LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062817\
Data File : BF096258.D
Acq On : 28 Jun 2017 19:19
Operator : SJ/MA
Sample : I3852-11 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-39-0-1.5

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-BF062717.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	2.216	21	22	28	rVB3	10403	13858	1.21%	0.141%
2	2.334	40	42	51	rVB5	14106	21596	1.89%	0.220%
3	4.334	379	382	387	rBV	94072	112491	9.86%	1.147%
4	4.963	485	489	496	rBV	338535	334122	29.28%	3.408%
5	5.387	557	561	566	rVB	303287	261953	22.95%	2.672%
6	6.398	730	733	739	rVB	444468	374405	32.81%	3.819%
7	6.545	754	758	762	rVB	405266	315529	27.65%	3.218%
8	6.781	795	798	802	rBV	1064441	895893	78.50%	9.137%
9	6.940	821	825	828	rVB	354105	303324	26.58%	3.094%
10	7.334	888	892	895	rBV	296242	222412	19.49%	2.268%
11	7.745	959	962	966	rBV4	11875	15060	1.32%	0.154%
12	8.063	1012	1016	1019	rBV	1400182	1141252	100.00%	11.640%
13	8.498	1086	1090	1095	rBV2	15327	20313	1.78%	0.207%
14	8.669	1115	1119	1124	rBV	27059	26267	2.30%	0.268%
15	8.775	1132	1137	1139	rVB4	14175	14686	1.29%	0.150%
16	9.098	1189	1192	1195	rBV	20723	16122	1.41%	0.164%
17	9.134	1195	1198	1202	rBV	447832	383882	33.64%	3.915%
18	9.234	1211	1215	1220	rBV	46059	50722	4.44%	0.517%
19	9.398	1241	1243	1249	rVB6	12214	15975	1.40%	0.163%
20	9.475	1254	1256	1259	rBV3	17138	19757	1.73%	0.202%
21	9.528	1263	1265	1268	rBV	47798	45960	4.03%	0.469%
22	9.551	1268	1269	1271	rVB	26635	15699	1.38%	0.160%
23	9.757	1302	1304	1309	rVB	54244	48820	4.28%	0.498%
24	9.816	1309	1314	1318	rBV	1195087	1036938	90.86%	10.576%
25	10.016	1346	1348	1351	rVB3	22619	18896	1.66%	0.193%
26	10.081	1357	1359	1362	rVB3	16357	16860	1.48%	0.172%
27	10.257	1387	1389	1392	rVB	64707	49651	4.35%	0.506%
28	10.480	1423	1427	1431	rBV	34480	35840	3.14%	0.366%
29	10.592	1443	1446	1450	rVB5	39796	34930	3.06%	0.356%
30	10.728	1466	1469	1471	rBV	71297	75560	6.62%	0.771%
31	11.175	1543	1545	1548	rBV	49522	42972	3.77%	0.438%
32	11.210	1548	1551	1556	rVB	41459	41487	3.64%	0.423%
33	11.263	1556	1560	1562	rBV3	22912	28392	2.49%	0.290%
34	11.292	1562	1565	1568	rVV	1083948	919242	80.55%	9.375%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062817\
Data File : BF096258.D
Acq On : 28 Jun 2017 19:19
Operator : SJ/MA
Sample : I3852-11 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-39-0-1.5

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-BF062717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.316	1568	1569	1573	rVB	69015	43661	3.83%	0.445%
36	11.363	1573	1577	1580	rBV2	30480	37375	3.27%	0.381%
37	11.604	1615	1618	1624	rVB2	51343	51284	4.49%	0.523%
38	11.822	1653	1655	1660	rVB5	37783	34637	3.04%	0.353%
39	11.904	1665	1669	1671	rBV5	26204	32499	2.85%	0.331%
40	12.010	1684	1687	1689	rVB	47808	33799	2.96%	0.345%
41	12.292	1733	1735	1737	rVB2	21696	17084	1.50%	0.174%
42	12.345	1741	1744	1747	rBV2	33263	40228	3.52%	0.410%
43	12.398	1751	1753	1755	rVB	57928	42442	3.72%	0.433%
44	12.504	1767	1771	1774	rBV	87464	88459	7.75%	0.902%
45	12.727	1806	1809	1812	rVB	70831	61371	5.38%	0.626%
46	12.769	1814	1816	1818	rVB	48515	33201	2.91%	0.339%
47	12.874	1831	1834	1838	rBV	397447	353203	30.95%	3.602%
48	13.121	1874	1876	1880	rVB	63162	56907	4.99%	0.580%
49	13.251	1896	1898	1900	rBV2	32487	26806	2.35%	0.273%
50	13.463	1932	1934	1937	rBV2	68822	63352	5.55%	0.646%
51	13.921	2009	2012	2016	rBV	999992	1017863	89.19%	10.381%
52	14.110	2041	2044	2047	rBV	92799	78131	6.85%	0.797%
53	15.351	2252	2255	2260	rVB	606445	721616	63.23%	7.360%

