8.192	1034	1038	1042	rBV	1255288	1136763	34.01%	3.765%
11	9.269	1216	1221	1224	rBV	3569776	3280307	98.14%	10.863%
12	9.657	1283	1287	1291	rBV	652423	542573	16.23%	1.797%
13	9.874	1316	1324	1328	rBV3	22387	34764	1.04%	0.115%
14	9.951	1333	1337	1341	rVB	1481247	1241568	37.15%	4.112%
15	10.321	1396	1400	1403	rBV	126581	108917	3.26%	0.361%
16	10.374	1406	1409	1411	rVB	51861	45666	1.37%	0.151%
17	10.739	1464	1471	1474	rBV	2151317	2048477	61.29%	6.784%
18	10.845	1486	1489	1498	rVB	72877	71031	2.13%	0.235%
19	11.439	1586	1590	1593	rBV	1436939	1202591	35.98%	3.983%
20	11.498	1593	1600	1604	rVB5	29242	35522	1.06%	0.118%
21	11.951	1674	1677	1682	rBV	50665	44375	1.33%	0.147%
22	13.021	1855	1859	1862	rBV	3065875	2773758	82.99%	9.186%
23	13.904	2006	2009	2015	rBV	191192	185425	5.55%	0.614%
24	14.074	2034	2038	2042	rBV	931588	790684	23.66%	2.619%
25	15.562	2286	2291	2300	rVB	543940	707484	21.17%	2.343%

Sum of corrected areas: 30196035

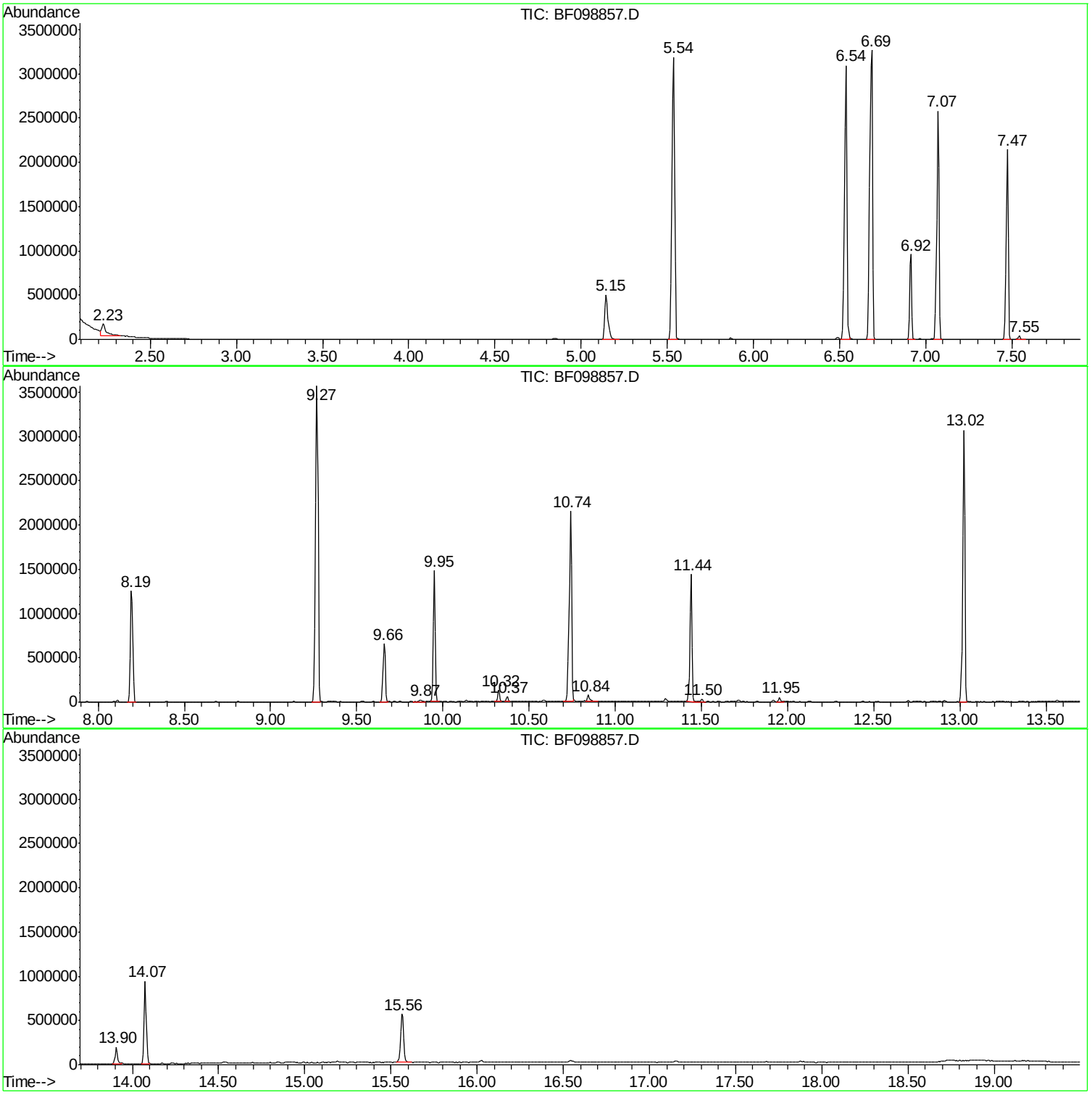
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098857.D
Acq On : 27 Sep 2017 12:24
Operator : SJ/JU
Sample : I5403-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-66(7-7.5)

