LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106343.D
Acq On : 12 Jun 2018 14:40
Operator : JU/SJ
Sample : J3245-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-061118-A

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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	4.101	296	300	306	rVB	20598	25826	1.37%	0.105%
2	5.195	482	486	493	rVB	172711	169698	8.99%	0.689%
3	5.590	549	553	556	rBV	1993168	1727610	91.47%	7.013%
4	6.254	663	666	671	rVB2	40976	39427	2.09%	0.160%
5	6.589	718	723	731	rBV	1867532	1751222	92.72%	7.109%
6	6.737	744	748	752	rBV	2060172	1769711	93.70%	7.184%
7	6.972	784	788	791	rVB	1361788	1085504	57.47%	4.406%
8	7.125	810	814	818	rVB	1729138	1420444	75.21%	5.766%
9	7.531	878	883	886	rBV	1290463	1101144	58.30%	4.470%
10	7.589	890	893	899	rVB3	16925	24695	1.31%	0.100%
11	8.254	1002	1006	1009	rBV	1626381	1318512	69.81%	5.352%
12	9.325	1184	1188	1191	rBV	2346103	1888680	100.00%	7.667%
13	9.666	1244	1246	1249	rVB2	44507	32024	1.70%	0.130%
14	9.719	1251	1255	1258	rBV	282576	226833	12.01%	0.921%
15	9.872	1274	1281	1285	rBV	36587	46133	2.44%	0.187%
16	9.925	1285	1290	1294	rVV2	41571	44542	2.36%	0.181%
17	10.013	1301	1305	1309	rBV	1460101	1259967	66.71%	5.115%
18	10.425	1369	1375	1379	rBV2	64620	76786	4.07%	0.312%
19	10.525	1387	1392	1395	rVB4	31278	28167	1.49%	0.114%
20	10.648	1407	1413	1416	rBV2	24438	34226	1.81%	0.139%
21	10.795	1435	1438	1442	rBV	984074	891748	47.22%	3.620%
22	10.901	1453	1456	1465	rBB	69658	79380	4.20%	0.322%
23	11.348	1529	1532	1535	rBV	41879	39421	2.09%	0.160%
24	11.501	1554	1558	1561	rBV	1330192	1161782	61.51%	4.716%
25	11.524	1561	1562	1566	rVV	179363	103905	5.50%	0.422%
26	11.577	1568	1571	1573	rVV	41552	30982	1.64%	0.126%
27	12.013	1640	1645	1647	rBV2	106709	139413	7.38%	0.566%
28	12.113	1659	1662	1665	rBV2	40315	46598	2.47%	0.189%
29	12.183	1672	1674	1677	rBV4	19143	22493	1.19%	0.091%
30	12.295	1691	1693	1695	rBV2	28059	24949	1.32%	0.101%
31	12.319	1695	1697	1703	rVB5	30672	33722	1.79%	0.137%
32	12.548	1734	1736	1739	rBV2	27425	25741	1.36%	0.104%
33	12.713	1761	1764	1768	rBV	406748	355090	18.80%	1.441%
34	12.866	1788	1790	1792	rBV3	26582	29696	1.57%	0.121%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106343.D
Acq On : 12 Jun 2018 14:40
Operator : JU/SJ
Sample : J3245-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-061118-A

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.948	1798	1804	1808	rVB	380524	388763	20.58%	1.578%
36	13.083	1823	1827	1830	rBV	1892888	1609888	85.24%	6.535%
37	13.271	1856	1859	1862	rVB3	55785	65598	3.47%	0.266%
38	13.977	1976	1979	1984	rBV5	102936	150104	7.95%	0.609%
39	14.118	2001	2003	2005	rBV	131750	125869	6.66%	0.511%
40	14.154	2005	2009	2012	rVV2	1546307	1698208	89.92%	6.894%
41	14.183	2012	2014	2026	rVB	293786	488575	25.87%	1.983%
42	14.630	2088	2090	2094	rVB2	153195	139780	7.40%	0.567%
43	15.248	2191	2195	2202	rVB	305030	631110	33.42%	2.562%
44	15.312	2203	2206	2208	rBV	198541	212405	11.25%	0.862%
45	15.571	2247	2250	2256	rVB	143716	174280	9.23%	0.707%
46	15.636	2258	2261	2266	rVB	161847	207013	10.96%	0.840%
47	15.707	2268	2273	2282	rBV	949930	1376575	72.89%	5.588%
48	16.189	2351	2355	2359	rVB	217265	310351	16.43%	1.260%

