LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096347.D
Acq On : 30 Jun 2017 20:20
Operator : SJ/MA
Sample : I3959-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-062717-B

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	4.939	482	485	489	rBV	120443	118176	4.92%	0.622%
2	5.363	553	557	561	rVB	980355	830674	34.55%	4.370%
3	6.381	726	730	736	rBV	1042304	866565	36.05%	4.559%
4	6.522	750	754	758	rBV	1007317	838305	34.87%	4.410%
5	6.757	790	794	798	rBV	1119176	969119	40.31%	5.098%
6	6.916	817	821	824	rVB	727623	594539	24.73%	3.128%
7	7.310	884	888	892	rBV	575620	494651	20.58%	2.602%
8	7.733	956	960	963	rBV2	31169	31704	1.32%	0.167%
9	8.039	1008	1012	1016	rBV	1496839	1311061	54.53%	6.897%
10	8.480	1084	1087	1089	rBV	36520	33667	1.40%	0.177%
11	8.598	1102	1107	1111	rBV5	16042	26169	1.09%	0.138%
12	8.645	1111	1115	1117	rBV4	24255	27224	1.13%	0.143%
13	8.739	1128	1131	1135	rVB4	24793	39486	1.64%	0.208%
14	9.074	1185	1188	1191	rBV	59035	54501	2.27%	0.287%
15	9.116	1191	1195	1199	rVB	1071986	824441	34.29%	4.337%
16	9.210	1207	1211	1215	rBV3	52266	67118	2.79%	0.353%
17	9.510	1259	1262	1264	rBV	177819	145578	6.06%	0.766%
18	9.533	1264	1266	1268	rVB	58729	44477	1.85%	0.234%
19	9.669	1286	1289	1292	rBV5	37414	37138	1.54%	0.195%
20	9.716	1294	1297	1299	rVB	73392	61429	2.56%	0.323%
21	9.739	1299	1301	1305	rBV4	38098	43629	1.81%	0.230%
22	9.792	1305	1310	1314	rBV	1303678	1198994	49.87%	6.307%
23	9.827	1314	1316	1318	rVB	72822	55473	2.31%	0.292%
24	9.998	1342	1345	1348	rVB	55184	54155	2.25%	0.285%
25	10.069	1354	1357	1361	rBV3	24947	28478	1.18%	0.150%
26	10.210	1378	1381	1384	rBV3	40731	33028	1.37%	0.174%
27	10.339	1400	1403	1406	rBV	93404	72574	3.02%	0.382%
28	10.457	1420	1423	1428	rVB3	22798	28941	1.20%	0.152%
29	10.574	1439	1443	1447	rBV	472020	382267	15.90%	2.011%
30	10.710	1463	1466	1468	rBV	40515	42122	1.75%	0.222%
31	11.168	1540	1544	1546	rBV2	26280	36225	1.51%	0.191%
32	11.274	1558	1562	1564	rBV	992155	875001	36.40%	4.603%
33	11.298	1564	1566	1569	rVV	271742	209006	8.69%	1.099%
34	11.345	1569	1574	1578	rVB	88185	81568	3.39%	0.429%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096347.D
Acq On : 30 Jun 2017 20:20
Operator : SJ/MA
Sample : I3959-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-062717-B

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	11.680	1627	1631	1634	rBV	960205	769303	32.00%	4.047%
36	11.804	1649	1652	1656	rBV	105783	95389	3.97%	0.502%
37	11.886	1663	1666	1668	rBV	58713	50731	2.11%	0.267%
38	12.362	1743	1747	1749	rBV	2618146	2404087	100.00%	12.647%
39	12.386	1749	1751	1759	rVB	1839019	1593093	66.27%	8.380%
40	12.474	1762	1766	1771	rBV2	457424	624768	25.99%	3.287%
41	12.592	1783	1786	1789	rBV4	33974	35909	1.49%	0.189%
42	12.710	1800	1806	1809	rBV	267097	291508	12.13%	1.533%
43	12.857	1827	1831	1834	rVB	587140	518907	21.58%	2.730%
44	13.039	1860	1862	1864	rBV2	38918	30985	1.29%	0.163%
45	13.104	1870	1873	1877	rBV4	60059	85346	3.55%	0.449%
46	13.192	1886	1888	1892	rBV	42309	41736	1.74%	0.220%
47	13.298	1903	1906	1911	rVB	55274	55743	2.32%	0.293%
48	13.757	1982	1984	1991	rVB2	87356	93945	3.91%	0.494%
49	13.904	2004	2009	2012	rBV	939117	978304	40.69%	5.146%
50	13.927	2012	2013	2016	rVB	83405	53056	2.21%	0.279%
51	15.321	2246	2250	2255	rBV2	543541	729530	30.35%	3.838%