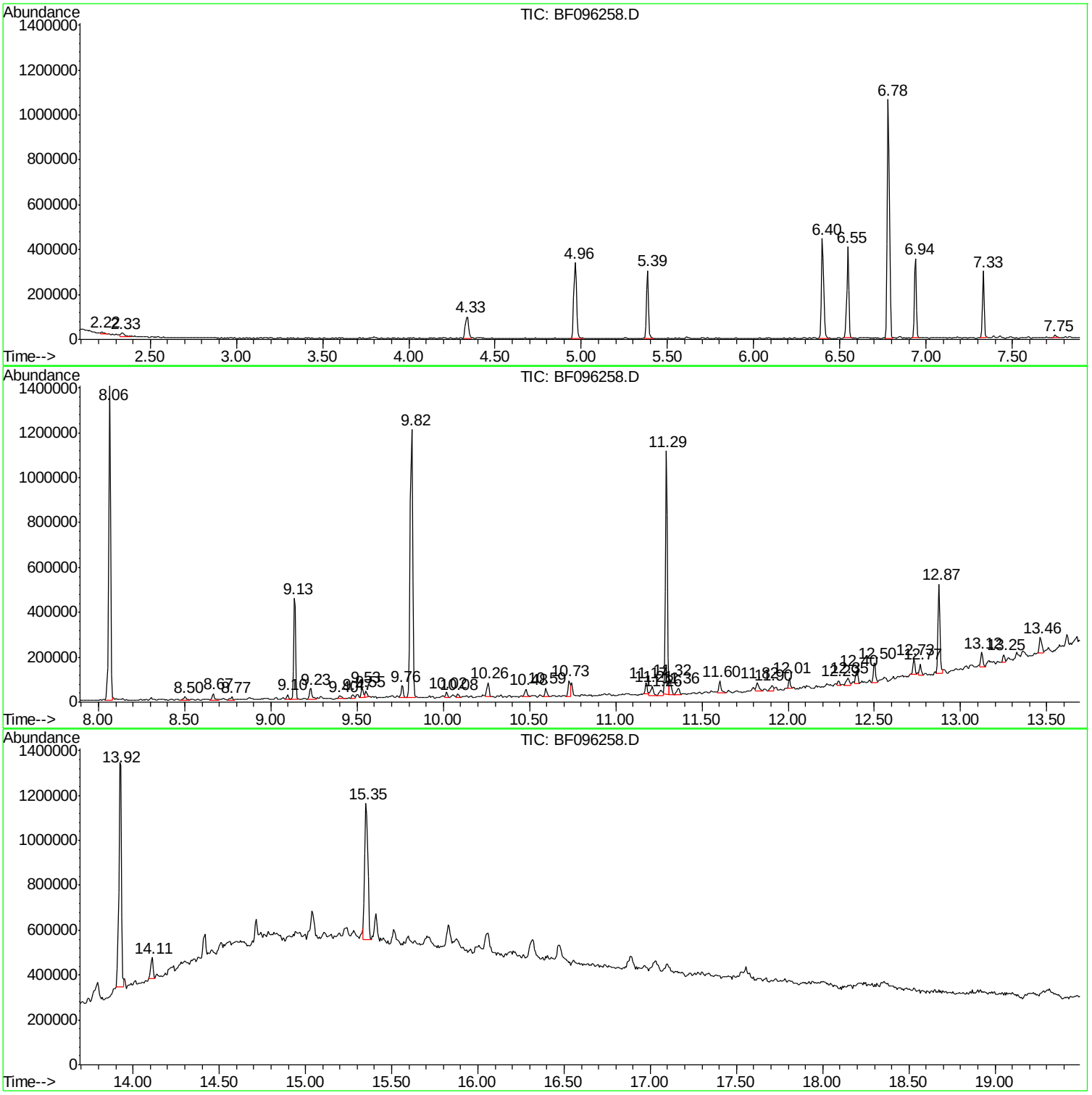
Sum of corrected areas: 9804784

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062817\
Data File : BF096258.D
Acq On : 28 Jun 2017 19:19
Operator : SJ/MA
Sample : I3852-11 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-39-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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\BF062817\
Data File : BF096258.D
Acq On : 28 Jun 2017 19:19
Operator : SJ/MA
Sample : I3852-11 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-39-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