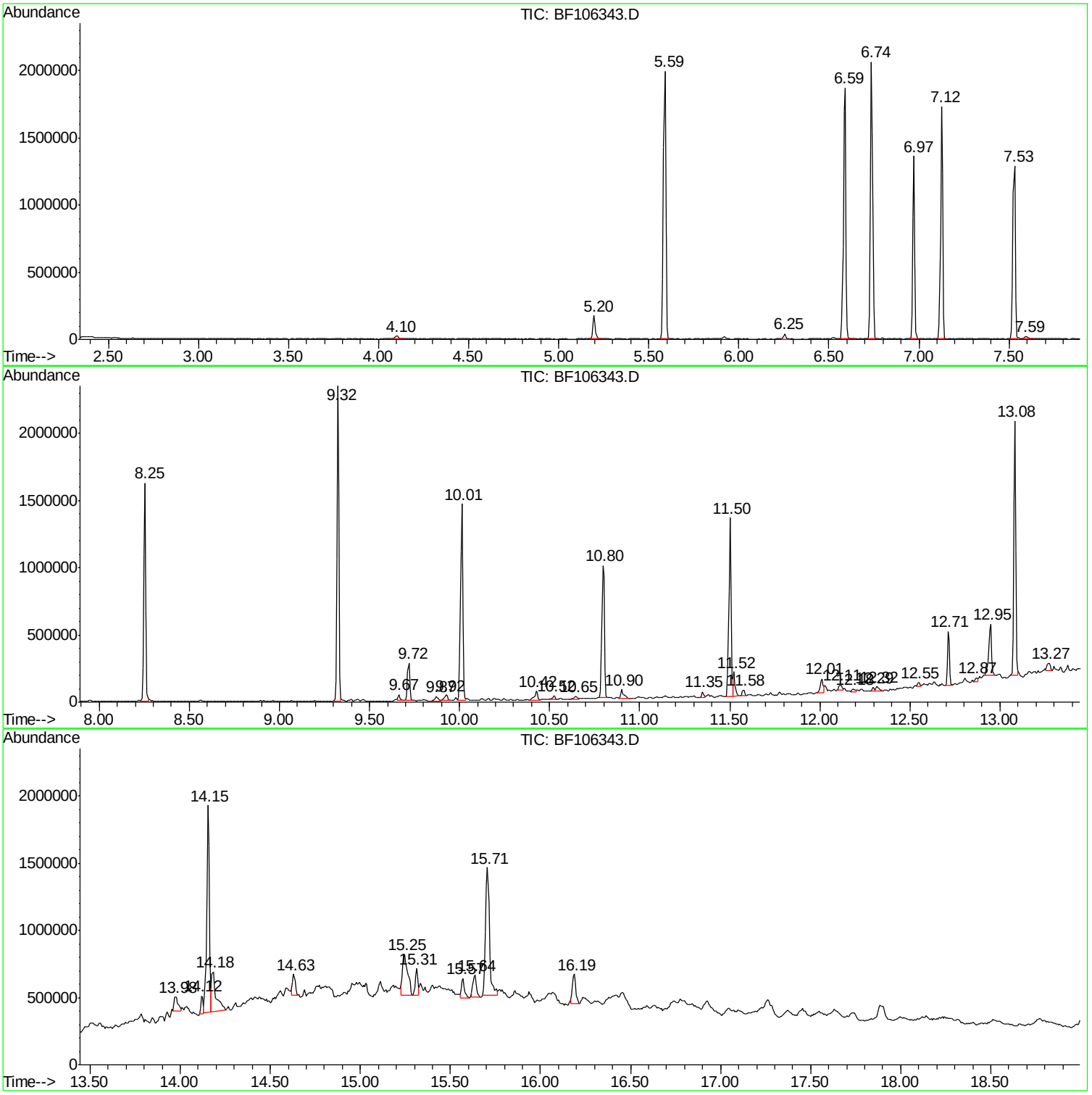
Sum of corrected areas: 24634590

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106343.D
Acq On : 12 Jun 2018 14:40
Operator : JU/SJ
Sample : J3245-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-01-061118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106343.D
Acq On : 12 Jun 2018 14:40
Operator : JU/SJ
Sample : J3245-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-061118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