Sum of corrected areas: 19009823

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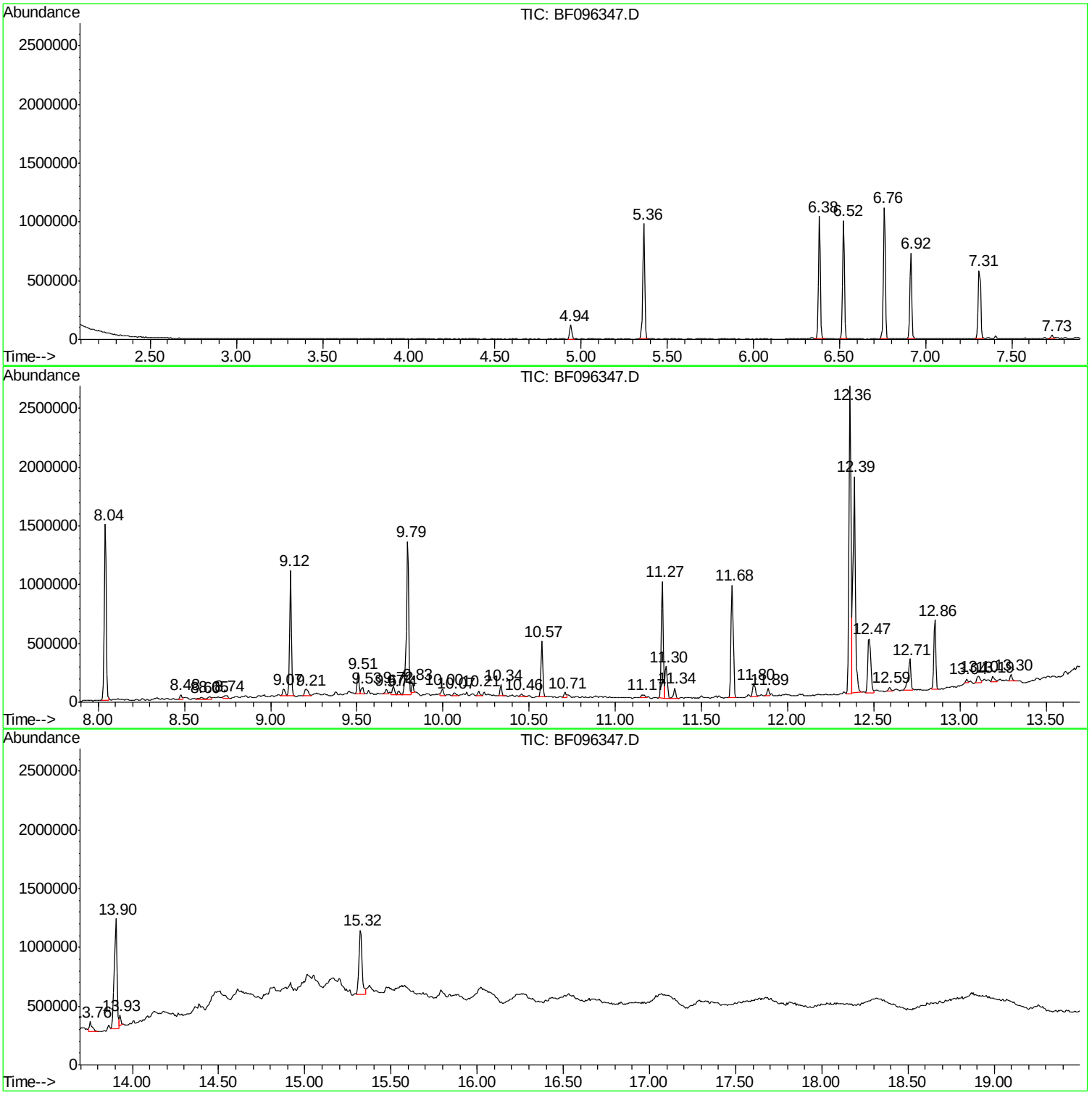
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-062717-B

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



Library Search Compound Report

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Data File : BF096347.D
Acq On : 30 Jun 2017 20:20
Operator : SJ/MA
Sample : I3959-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-062717-B

