LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098792.D
Acq On : 25 Sep 2017 19:39
Operator : SJ/JU
Sample : I5395-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

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	2.222	19	23	38	rVB	86081	129883	3.78%	0.401%
2	5.145	516	520	528	rBV	505476	609281	17.73%	1.880%
3	5.534	581	586	589	rBV	3244452	3314373	96.43%	10.225%
4	6.539	751	757	766	rVB	3036476	3437053	100.00%	10.603%
5	6.681	776	781	785	rBV	3207405	3390414	98.64%	10.459%
6	6.916	817	821	824	rBV	892235	795100	23.13%	2.453%
7	7.069	843	847	851	rVB	2795694	2449062	71.25%	7.555%
8	7.475	911	916	919	rBV	2160619	2050107	59.65%	6.324%
9	8.192	1034	1038	1042	rBV	1217537	1087652	31.64%	3.355%
10	9.269	1216	1221	1224	rBV	3677671	3429100	99.77%	10.579%
11	9.657	1283	1287	1290	rBV	570635	450873	13.12%	1.391%
12	9.951	1332	1337	1341	rVB	1398955	1198804	34.88%	3.698%
13	10.251	1382	1388	1393	rBV	27830	35087	1.02%	0.108%
14	10.374	1401	1409	1412	rBV2	67189	71345	2.08%	0.220%
15	10.739	1464	1471	1474	rBV	2259254	2210337	64.31%	6.819%
16	10.845	1486	1489	1498	rBV	84639	79732	2.32%	0.246%
17	11.439	1586	1590	1593	rBV	1454284	1236439	35.97%	3.814%
18	11.951	1673	1677	1681	rBV	117646	101668	2.96%	0.314%
19	13.021	1854	1859	1863	rBV	3383652	3392932	98.72%	10.467%
20	13.904	2005	2009	2022	rBV	440533	416514	12.12%	1.285%
21	14.074	2034	2038	2042	rVB	1266173	1120197	32.59%	3.456%
22	14.539	2112	2117	2123	rBV3	59430	85639	2.49%	0.264%
23	15.192	2224	2228	2231	rBV	36000	48123	1.40%	0.148%
24	15.568	2286	2292	2299	rBV	782704	1045186	30.41%	3.224%
25	16.027	2366	2370	2375	rBV	40739	62585	1.82%	0.193%
26	16.080	2375	2379	2384	rVV2	39824	60773	1.77%	0.187%
27	16.550	2455	2459	2464	rVB2	37763	60794	1.77%	0.188%
28	17.168	2560	2564	2569	rVB4	25004	46350	1.35%	0.143%

