LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098829.D
Acq On : 26 Sep 2017 13:49
Operator : SJ/JU
Sample : I5394-04 10X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20-41

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	2.334	39	42	65	rVB3	63037	182928	13.73%	1.693%
2	2.528	73	75	80	rVB2	14858	19630	1.47%	0.182%
3	5.122	512	516	521	rBV	82570	75516	5.67%	0.699%
4	5.516	579	583	587	rBV	500020	410550	30.81%	3.799%
5	6.522	750	754	759	rBV	548772	434865	32.63%	4.024%
6	6.675	776	780	783	rBV	572673	451905	33.91%	4.182%
7	6.910	816	820	824	rVB	1136908	921649	69.16%	8.529%
8	7.063	843	846	850	rVB	390866	335684	25.19%	3.106%
9	7.469	911	915	918	rBV	309353	258817	19.42%	2.395%
10	8.163	1028	1033	1034	rBV2	11439	14693	1.10%	0.136%
11	8.192	1034	1038	1041	rVV	1509686	1245316	93.44%	11.524%
12	9.263	1216	1220	1224	rBV	674308	534209	40.08%	4.944%
13	9.657	1284	1287	1294	rBV	61798	49262	3.70%	0.456%
14	9.810	1305	1313	1316	rBV2	18932	23055	1.73%	0.213%
15	9.869	1316	1323	1328	rVB6	6236	14983	1.12%	0.139%
16	9.951	1331	1337	1340	rBV	1522385	1332698	100.00%	12.333%
17	10.133	1364	1368	1372	rBV5	11929	14954	1.12%	0.138%
18	10.733	1466	1470	1473	rBV	305696	261932	19.65%	2.424%
19	11.080	1525	1529	1535	rVB7	11496	17529	1.32%	0.162%
20	11.433	1585	1589	1592	rBV	1455417	1294717	97.15%	11.982%
21	11.457	1592	1593	1596	rVB2	28985	18247	1.37%	0.169%
22	11.816	1650	1654	1657	rBV	21004	18433	1.38%	0.171%
23	11.945	1671	1676	1681	rBV5	75453	104132	7.81%	0.964%
24	12.233	1722	1725	1727	rBV	34911	34426	2.58%	0.319%
25	12.480	1763	1767	1770	rVB3	14964	16179	1.21%	0.150%
26	12.645	1792	1795	1800	rBV	52908	48307	3.62%	0.447%
27	12.733	1807	1810	1816	rBV2	74823	79774	5.99%	0.738%
28	12.874	1831	1834	1837	rBV	57605	45142	3.39%	0.418%
29	13.015	1854	1858	1861	rVB	539391	452375	33.94%	4.186%
30	13.204	1883	1890	1895	rBV8	21404	47969	3.60%	0.444%
31	13.704	1973	1975	1980	rVB5	12546	16584	1.24%	0.153%
32	13.904	2006	2009	2016	rVB8	28205	49743	3.73%	0.460%
33	14.074	2033	2038	2041	rBV	1015574	947886	71.13%	8.772%
34	14.098	2041	2042	2047	rVB	36707	29525	2.22%	0.273%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098829.D
Acq On : 26 Sep 2017 13:49
Operator : SJ/JU
Sample : I5394-04 10X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20-41

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

35	15.127	2213	2217	2224	rVB3	48855	81853	6.14%	0.757%
36	15.268	2239	2241	2246	rBV6	21210	24457	1.84%	0.226%
37	15.562	2286	2291	2306	rVB	673253	896027	67.23%	8.292%