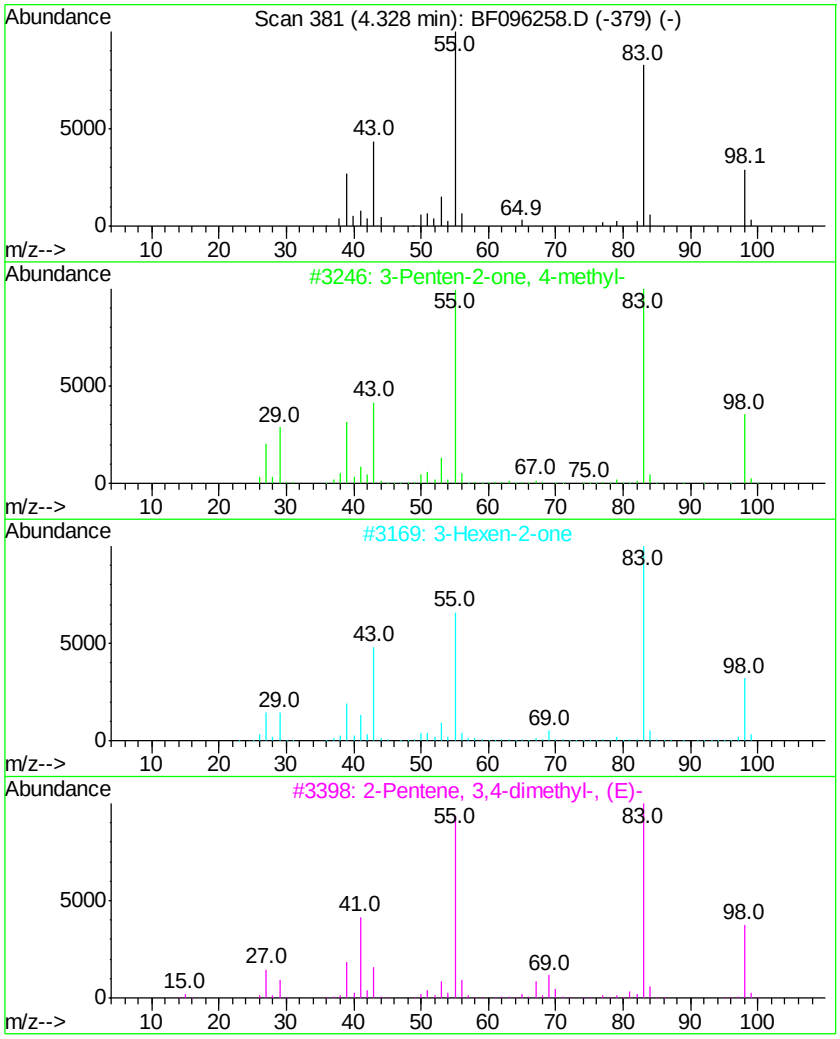
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

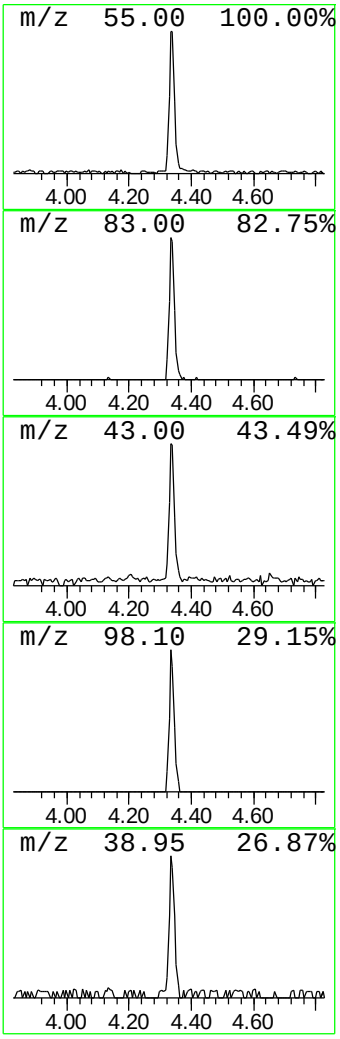
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	2.51 ng	112491	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	80
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	80
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062817\
Data File : BF096258.D
Acq On : 28 Jun 2017 19:19
Operator : SJ/MA
Sample : I3852-11 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-39-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