Sum of corrected areas: 32415403

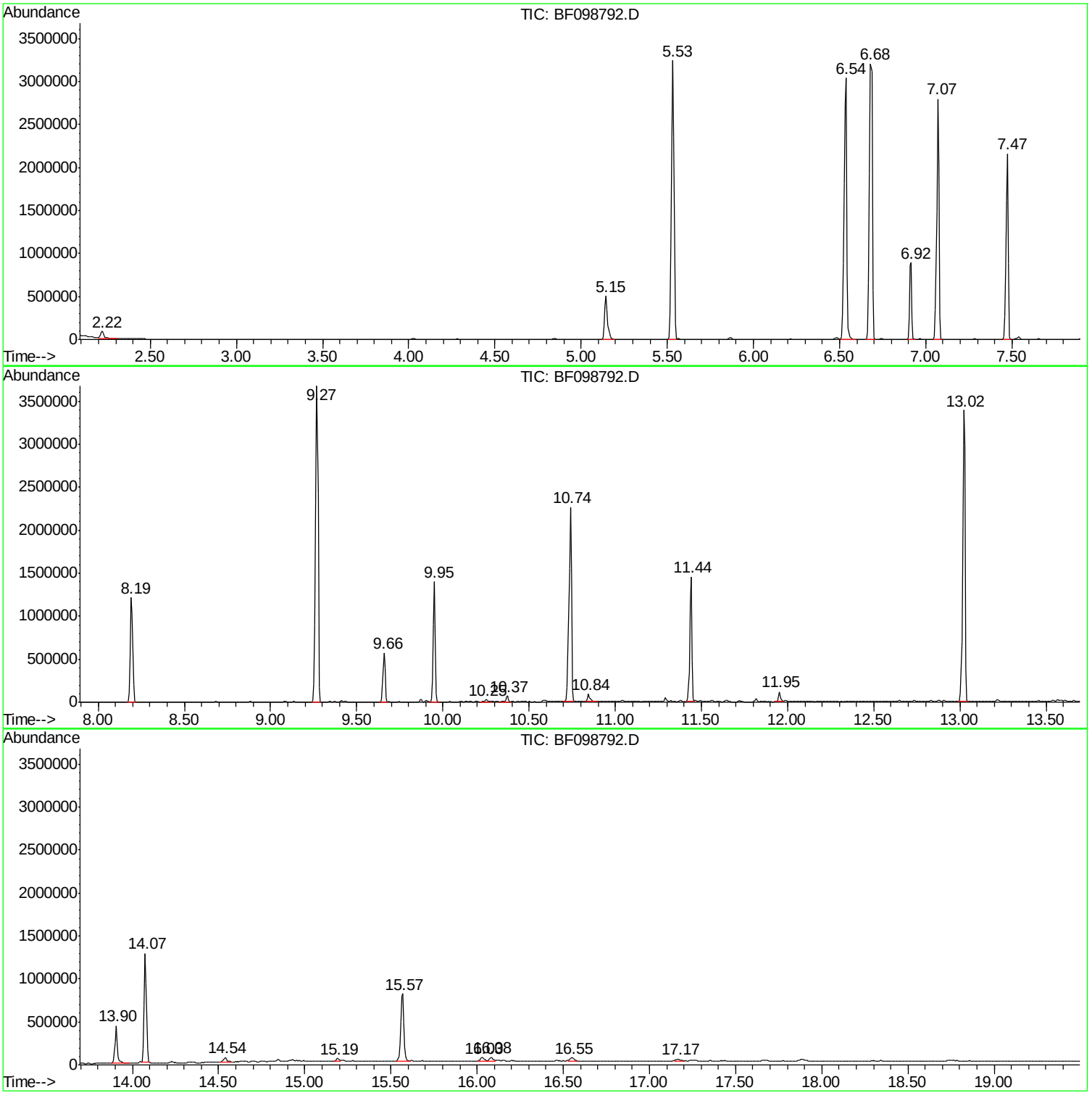
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098792.D
Acq On : 25 Sep 2017 19:39
Operator : SJ/JU
Sample : I5395-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-(0-5)

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\BF092517\
Data File : BF098792.D
Acq On : 25 Sep 2017 19:39
Operator : SJ/JU
Sample : I5395-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