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

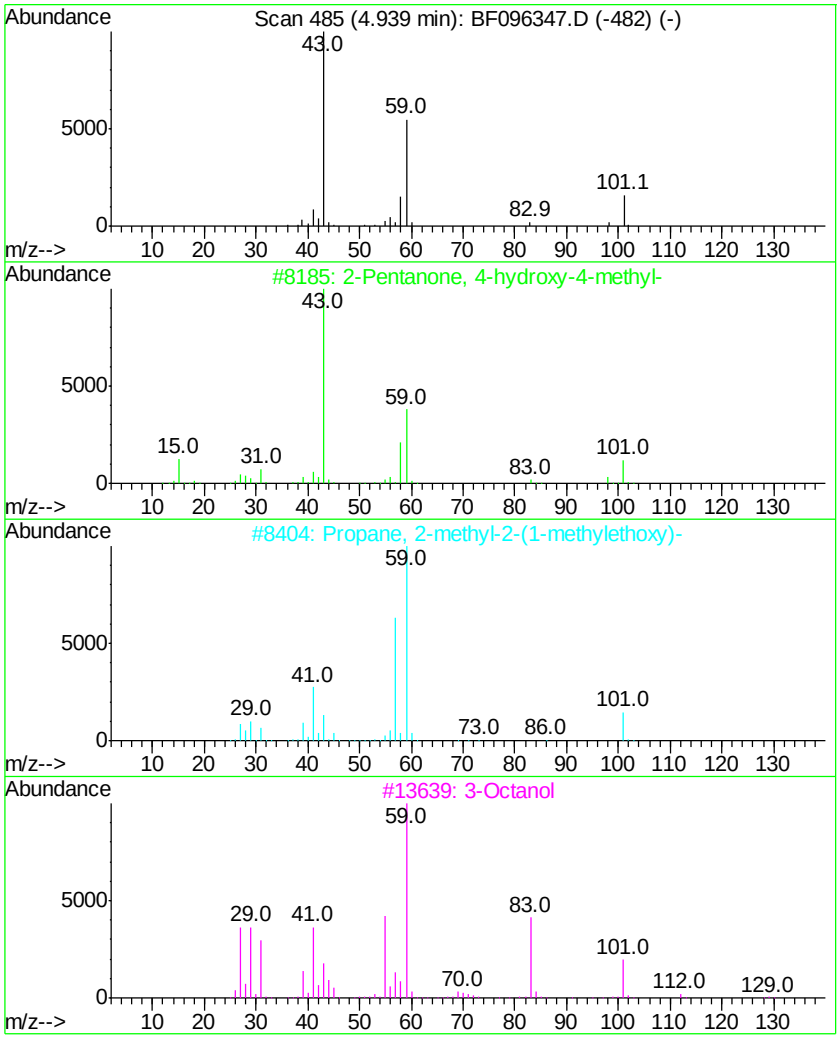
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

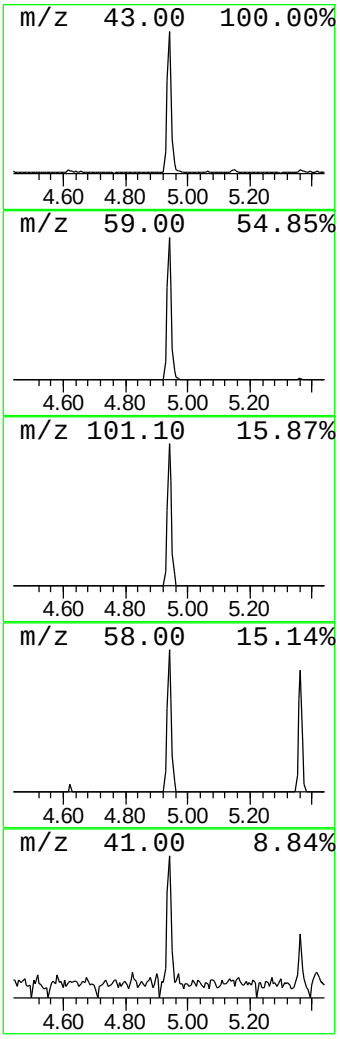
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	2.44 ng	118176	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Octanol	130	C8H18O	000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
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Acq On : 30 Jun 2017 20:20
Operator : SJ/MA
Sample : I3959-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-062717-B

