LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096518.D
Acq On : 6 Jul 2017 7:56
Operator : SJ/MA
Sample : I3975-10 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B8-4-6

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-BF070117.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	2.710	100	106	112	rVB6	6089	11167	1.79%	0.148%
2	3.663	260	268	273	rBV2	11882	19943	3.20%	0.265%
3	4.310	373	378	382	rBV5	7717	12067	1.93%	0.160%
4	4.881	472	475	482	rBV	60261	68130	10.92%	0.905%
5	5.175	522	525	528	rVB	10296	8659	1.39%	0.115%
6	5.287	540	544	545	rBV	26110	24519	3.93%	0.326%
7	5.316	545	549	559	rVB	445050	415522	66.58%	5.517%
8	5.545	586	588	593	rVB	18771	18641	2.99%	0.248%
9	5.628	598	602	605	rBV	9998	9384	1.50%	0.125%
10	6.251	705	708	714	rVB5	13620	17525	2.81%	0.233%
11	6.345	720	724	730	rBV	435219	401272	64.30%	5.328%
12	6.481	743	747	750	rBV	464148	398873	63.91%	5.296%
13	6.539	755	757	759	rBV	12242	8623	1.38%	0.114%
14	6.710	783	786	790	rBV	578528	507343	81.29%	6.736%
15	6.739	790	791	794	rVB	11195	8659	1.39%	0.115%
16	6.869	809	813	816	rBV	374965	298181	47.78%	3.959%
17	6.992	830	834	838	rBV3	9705	9229	1.48%	0.123%
18	7.269	873	881	884	rBV	238301	214216	34.32%	2.844%
19	7.328	888	891	894	rVV	19711	16909	2.71%	0.225%
20	7.363	894	897	901	rVB4	8858	12320	1.97%	0.164%
21	7.639	942	944	949	rVB2	8024	8728	1.40%	0.116%
22	7.704	949	955	957	rBV4	7020	12613	2.02%	0.167%
23	7.763	962	965	969	rVB2	9300	10564	1.69%	0.140%
24	7.992	1001	1004	1007	rBV	705118	624109	100.00%	8.287%
25	8.075	1016	1018	1020	rVB	15391	10377	1.66%	0.138%
26	8.386	1068	1071	1074	rVB4	8030	7961	1.28%	0.106%
27	8.433	1076	1079	1084	rBV	25329	26150	4.19%	0.347%
28	8.551	1095	1099	1105	rBV3	6496	9356	1.50%	0.124%
29	8.604	1105	1108	1112	rBV	26266	24547	3.93%	0.326%
30	8.710	1120	1126	1130	rVB	35332	34172	5.48%	0.454%
31	8.810	1140	1143	1147	rBV	24179	23571	3.78%	0.313%
32	9.033	1178	1181	1184	rVB	19563	14847	2.38%	0.197%
33	9.069	1184	1187	1191	rBV	405015	347757	55.72%	4.617%
34	9.169	1199	1204	1208	rVB	40888	39506	6.33%	0.525%