Sum of corrected areas: 10805951

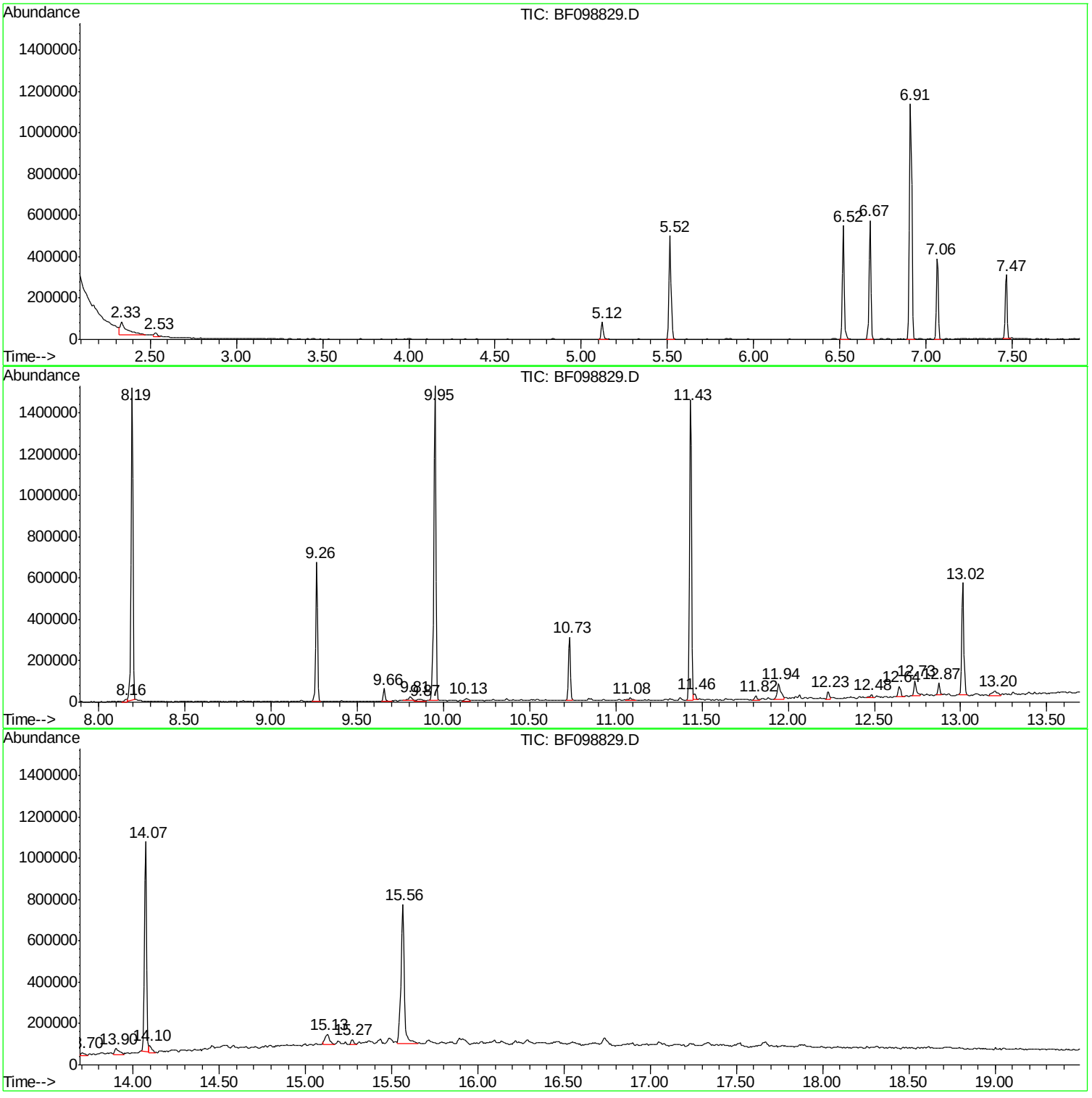
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098829.D
Acq On : 26 Sep 2017 13:49
Operator : SJ/JU
Sample : I5394-04 10X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20-41

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\BF092617\
Data File : BF098829.D
Acq On : 26 Sep 2017 13:49
Operator : SJ/JU
Sample : I5394-04 10X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20-41