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

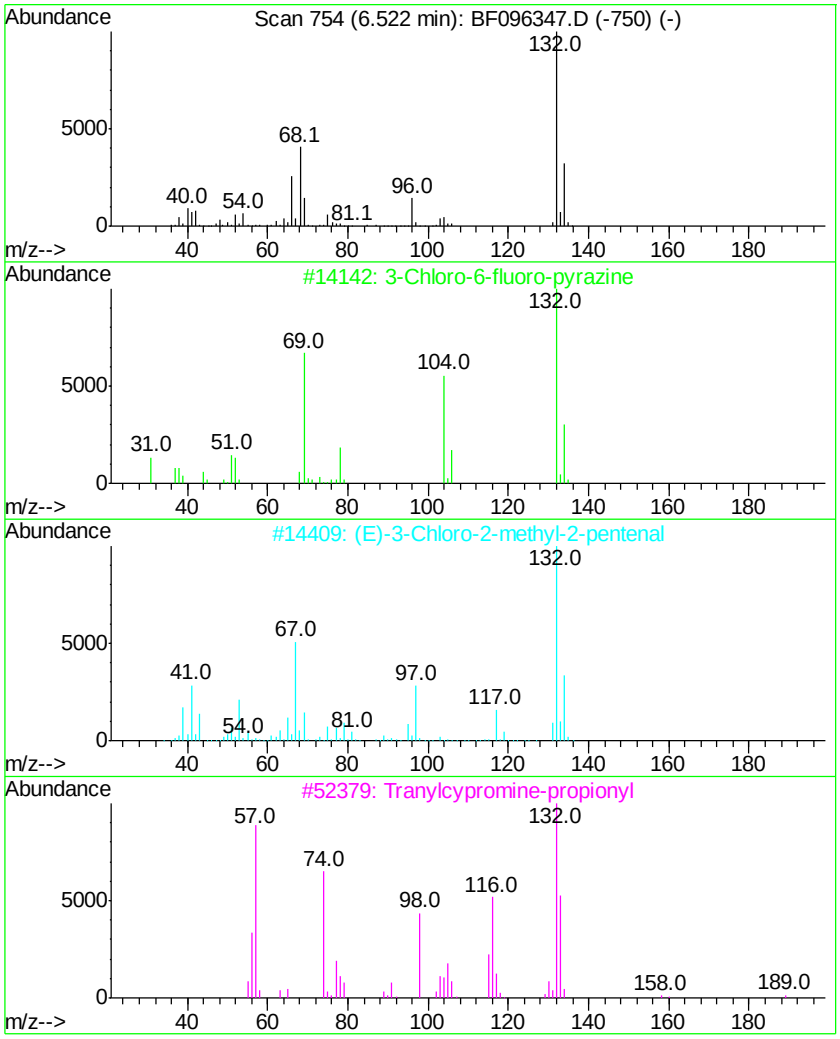
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

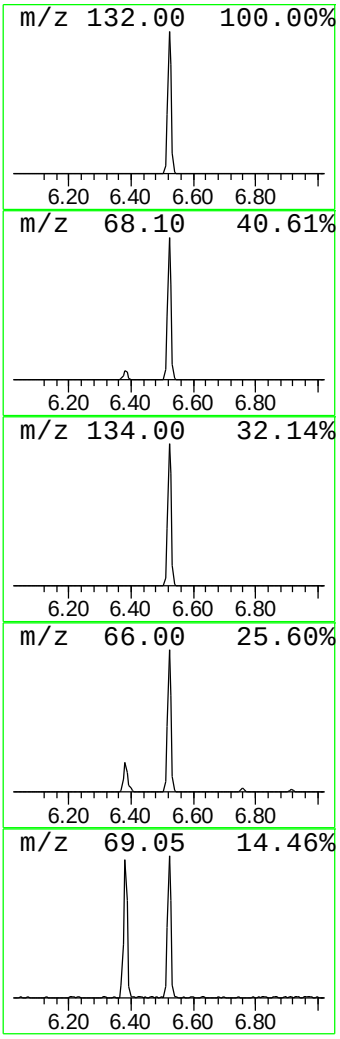
****

Peak Number 2 unknown6.52 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	17.30 ng	838305	1,4-Dichlorobenzene-d4	6.76

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096347.D
Acq On : 30 Jun 2017 20:20
Operator : SJ/MA
Sample : I3959-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-062717-B