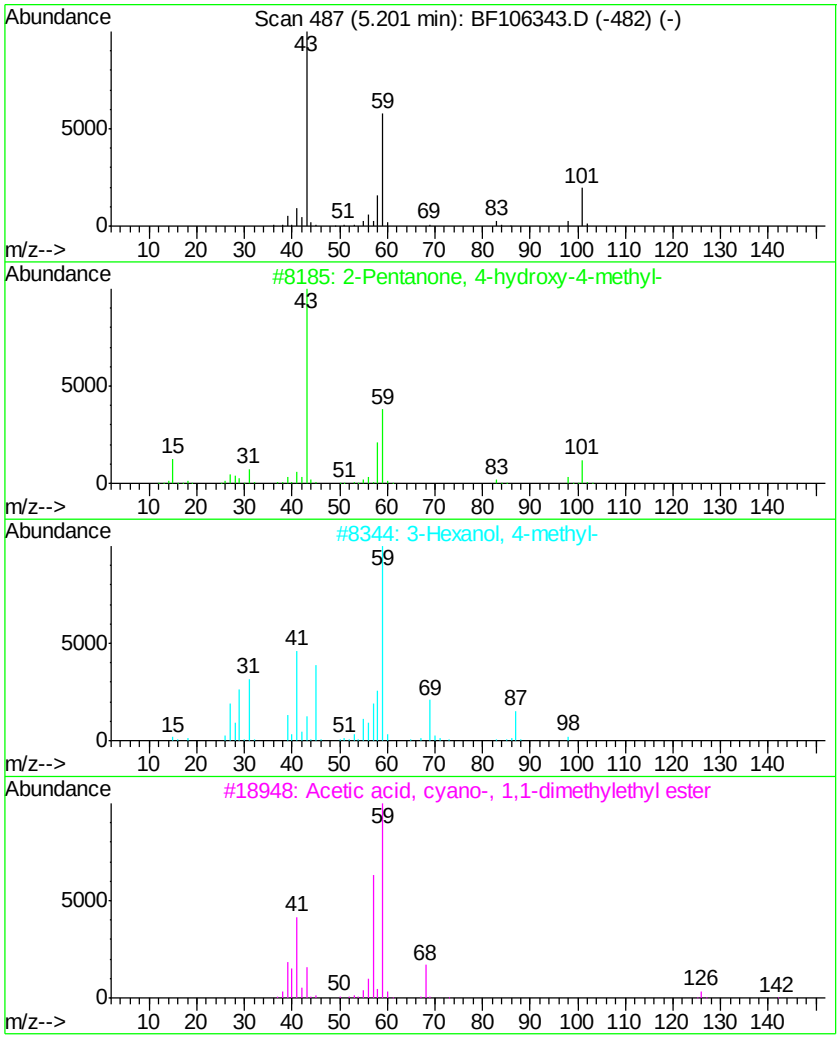
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

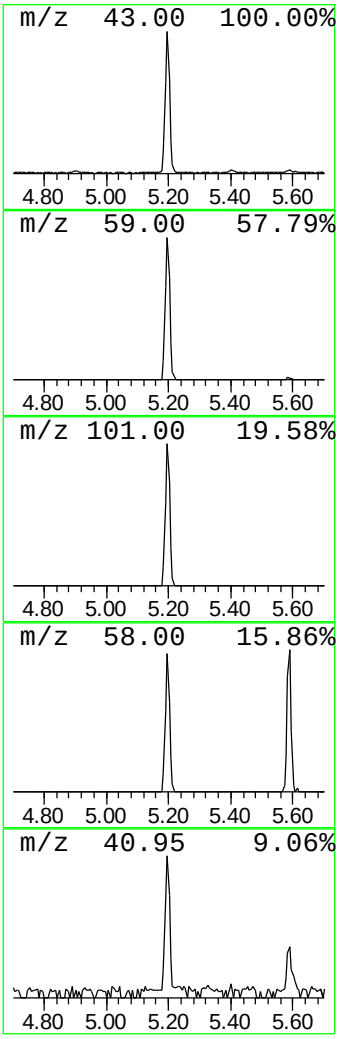
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.13 ng	169698	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106343.D
Acq On : 12 Jun 2018 14:40
Operator : JU/SJ
Sample : J3245-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-061118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