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

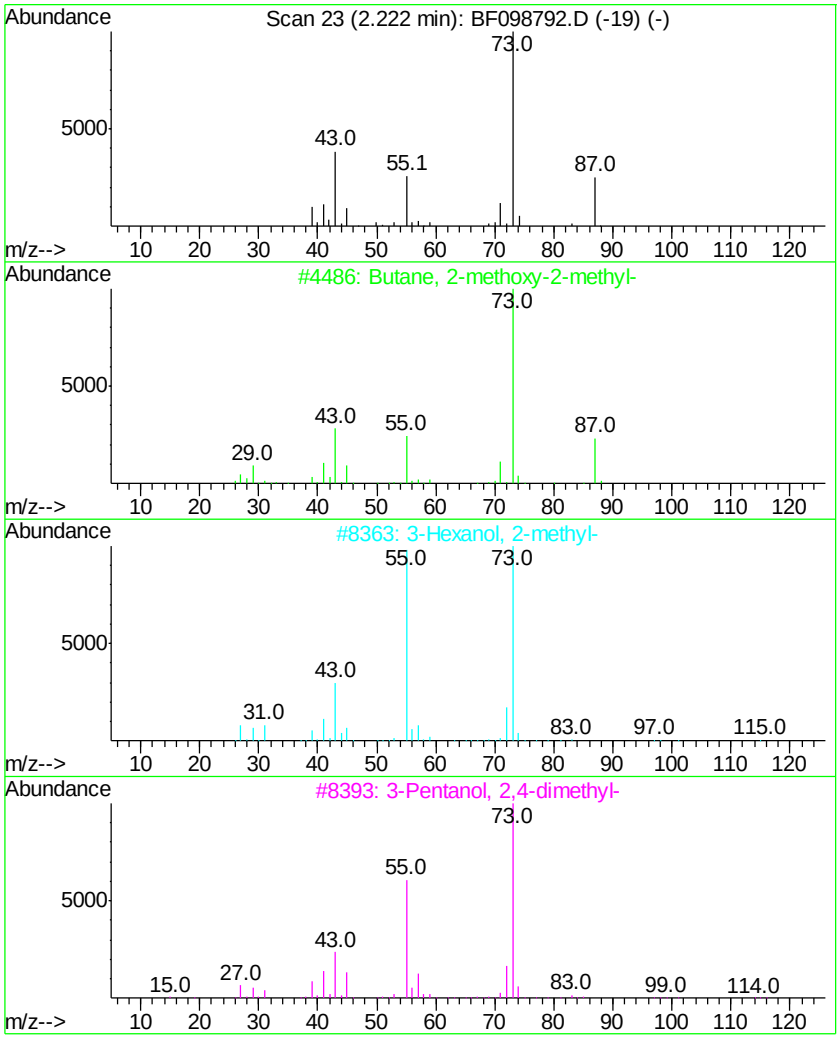
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

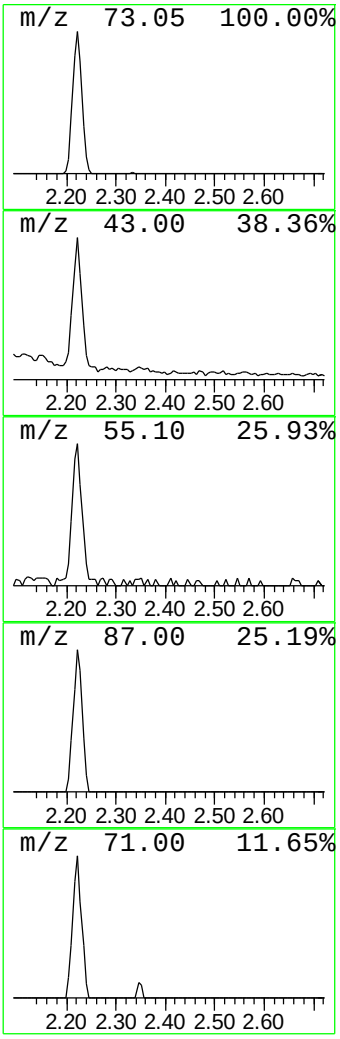
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	3.27 ng	129883	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	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098792.D
Acq On : 25 Sep 2017 19:39
Operator : SJ/JU
Sample : I5395-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