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

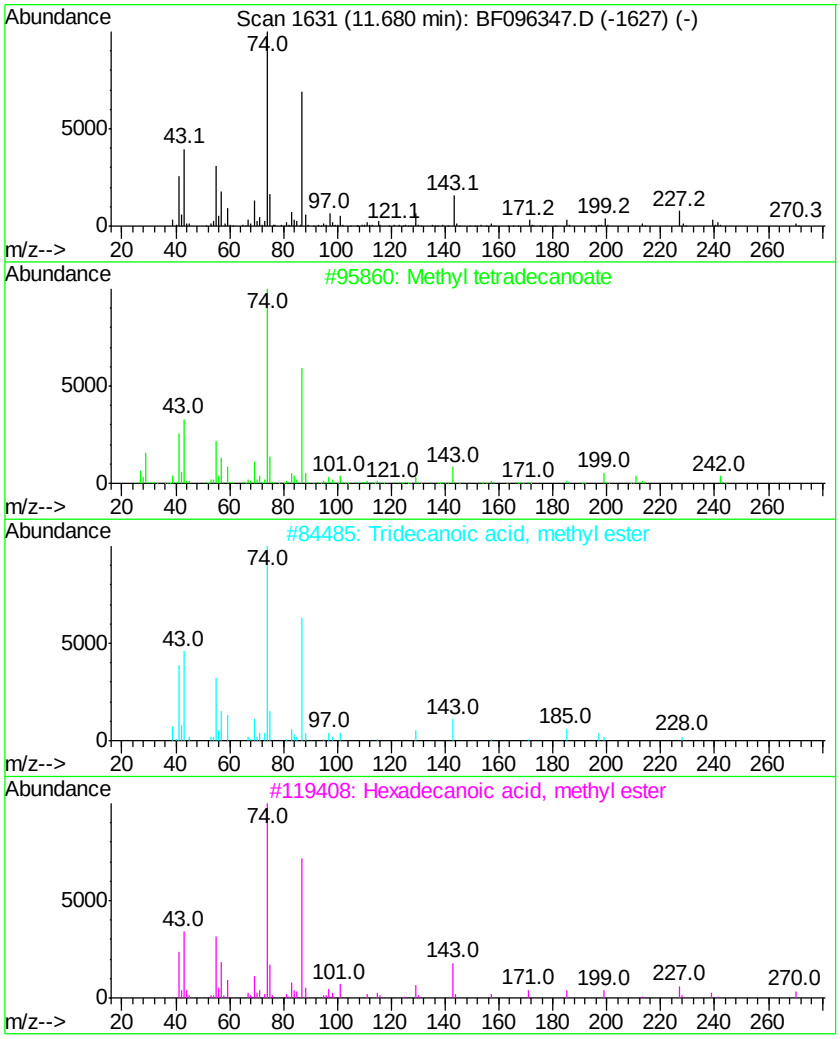
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

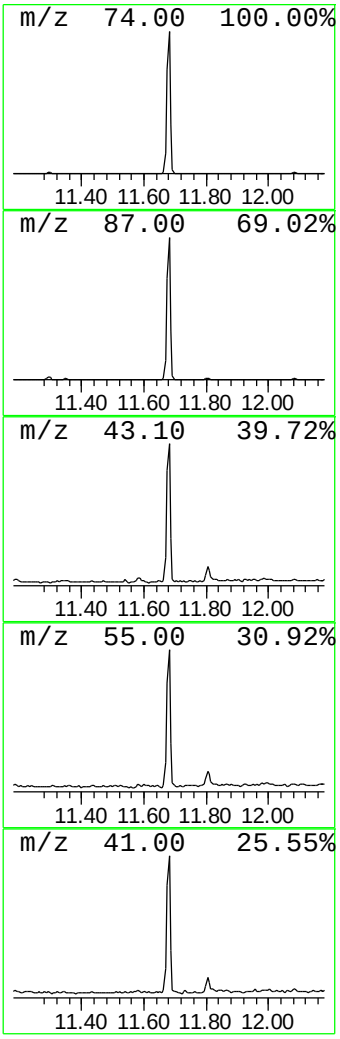
****

Peak Number 4 Methyl tetradecanoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	17.58 ng	769303	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl tetradecanoate	242	C15H30O2	000124-10-7	97
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
3	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
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Acq On : 30 Jun 2017 20:20
Operator : SJ/MA
Sample : I3959-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-062717-B