LSC Area Percent Report

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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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.222	1208	1213	1216	rBV6	6440	9944	1.59%	0.132%
36	9.339	1229	1233	1237	rBV4	10578	15948	2.56%	0.212%
37	9.410	1239	1245	1247	rBV	21523	23501	3.77%	0.312%
38	9.433	1247	1249	1252	rVB	12290	10675	1.71%	0.142%
39	9.463	1252	1254	1257	rBV	139238	116128	18.61%	1.542%
40	9.486	1257	1258	1261	rVB	24474	16256	2.60%	0.216%
41	9.669	1286	1289	1291	rVB2	9496	7917	1.27%	0.105%
42	9.698	1291	1294	1298	rBV	38709	32721	5.24%	0.434%
43	9.751	1298	1303	1306	rBV	593678	544014	87.17%	7.223%
44	9.957	1335	1338	1341	rVB2	19727	18988	3.04%	0.252%
45	9.992	1341	1344	1346	rBV2	9396	10780	1.73%	0.143%
46	10.022	1346	1349	1352	rBV4	13081	14359	2.30%	0.191%
47	10.092	1359	1361	1364	rVB2	8652	7884	1.26%	0.105%
48	10.163	1369	1373	1376	rBV4	10317	16338	2.62%	0.217%
49	10.192	1376	1378	1382	rVB	34040	29826	4.78%	0.396%
50	10.292	1393	1395	1397	rVB2	17449	12511	2.00%	0.166%
51	10.322	1397	1400	1403	rVB4	7562	8850	1.42%	0.118%
52	10.357	1403	1406	1409	rBV5	7459	9014	1.44%	0.120%
53	10.416	1412	1416	1419	rVV	33241	36427	5.84%	0.484%
54	10.451	1420	1422	1428	rVB7	10687	13948	2.23%	0.185%
55	10.533	1432	1436	1441	rBV	195123	184932	29.63%	2.455%
56	10.669	1455	1459	1460	rBV	54116	52998	8.49%	0.704%
57	10.680	1460	1461	1468	rVB	68790	49969	8.01%	0.663%
58	10.733	1468	1470	1473	rBV4	6607	9132	1.46%	0.121%
59	10.975	1506	1511	1512	rBV4	8244	11273	1.81%	0.150%
60	11.033	1519	1521	1526	rBV6	6046	10739	1.72%	0.143%
61	11.086	1526	1530	1532	rVV5	9185	14088	2.26%	0.187%
62	11.116	1532	1535	1537	rVV	41124	39210	6.28%	0.521%
63	11.145	1537	1540	1545	rVB	43403	44697	7.16%	0.593%
64	11.227	1551	1554	1557	rBV	600595	522637	83.74%	6.939%
65	11.251	1557	1558	1561	rVV	67932	43324	6.94%	0.575%
66	11.304	1565	1567	1569	rVB	26038	19781	3.17%	0.263%
67	11.457	1591	1593	1597	rBV5	10575	17336	2.78%	0.230%
68	11.498	1597	1600	1602	rVV2	8422	9686	1.55%	0.129%
69	11.539	1604	1607	1610	rBV2	35394	35325	5.66%	0.469%
70	11.704	1633	1635	1637	rBV3	8041	9843	1.58%	0.131%
71	11.733	1637	1640	1642	rVV4	24043	26984	4.32%	0.358%

LSC Area Percent Report

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Acq On : 6 Jul 2017 7:56
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Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B8-4-6

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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	11.757	1642	1644	1649	rVV	30224	32837	5.26%	0.436%
73	11.804	1649	1652	1655	rVB3	14568	14935	2.39%	0.198%
74	11.839	1655	1658	1660	rBV	35220	37628	6.03%	0.500%
75	11.863	1660	1662	1664	rVB2	21937	17279	2.77%	0.229%
76	11.945	1674	1676	1679	rBV	31647	29628	4.75%	0.393%
77	12.104	1701	1703	1704	rBV2	11685	9610	1.54%	0.128%
78	12.163	1710	1713	1714	rBV3	9918	10764	1.72%	0.143%
79	12.227	1722	1724	1727	rVB4	19101	15985	2.56%	0.212%
80	12.280	1730	1733	1737	rBV2	28976	33592	5.38%	0.446%
81	12.333	1740	1742	1745	rVV	36637	32166	5.15%	0.427%
82	12.369	1745	1748	1751	rVV4	13350	14306	2.29%	0.190%
83	12.439	1757	1760	1764	rBV	125817	116857	18.72%	1.552%
84	12.663	1795	1798	1801	rVB	85735	75357	12.07%	1.001%
85	12.704	1803	1805	1808	rVB2	20977	16569	2.65%	0.220%
86	12.810	1820	1823	1827	rBV	362901	338373	54.22%	4.493%
87	13.063	1863	1866	1868	rVB2	44281	35803	5.74%	0.475%
88	13.263	1898	1900	1902	rBV2	30559	26556	4.26%	0.353%
89	13.298	1904	1906	1913	rVB	82869	91338	14.63%	1.213%
90	13.404	1922	1924	1926	rBV2	39267	29635	4.75%	0.393%
91	13.863	1998	2002	2005	rBV	563857	540770	86.65%	7.180%
92	15.274	2239	2242	2246	rVB	264567	278072	44.56%	3.692%