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\BF092717\
Data File : BF098857.D
Acq On : 27 Sep 2017 12:24
Operator : SJ/JU
Sample : I5403-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-66(7-7.5)

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

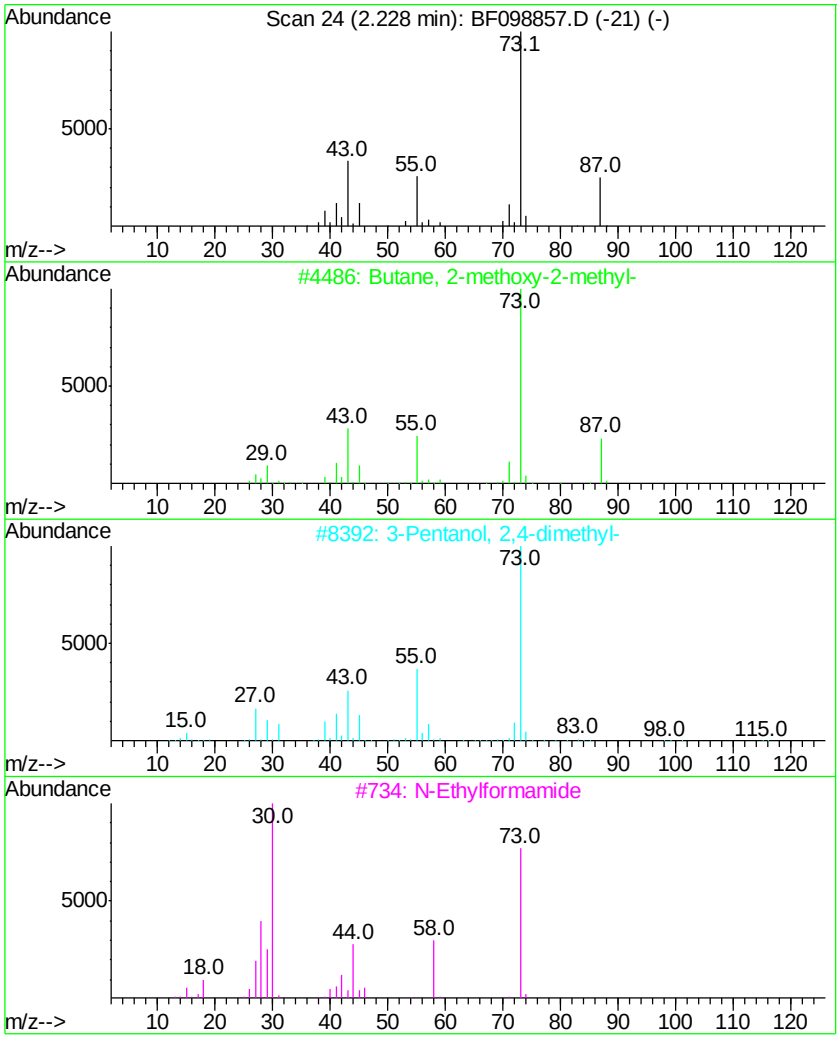
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