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

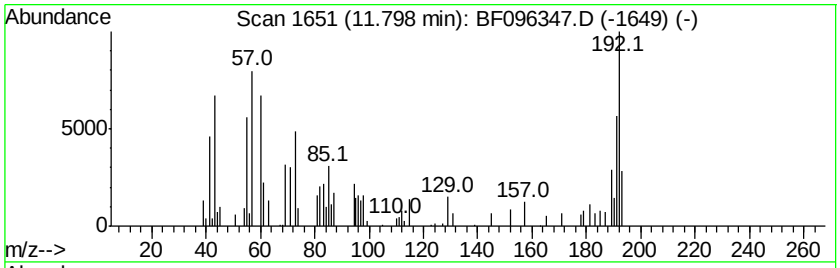
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

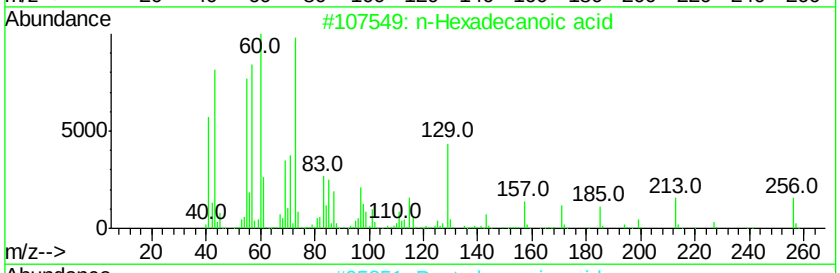
****

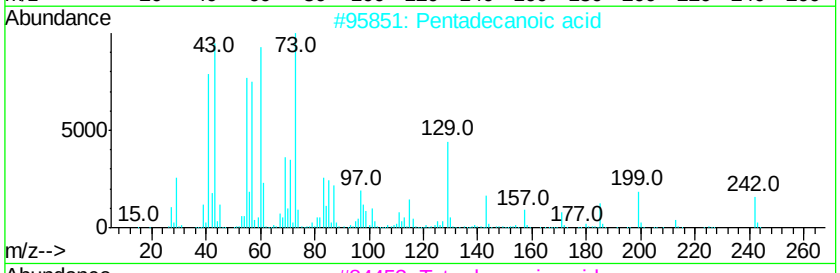
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

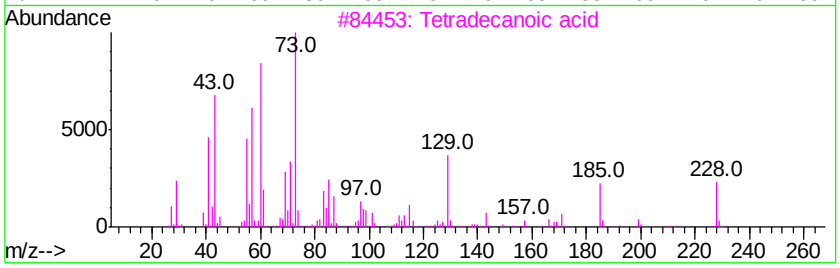
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.18 ng	95389	Phenanthrene-d10	11.27

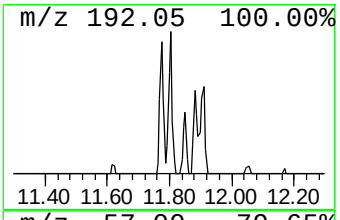
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4	Tridecanoic acid	214	C13H26O2	000638-53-9	38
5	n-Decanoic acid	172	C10H20O2	000334-48-5	35