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

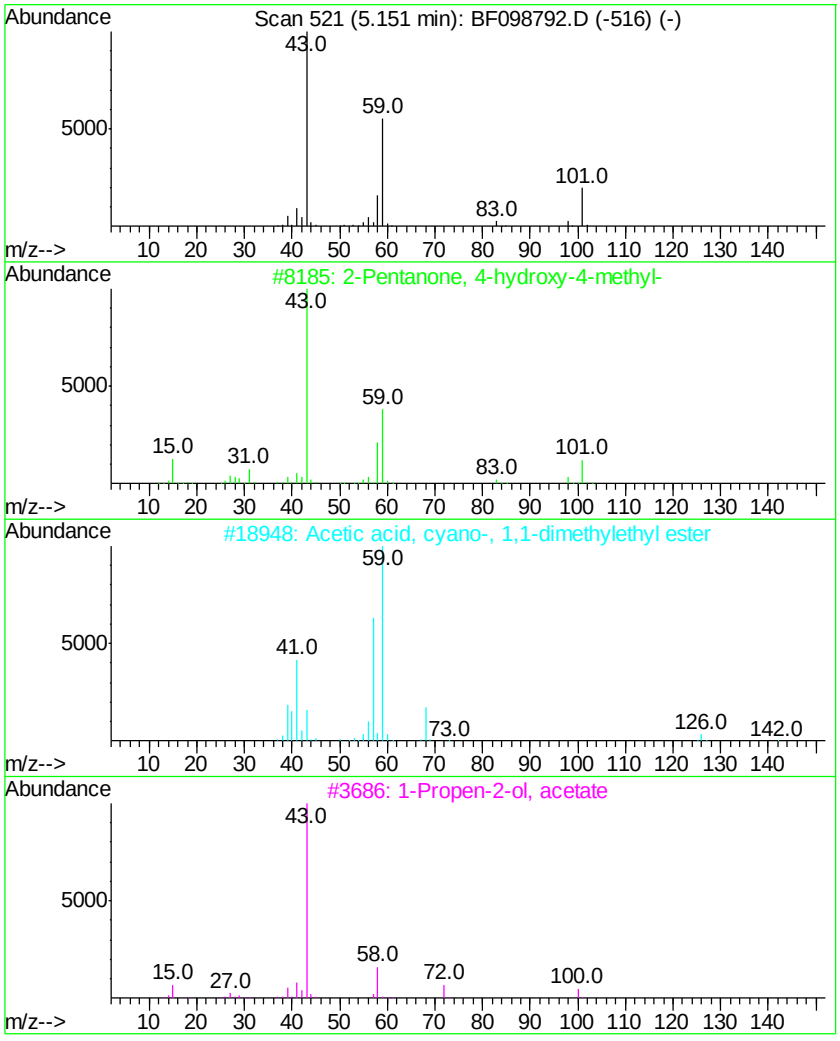
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

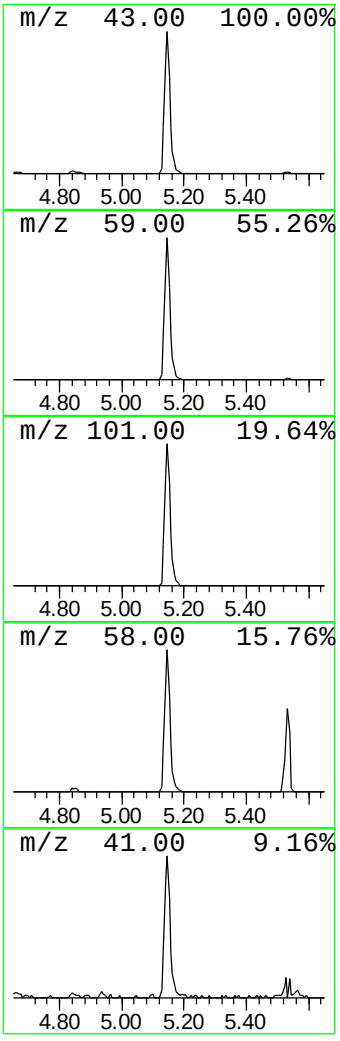
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	15.33 ng	609281	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	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098792.D
Acq On : 25 Sep 2017 19:39
Operator : SJ/JU
Sample : I5395-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