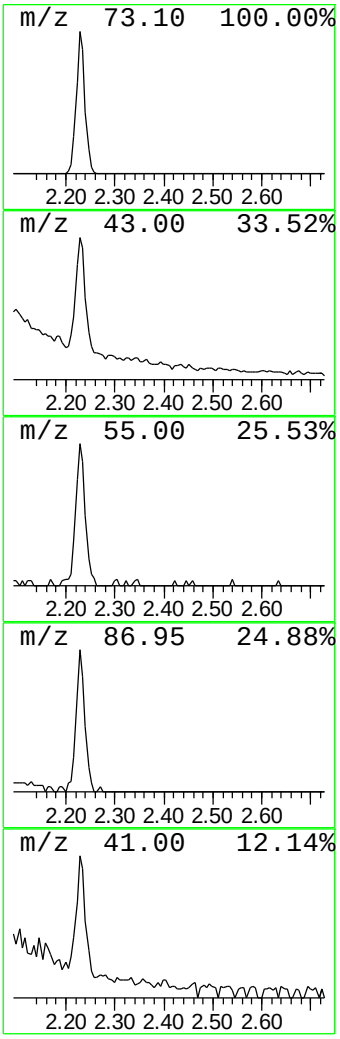
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	5.86 ng	241027	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	78
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098857.D
Acq On : 27 Sep 2017 12:24
Operator : SJ/JU
Sample : I5403-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-66(7-7.5)

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

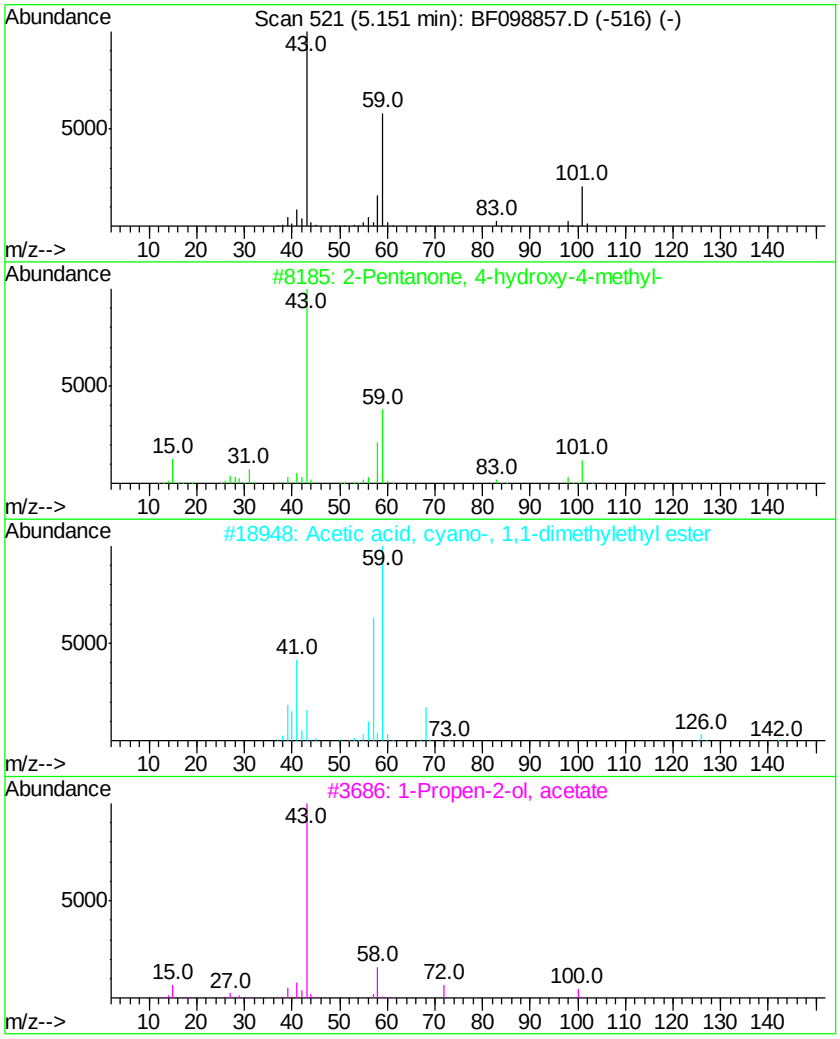
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