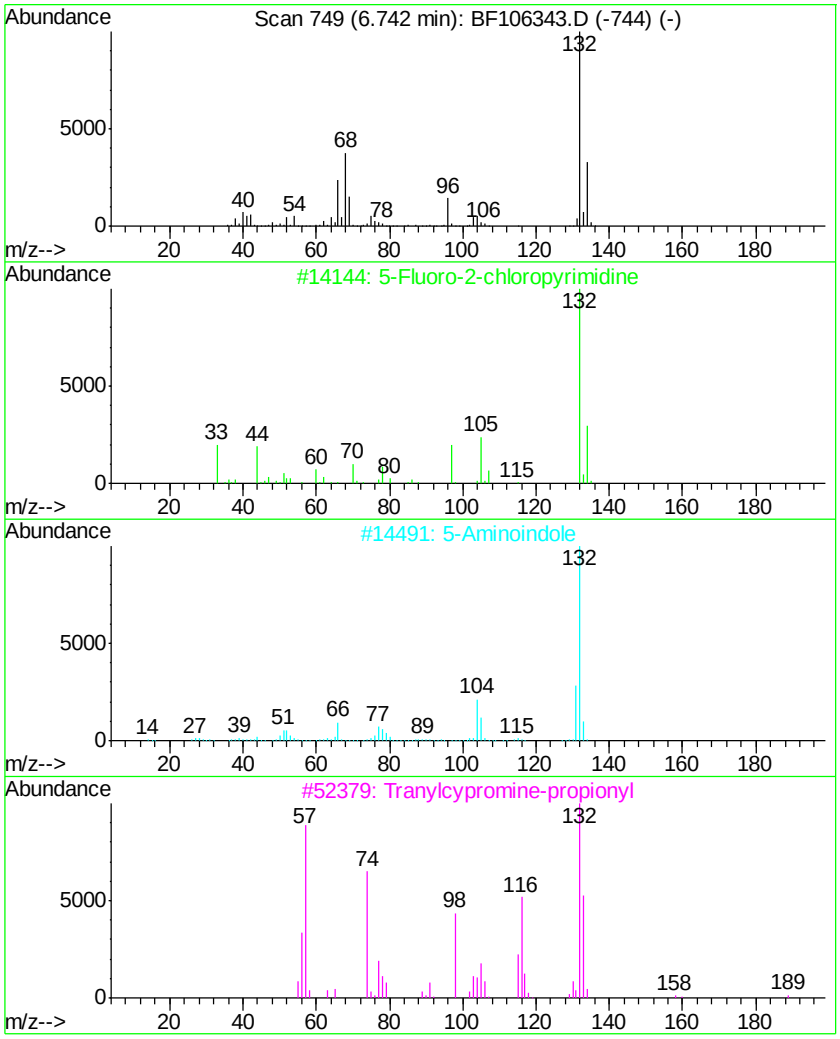
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

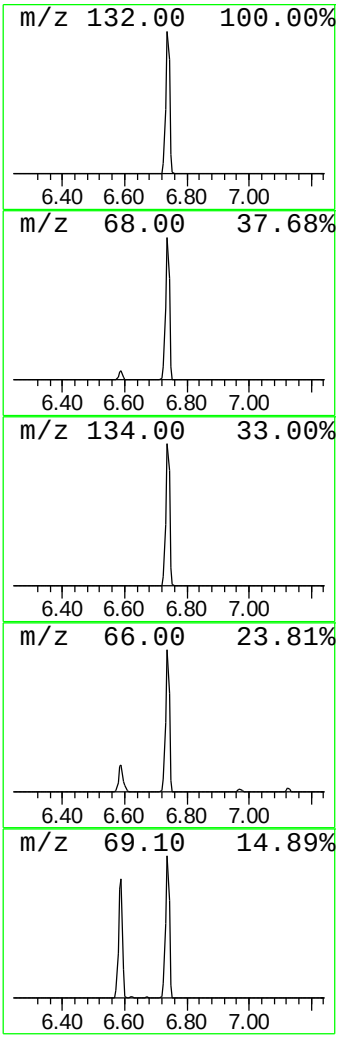
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	32.61 ng	1769710	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106343.D
Acq On : 12 Jun 2018 14:40
Operator : JU/SJ
Sample : J3245-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-061118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