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

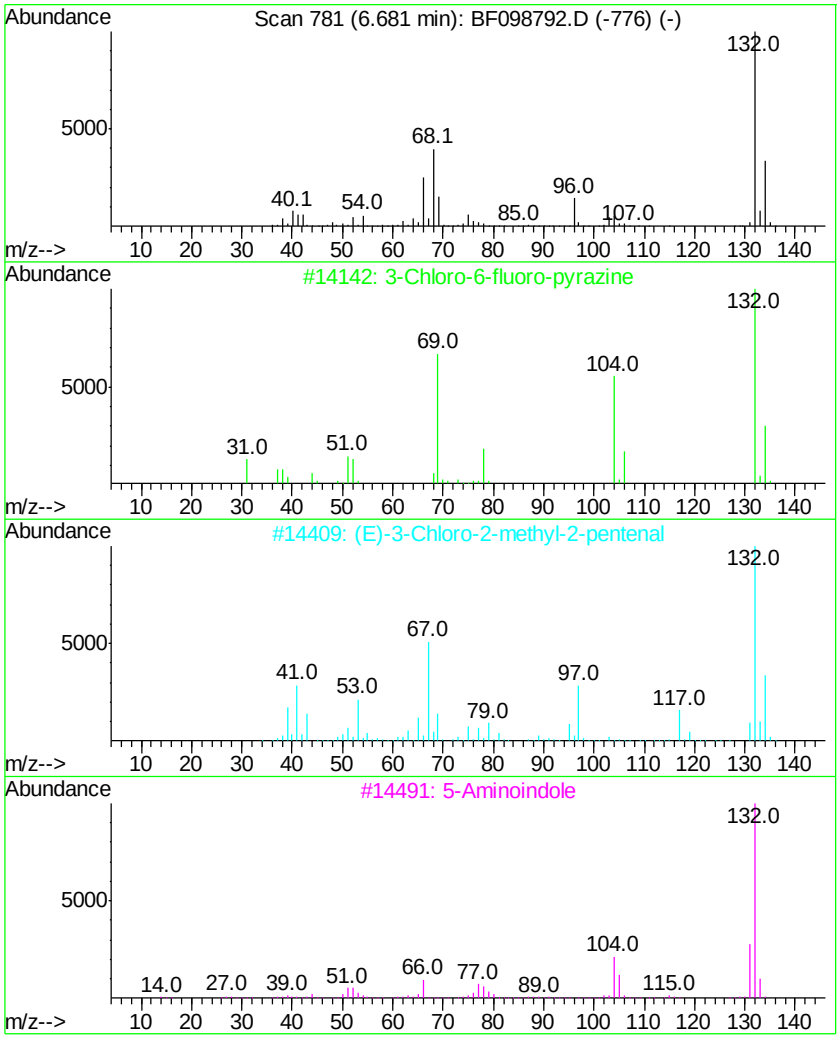
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

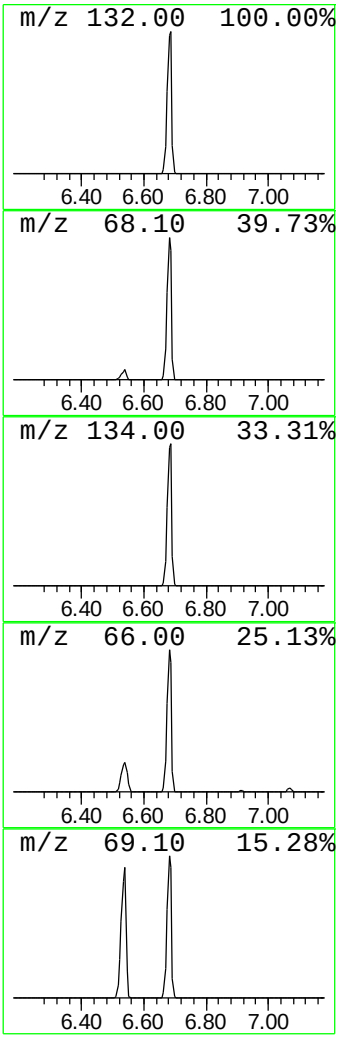
****

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	85.28 ng	3390410	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	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098792.D
Acq On : 25 Sep 2017 19:39
Operator : SJ/JU
Sample : I5395-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