Sum of corrected areas: 7531483

LSC Report - Integrated Chromatogram

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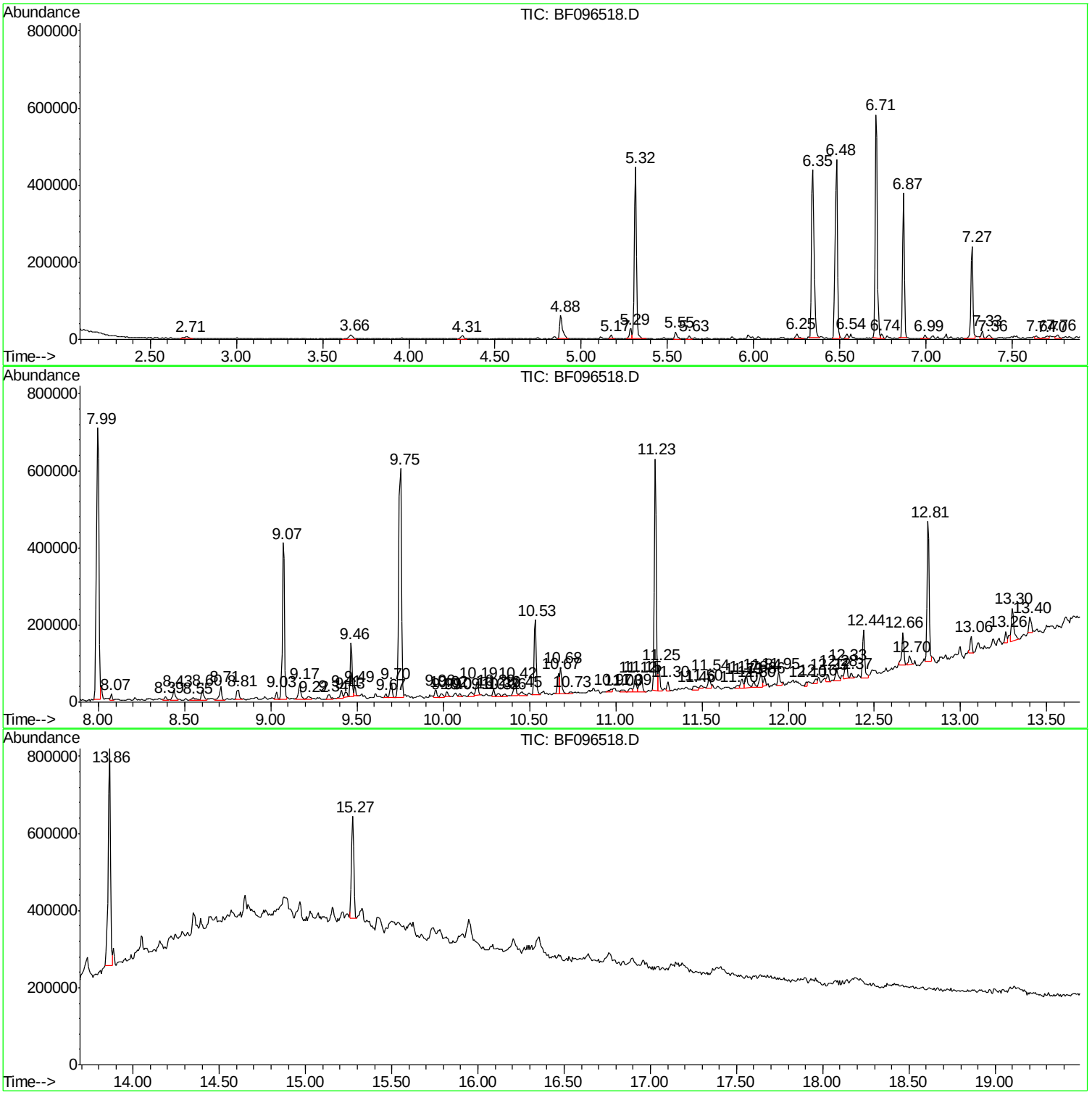
Data File : BF096518.D
Acq On : 6 Jul 2017 7:56
Operator : SJ/MA
Sample : I3975-10 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B8-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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\BF070517\
Data File : BF096518.D
Acq On : 6 Jul 2017 7:56
Operator : SJ/MA
Sample : I3975-10 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