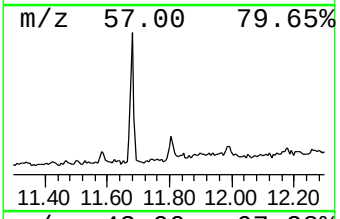


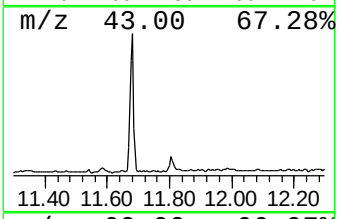


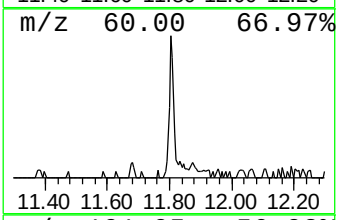


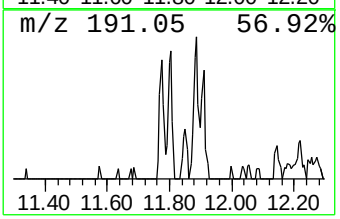












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

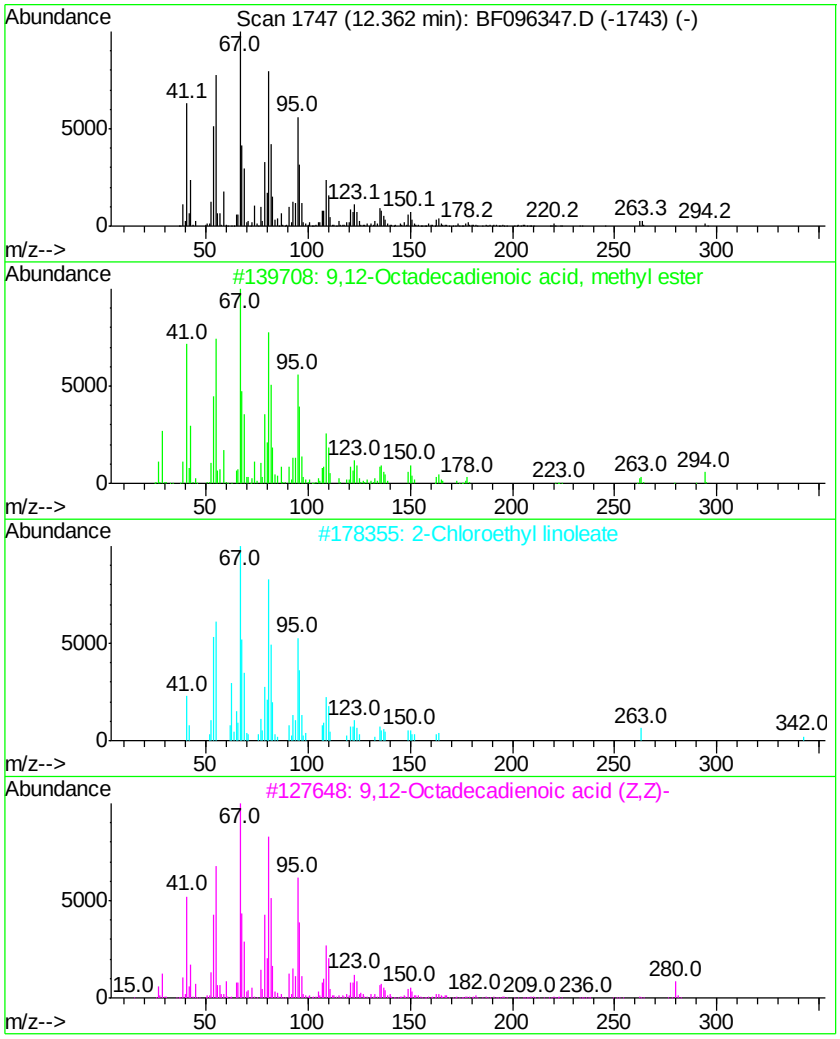
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

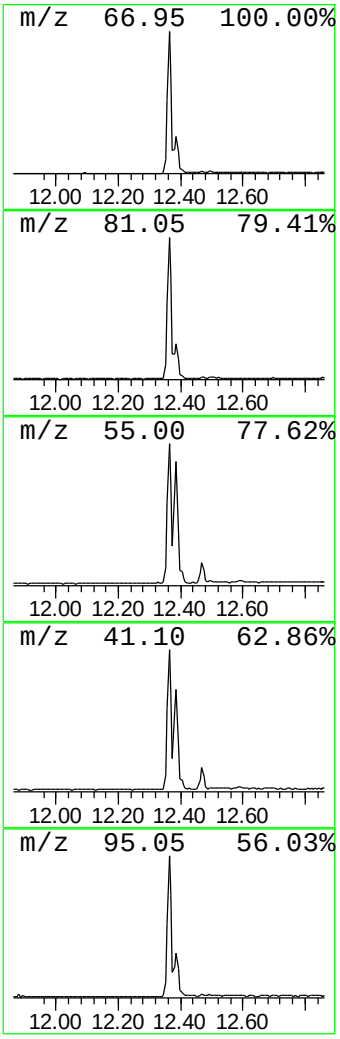
****

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	54.95 ng	2404090	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	94
2	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	94
3	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	93
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	91
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	91