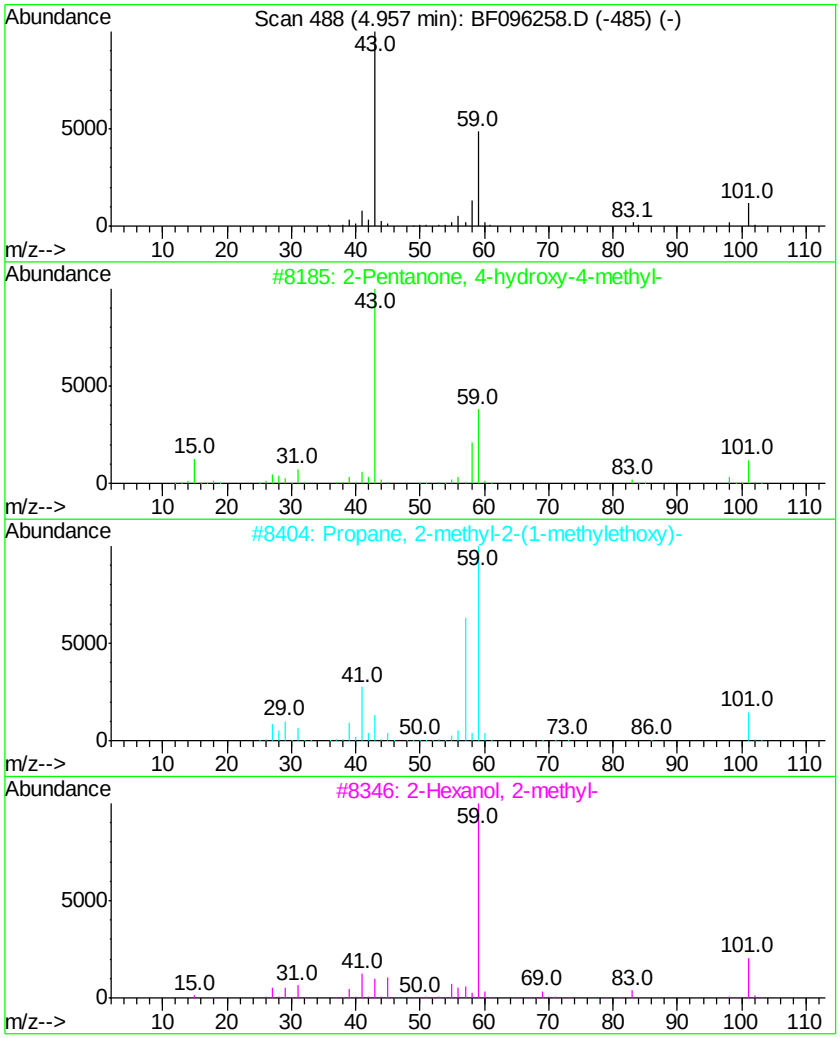
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

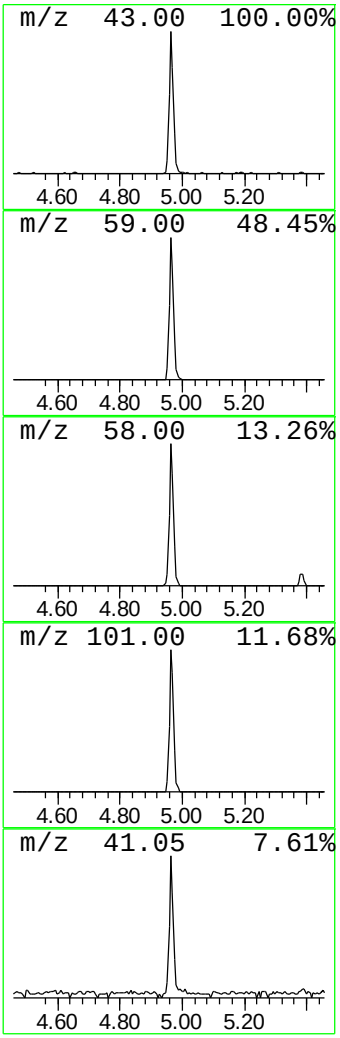
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	7.46 ng	334122	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062817\
Data File : BF096258.D
Acq On : 28 Jun 2017 19:19
Operator : SJ/MA
Sample : I3852-11 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-39-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