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

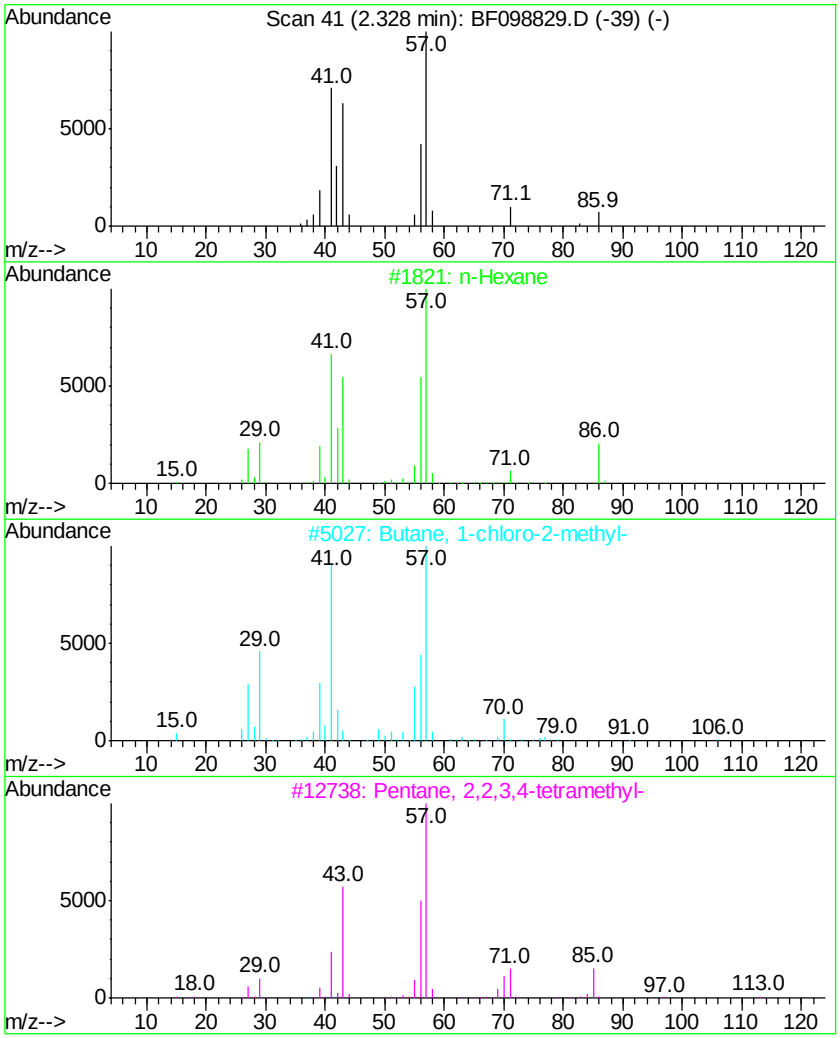
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

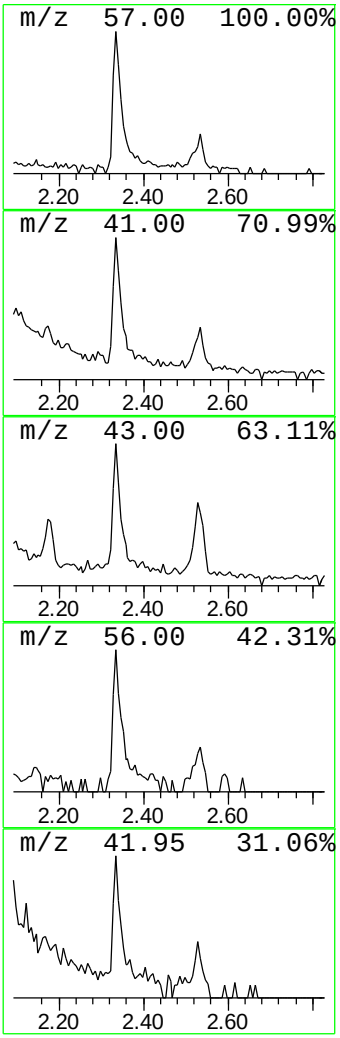
****

Peak Number 1 n-Hexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	3.97 ng	182928	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	83
2	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	45
3	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	36
5	Butanal, 2-methyl-	86	C5H10O	000096-17-3	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098829.D
Acq On : 26 Sep 2017 13:49
Operator : SJ/JU
Sample : I5394-04 10X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20-41