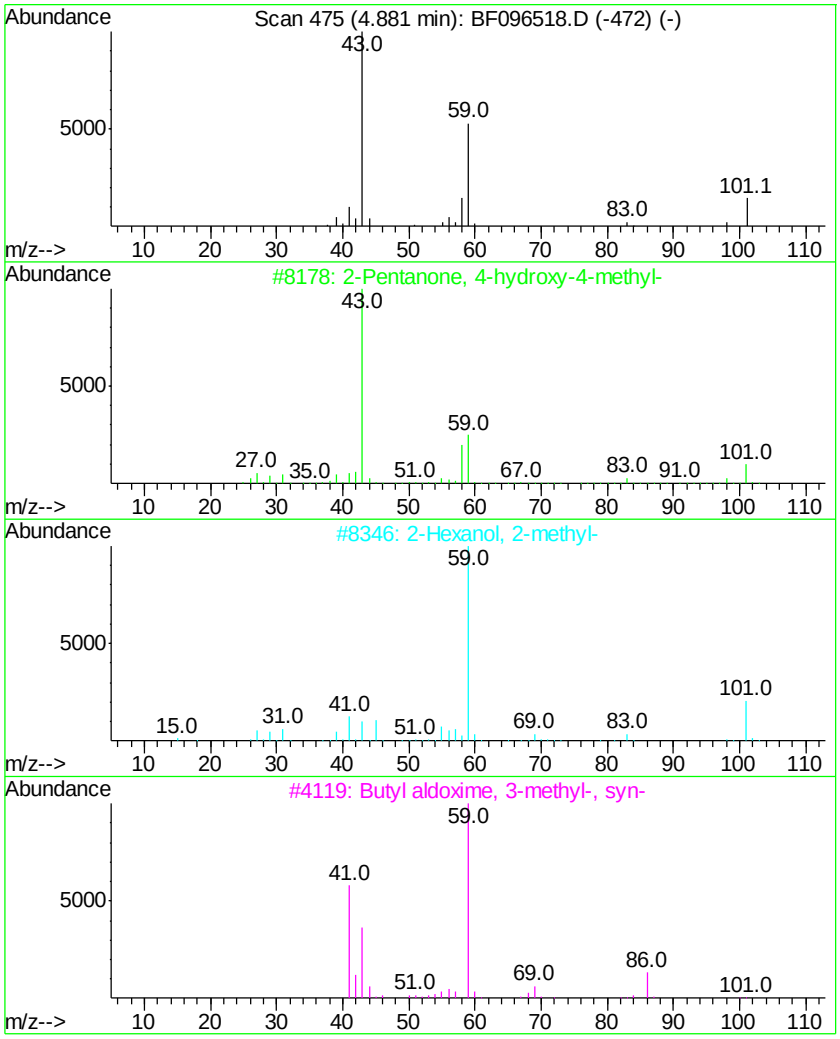
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

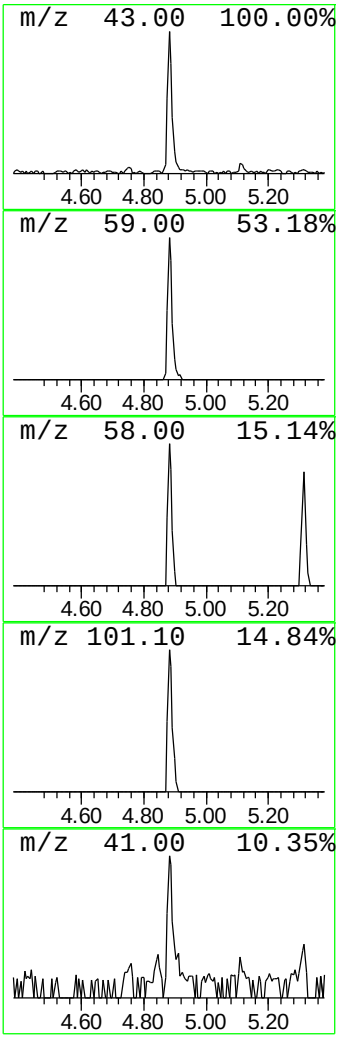
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	2.69 ng	68130	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5	3-Hexanol	102	C6H14O	000623-37-0	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