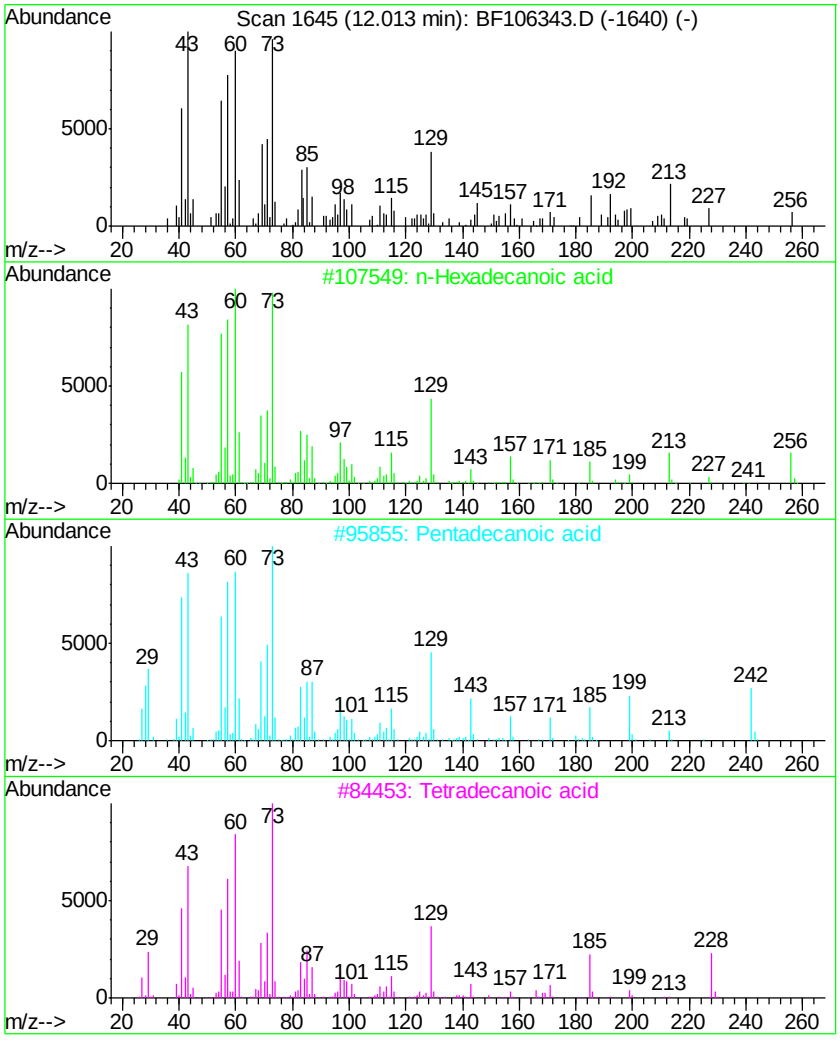
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

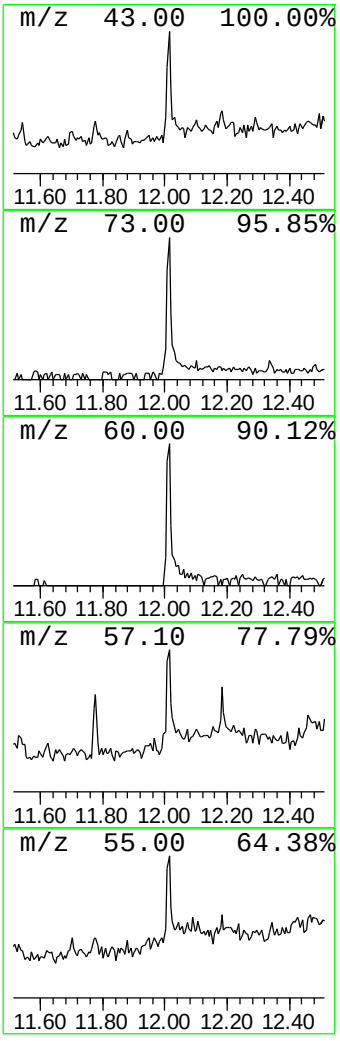
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.40 ng	139413	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Nonanoic acid	158	C9H18O2	000112-05-0	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106343.D
Acq On : 12 Jun 2018 14:40
Operator : JU/SJ
Sample : J3245-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-061118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