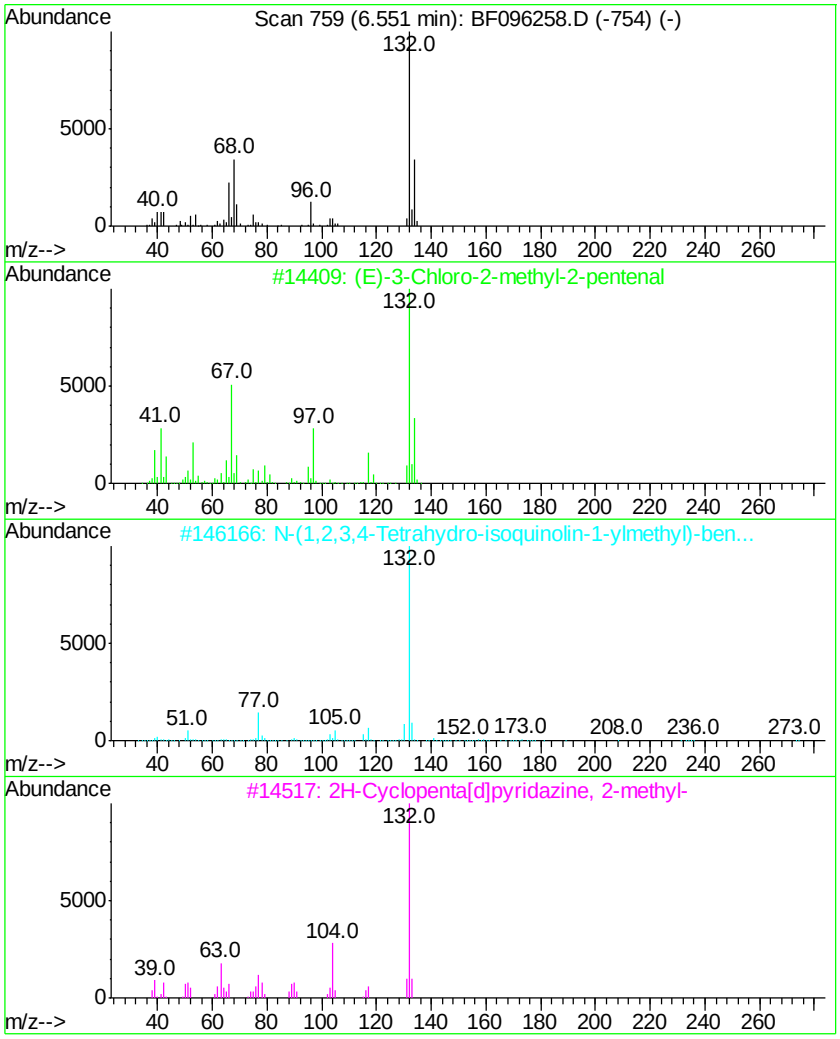
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

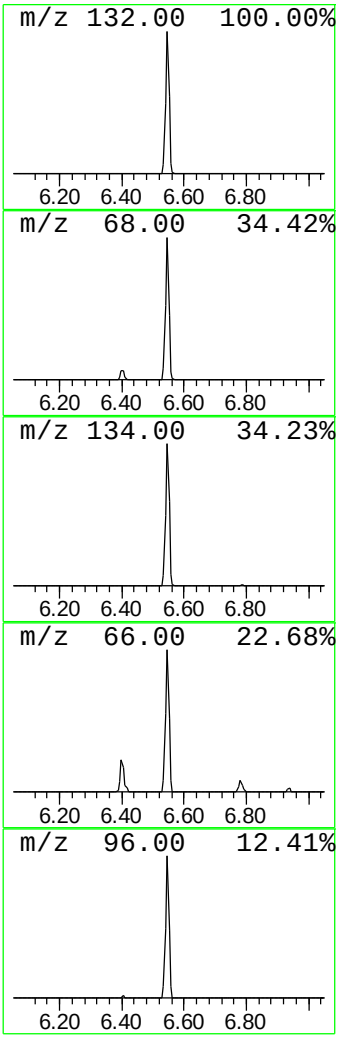
****

Peak Number 3 unknown6.55 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	7.04 ng	315529	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	N-(1,2,3,4-Tetrahydro-isoquinoli...	302	C16H18N2O2S	1000274-62-8	10
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	1-Aminoindan	133	C9H11N	034698-41-4	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062817\
Data File : BF096258.D
Acq On : 28 Jun 2017 19:19
Operator : SJ/MA
Sample : I3852-11 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-39-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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
3-Penten-2-one, 4...	4.33	2.5	ng	112491	1	6.78	895893	20.0
2-Pentanone, 4-hy...	4.96	7.5	ng	334122	1	6.78	895893	20.0
unknown6.55	6.55	7.0	ng	315529	1	6.78	895893	20.0