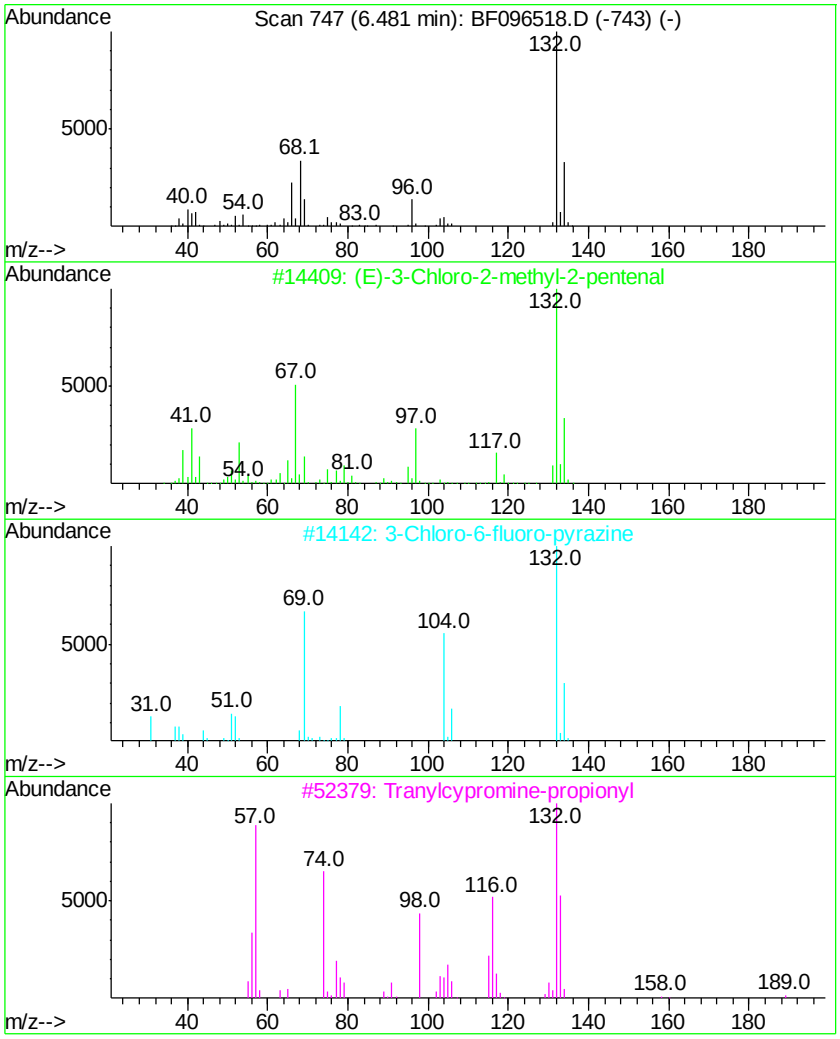
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

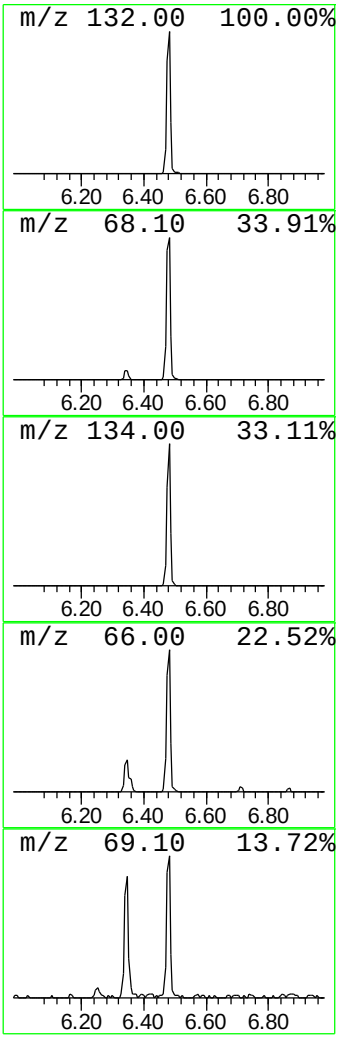
****

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	15.72 ng	398873	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Xenon	132	Xe	007440-63-3	9