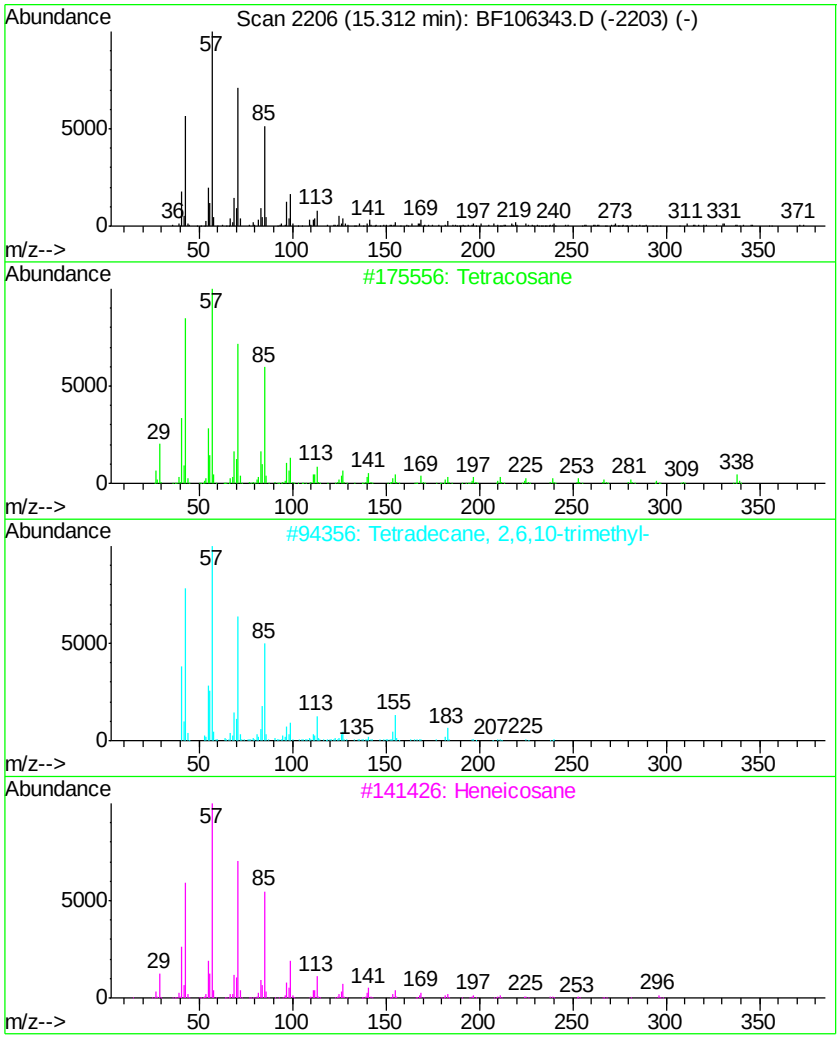
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

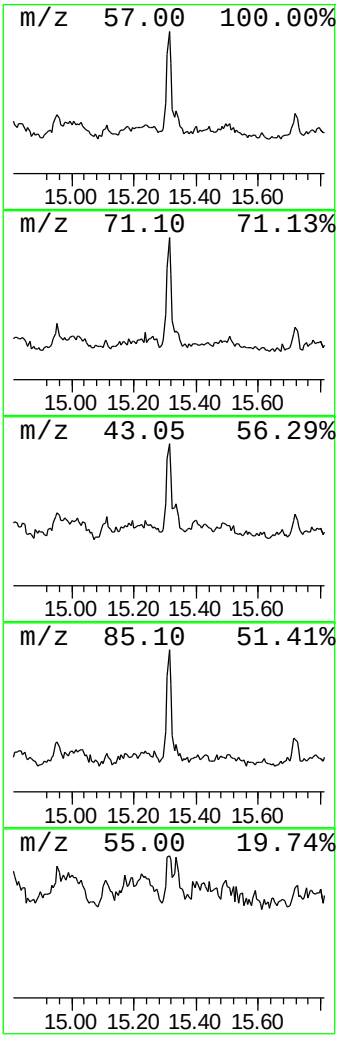
****

Peak Number 5 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	3.09 ng	212405	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
3	Heneicosane	296	C21H44	000629-94-7	86
4	Tetradecane	198	C14H30	000629-59-4	74
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106343.D
Acq On : 12 Jun 2018 14:40
Operator : JU/SJ
Sample : J3245-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-061118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