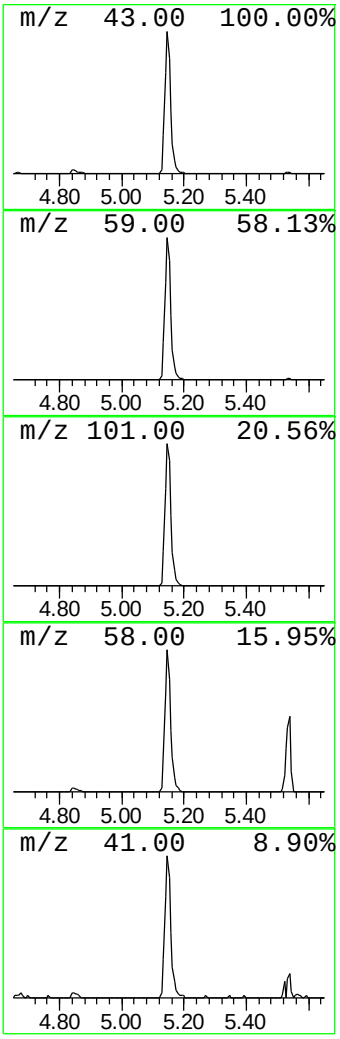
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	15.87 ng	652906	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098857.D
Acq On : 27 Sep 2017 12:24
Operator : SJ/JU
Sample : I5403-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-66(7-7.5)

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

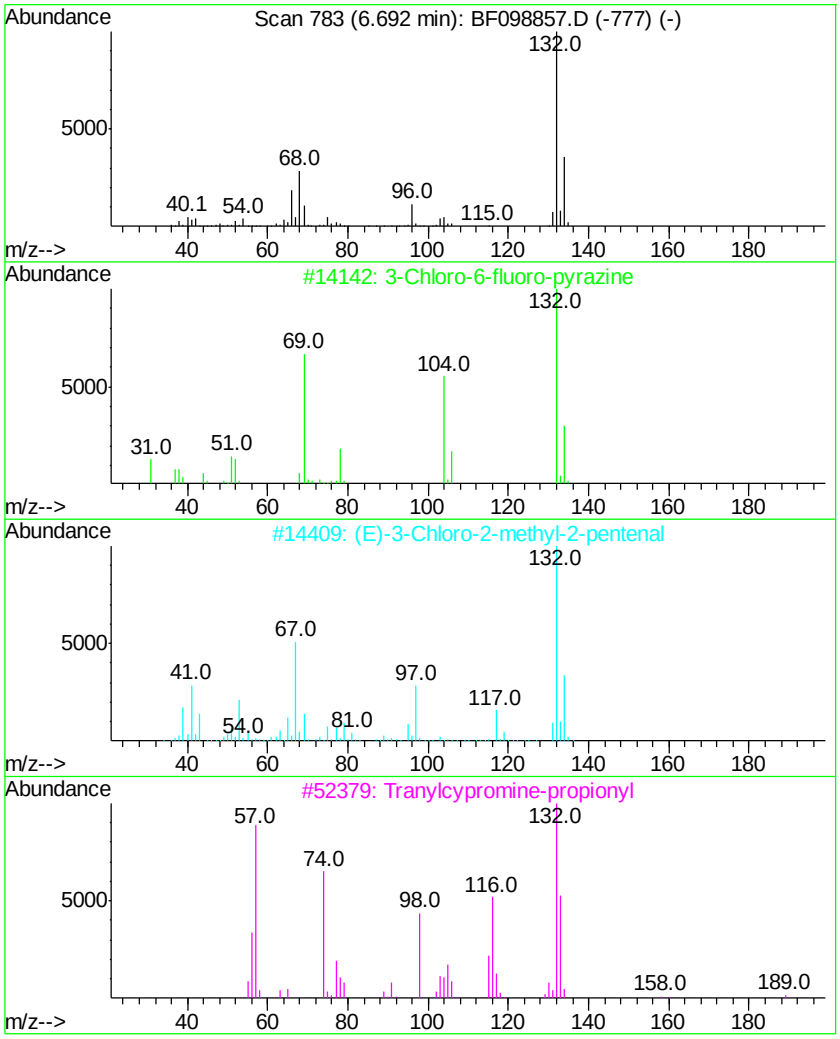
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