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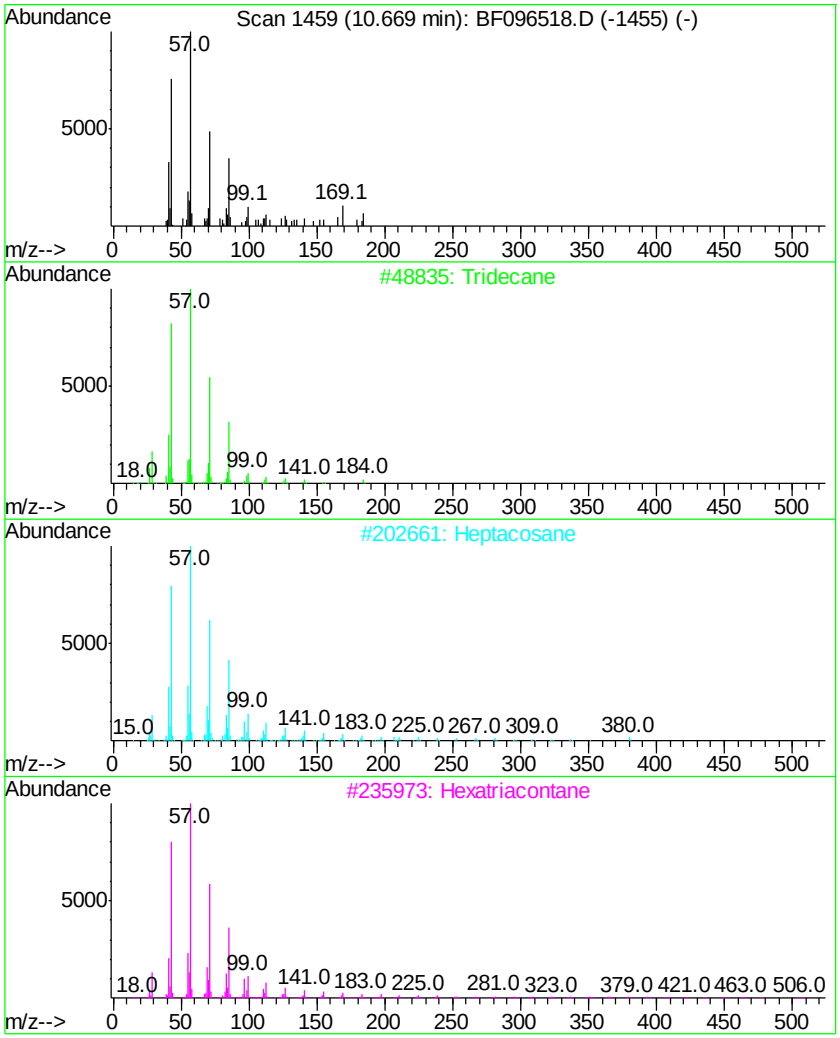
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

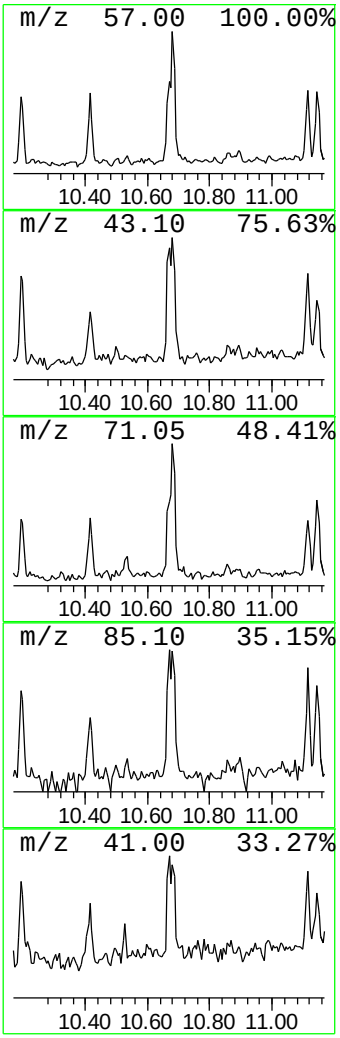
****

Peak Number 4 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.03 ng	52998	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Heptacosane	380	C27H56	000593-49-7	74
3	Hexatriacontane	507	C36H74	000630-06-8	72
4	Tetracosane	338	C24H50	000646-31-1	72
5	Octadecane	254	C18H38	000593-45-3	72