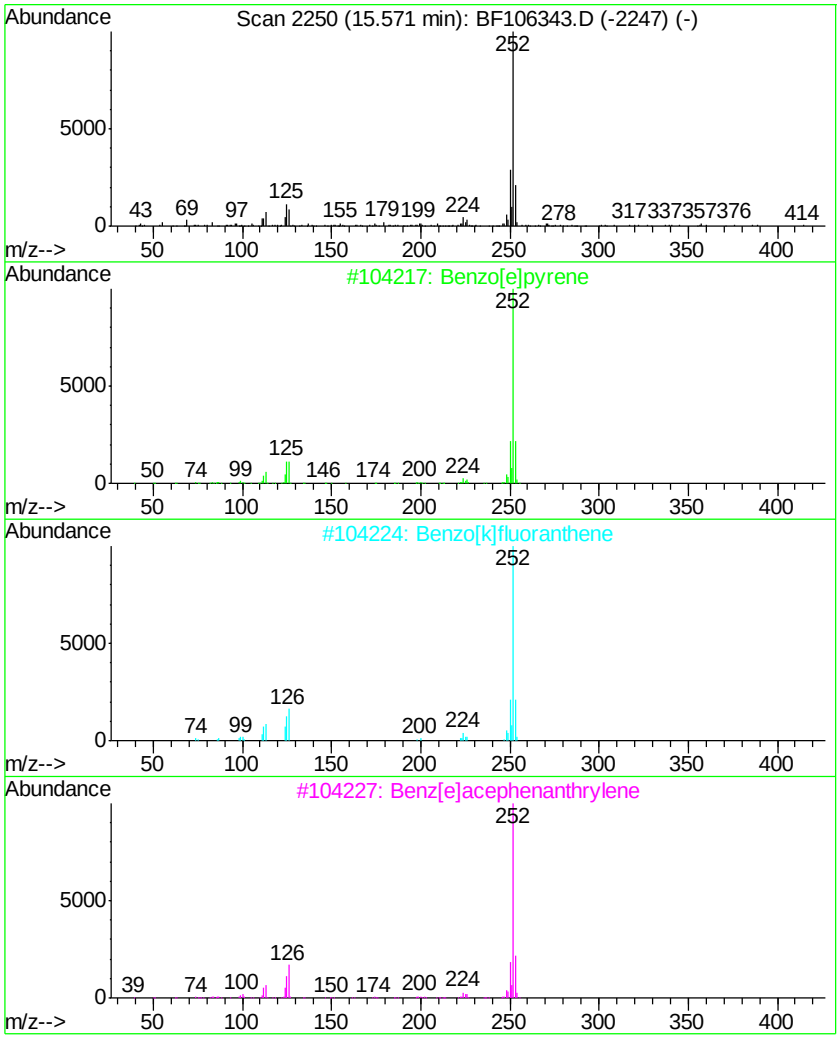
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

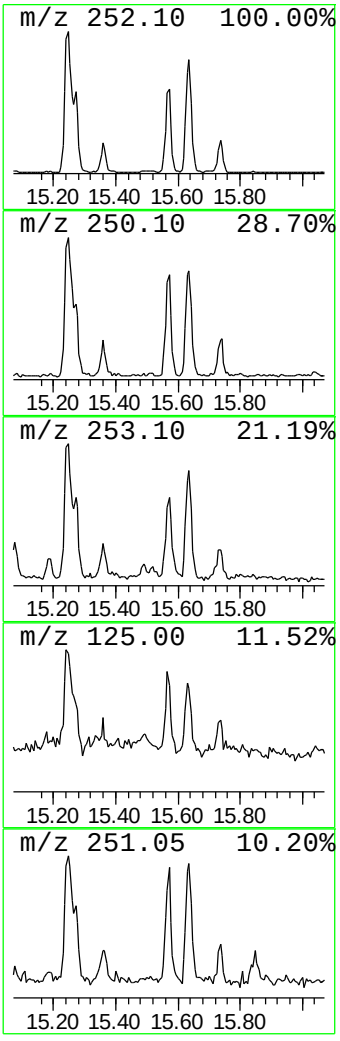
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	2.53 ng	174280	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	91
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Perylene	252	C20H12	000198-55-0	89





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106343.D
Acq On : 12 Jun 2018 14:40
Operator : JU/SJ
Sample : J3245-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-061118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