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

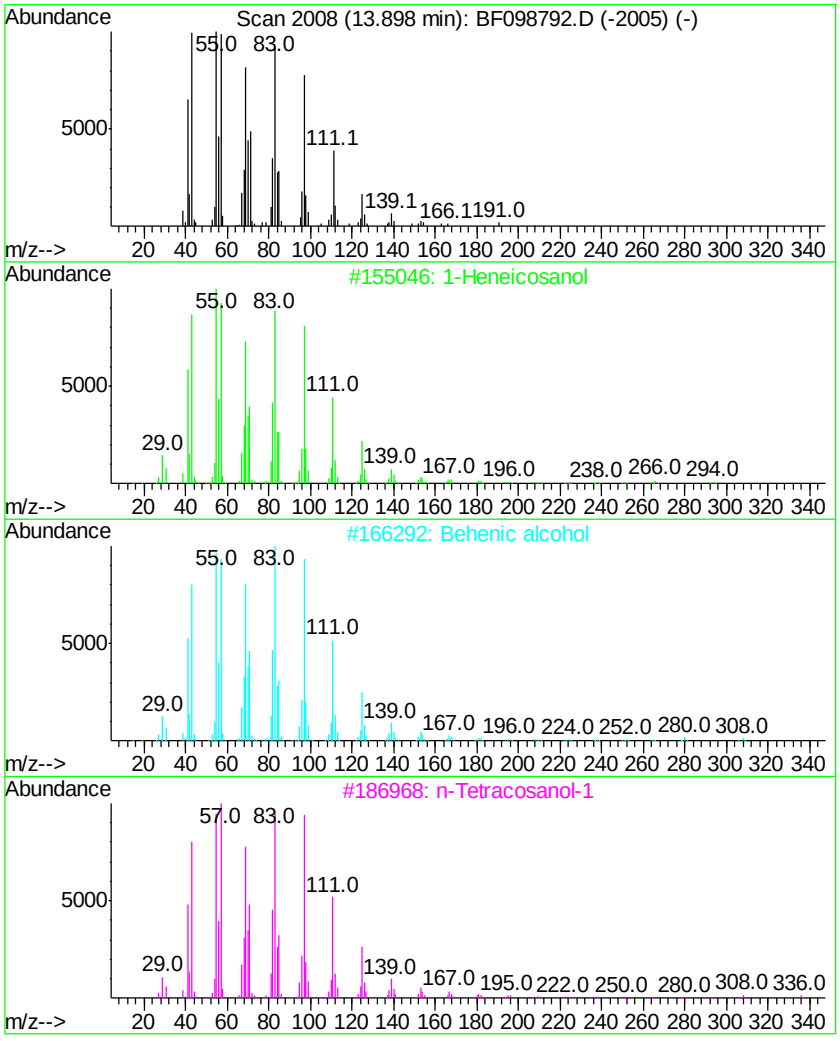
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

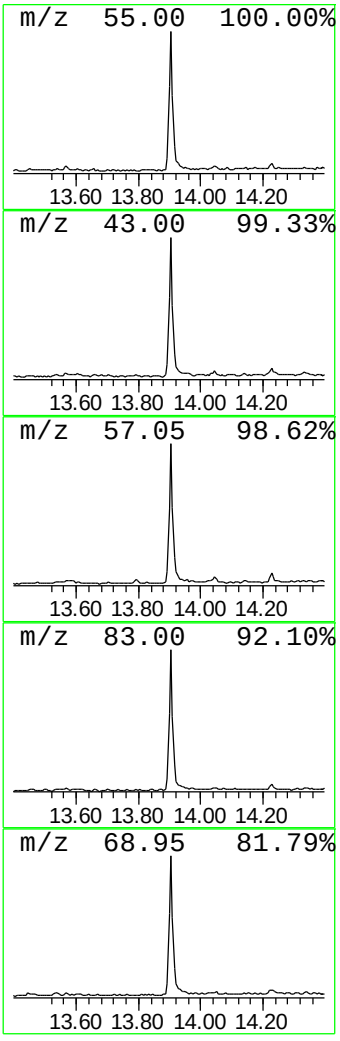
****

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	7.44 ng	416514	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098792.D
Acq On : 25 Sep 2017 19:39
Operator : SJ/JU
Sample : I5395-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

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...	2.22	3.3	ng	129883	1	6.92	795100	20.0
2-Pentanone, 4-hy...	5.15	15.3	ng	609281	1	6.92	795100	20.0
unknown6.68	6.68	85.3	ng	3390410	1	6.92	795100	20.0
1-Heneicosanol	13.90	7.4	ng	416514	5	14.07	1120200	20.0