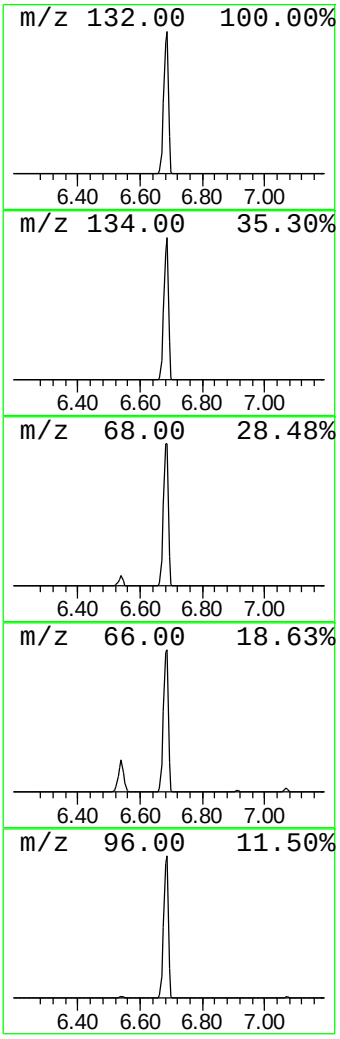
****

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	81.23 ng	3342470	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	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098857.D
Acq On : 27 Sep 2017 12:24
Operator : SJ/JU
Sample : I5403-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-66(7-7.5)

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

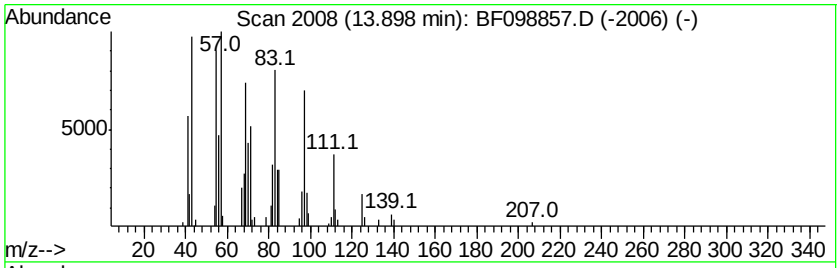
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