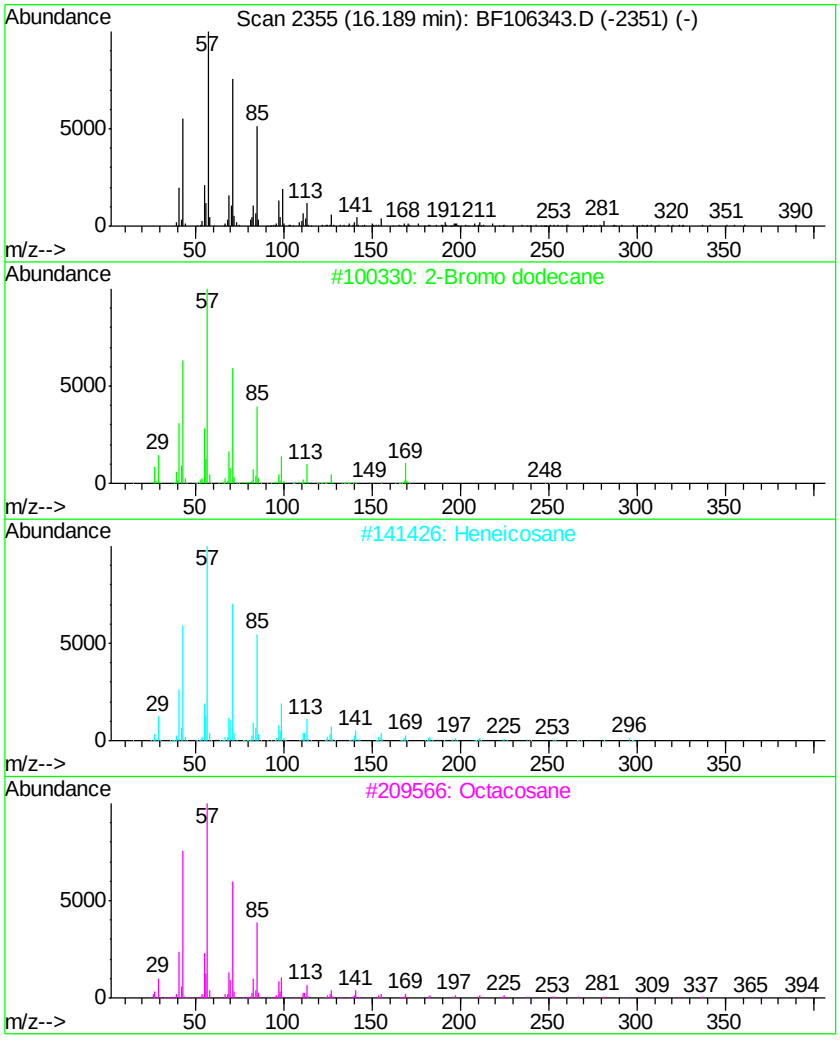
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

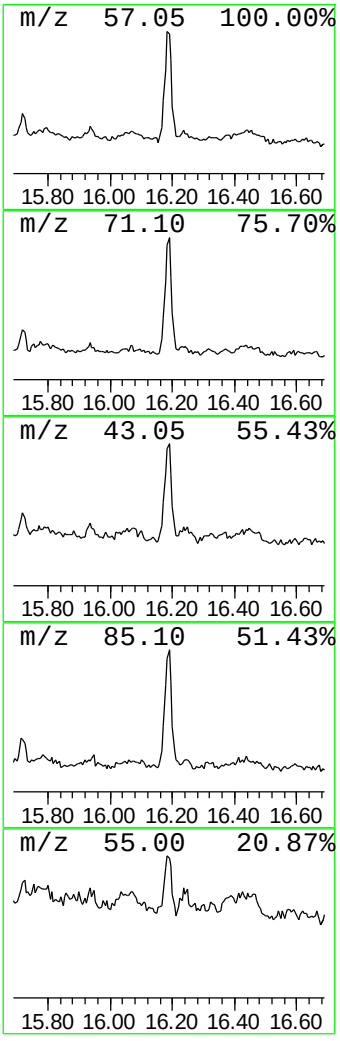
****

Peak Number 7 2-Bromo dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	4.51 ng	310351	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061218\
Data File : BF106343.D
Acq On : 12 Jun 2018 14:40
Operator : JU/SJ
Sample : J3245-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-061118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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...	5.20	3.1	ng	169698	1	6.97	1085500	20.0
unknown6.74	6.74	32.6	ng	1769710	1	6.97	1085500	20.0
n-Hexadecanoic acid	12.01	2.4	ng	139413	4	11.50	1161780	20.0
Tetracosane	15.31	3.1	ng	212405	6	15.71	1376580	20.0
Benzo[e]pyrene	15.57	2.5	ng	174280	6	15.71	1376580	20.0
2-Bromo dodecane	16.19	4.5	ng	310351	6	15.71	1376580	20.0