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

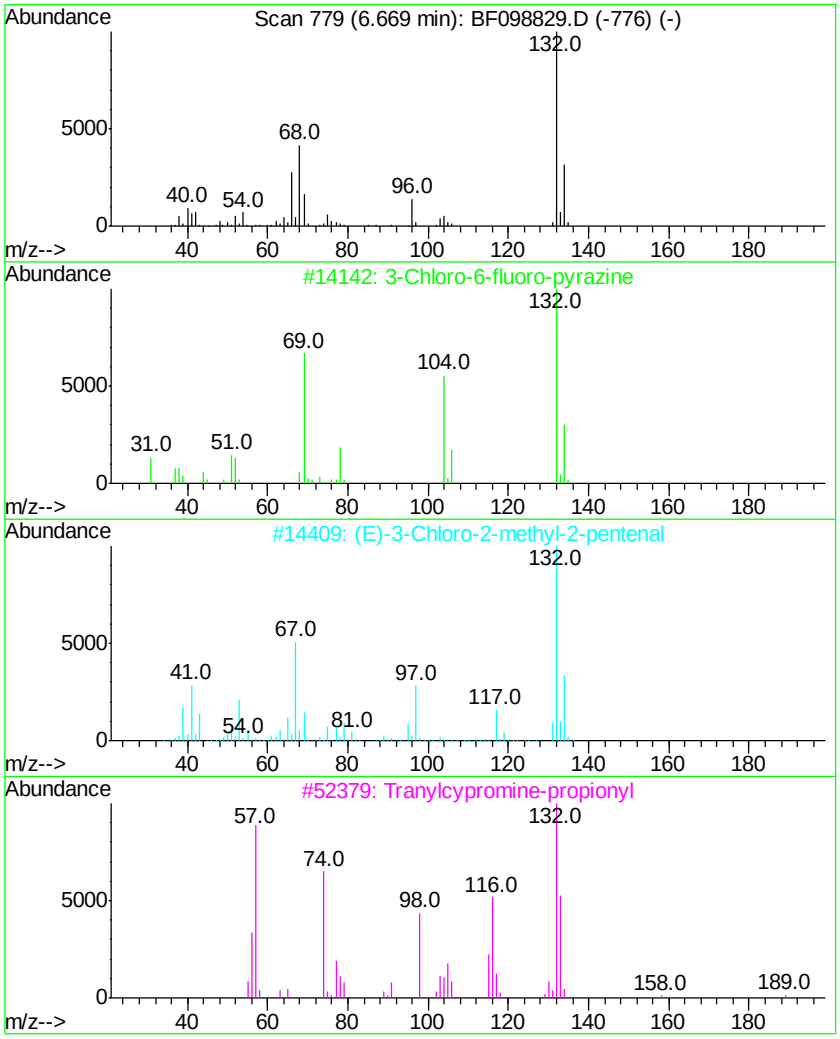
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

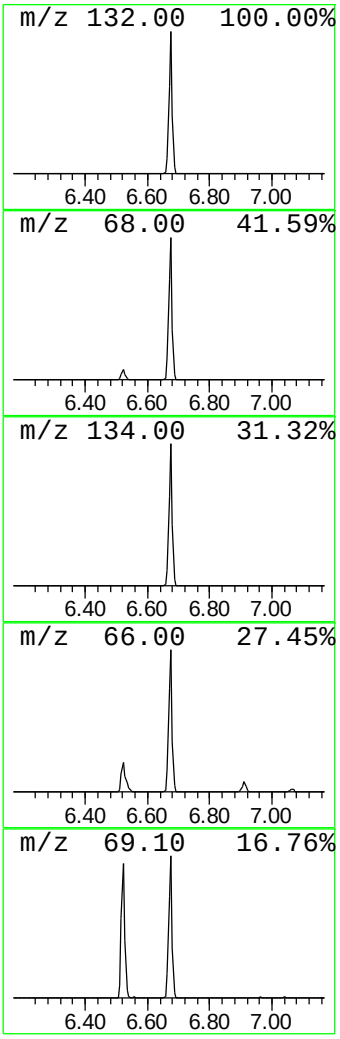
****

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	9.81 ng	451905	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
Data File : BF098829.D
Acq On : 26 Sep 2017 13:49
Operator : SJ/JU
Sample : I5394-04 10X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20-41

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
n-Hexane	2.33	4.0	ng	182928	1	6.91	921649	20.0
unknown6.67	6.67	9.8	ng	451905	1	6.91	921649	20.0