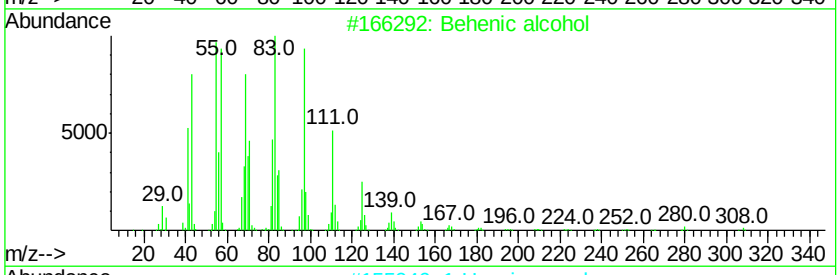
****

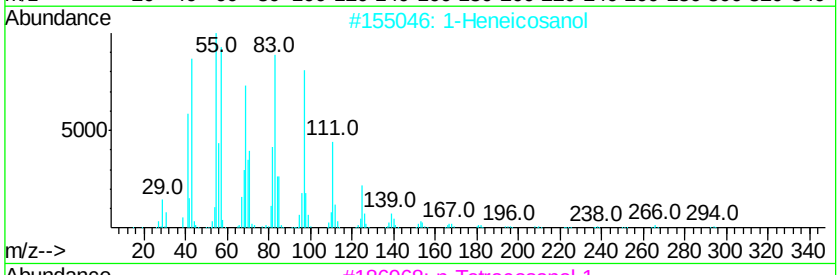
Peak Number 5 Behenic alcohol Concentration Rank 5

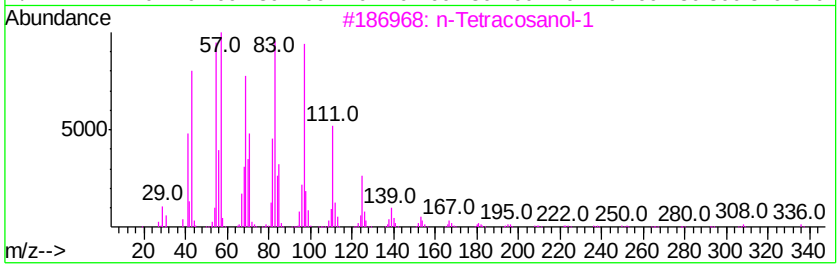
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.69 ng	185425	Chrysene-d12	14.07

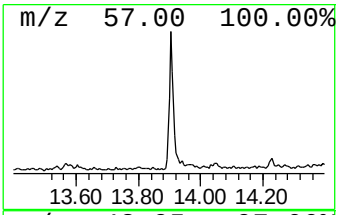
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91

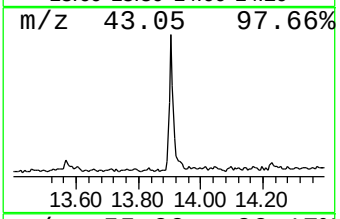


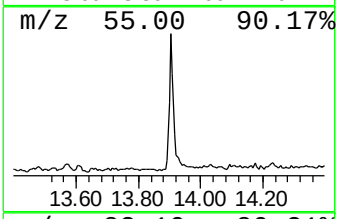


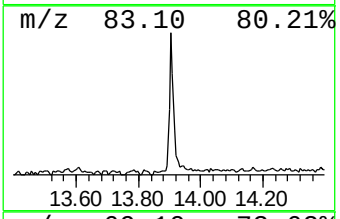


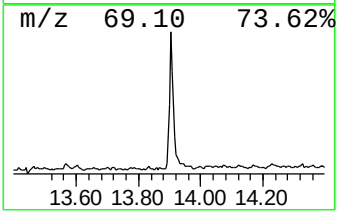












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098857.D
Acq On : 27 Sep 2017 12:24
Operator : SJ/JU
Sample : I5403-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-66(7-7.5)

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...	2.23	5.9	ng	241027	1	6.92	823014	20.0
2-Pentanone, 4-hy...	5.15	15.9	ng	652906	1	6.92	823014	20.0
unknown6.69	6.69	81.2	ng	3342470	1	6.92	823014	20.0
Behenic alcohol	13.90	4.7	ng	185425	5	14.07	790684	20.0