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

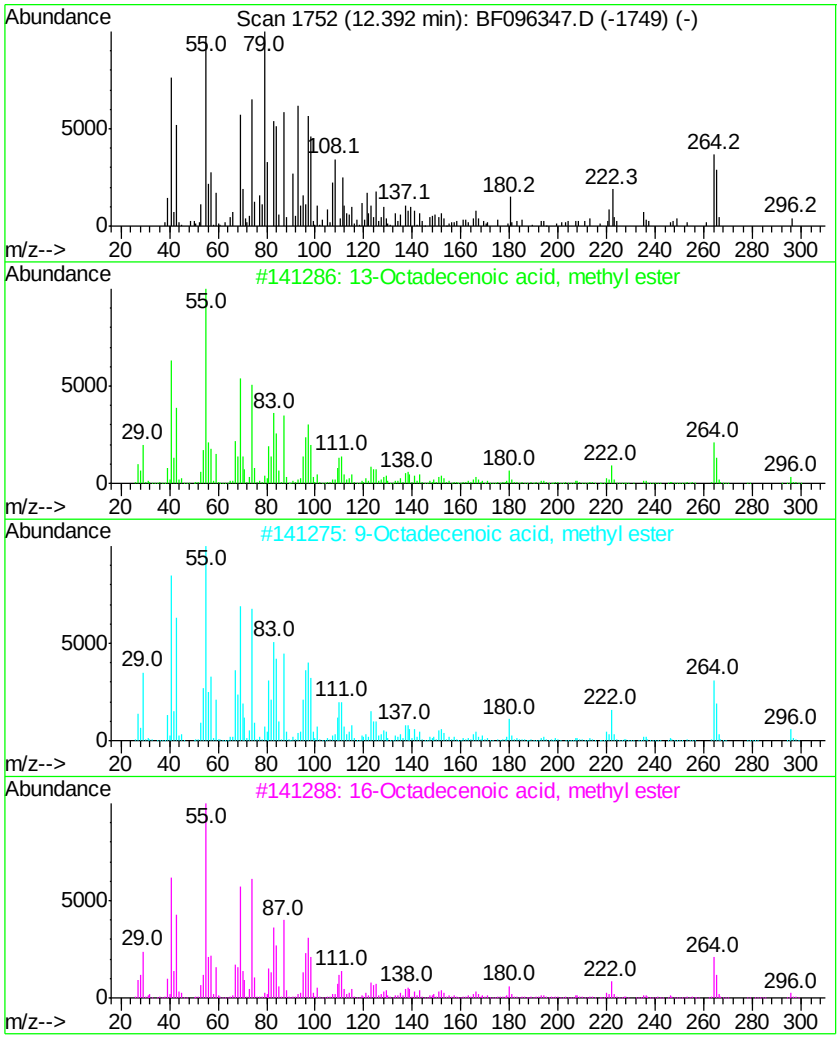
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

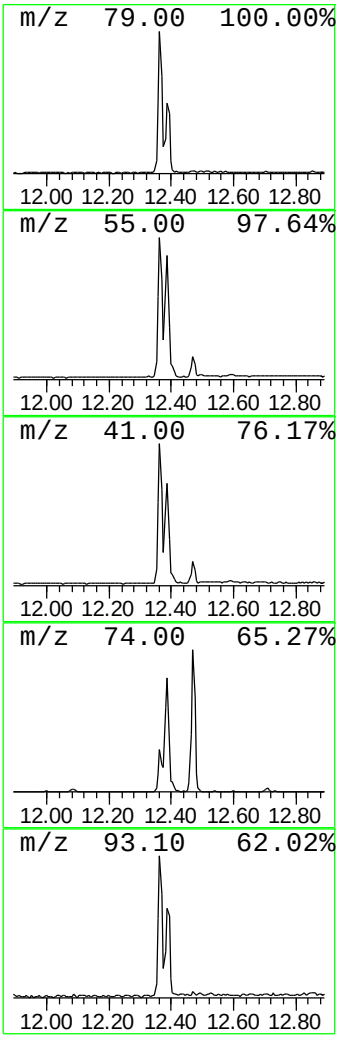
****

Peak Number 7 13-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	36.41 ng	1593090	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	95
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	95
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
Data File : BF096347.D
Acq On : 30 Jun 2017 20:20
Operator : SJ/MA
Sample : I3959-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-062717-B

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
2-Pentanone, 4-hy...	4.94	2.4	ng	118176	1	6.76	969119	20.0
unknown6.52	6.52	17.3	ng	838305	1	6.76	969119	20.0
Methyl tetradecan...	11.68	17.6	ng	769303	4	11.27	875001	20.0
n-Hexadecanoic acid	11.80	2.2	ng	95389	4	11.27	875001	20.0
9,12-Octadecadien...	12.36	55.0	ng	2404090	4	11.27	875001	20.0
13-Octadecenoic a...	12.39	36.4	ng	1593090	4	11.27	875001	20.0