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
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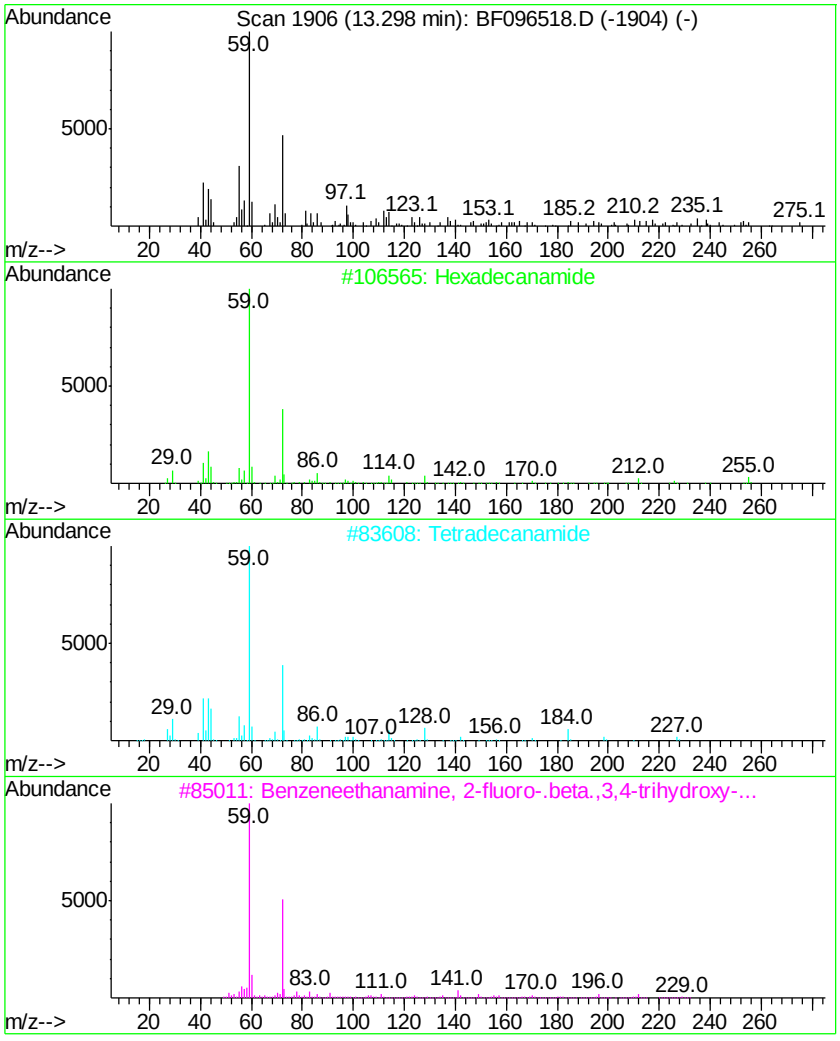
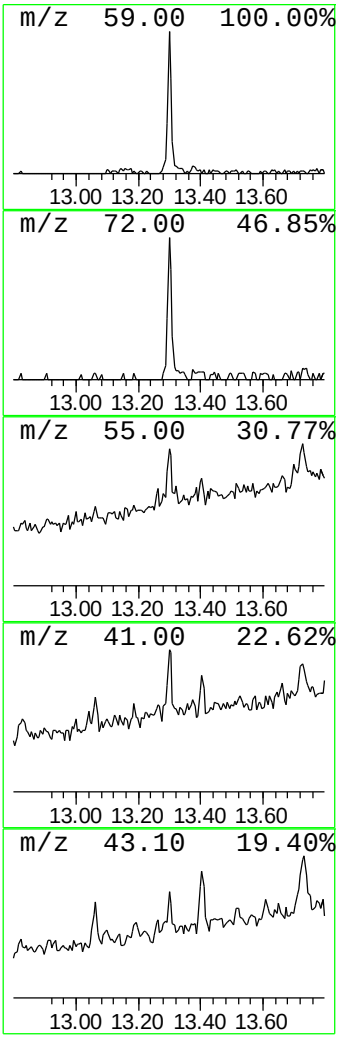
****

Peak Number 5 Hexadecanamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	3.38 ng	91338	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	81
2	Tetradecanamide	227	C14H29NO	000638-58-4	81
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	76
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59
5	Dodecanamide	199	C12H25NO	001120-16-7	53





Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument : BNA_F
ClientSampleId : B8-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.88	2.7	ng	68130	1	6.71	507343	20.0
unknown6.48	6.48	15.7	ng	398873	1	6.71	507343	20.0
Tridecane	10.67	2.0	ng	52998	4	11.23	522637	20.0
Hexadecanamide	13.30	3.4	ng	91338	5	13.86	540770	20.0