LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107545.D
Acq On : 21 Jul 2018 00:56
Operator : JU/SJ
Sample : J3828-11 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-071818-C

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-BF072018.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	5.189	482	485	497	rBV	337840	389939	13.17%	1.113%
2	5.595	550	554	577	rBV	1690446	2583130	87.22%	7.374%
3	6.601	721	725	745	rBV	1824197	2887893	97.51%	8.244%
4	6.742	745	749	774	rVB	2588558	2961753	100.00%	8.455%
5	6.972	784	788	811	rBV	1695819	1970532	66.53%	5.625%
6	7.125	811	814	830	rBV	1864181	2081897	70.29%	5.943%
7	7.530	880	883	903	rBV	1290052	1723498	58.19%	4.920%
8	8.254	1002	1006	1025	rBV	2304926	2522832	85.18%	7.202%
9	9.330	1185	1189	1198	rBV	2933596	2950832	99.63%	8.424%
10	9.395	1198	1200	1204	rVB2	37354	42108	1.42%	0.120%
11	9.719	1252	1255	1260	rBV	225019	229744	7.76%	0.656%
12	9.924	1287	1290	1294	rBV2	39027	40589	1.37%	0.116%
13	10.013	1299	1305	1319	rBV	2300404	2477321	83.64%	7.072%
14	10.324	1356	1358	1363	rBV6	23172	31235	1.05%	0.089%
15	10.424	1372	1375	1378	rVB2	53817	51693	1.75%	0.148%
16	10.648	1408	1413	1417	rBV2	46255	64448	2.18%	0.184%
17	10.807	1436	1440	1450	rBV	1497305	1575405	53.19%	4.497%
18	10.913	1454	1458	1462	rVV2	74678	120269	4.06%	0.343%
19	11.348	1530	1532	1535	rBV	77619	67617	2.28%	0.193%
20	11.383	1535	1538	1545	rVB3	56454	79291	2.68%	0.226%
21	11.507	1555	1559	1567	rBV	2199996	2174090	73.41%	6.206%
22	11.777	1603	1605	1608	rBV	77717	59829	2.02%	0.171%
23	12.018	1643	1646	1652	rBV8	87698	146064	4.93%	0.417%
24	12.183	1672	1674	1677	rBV	67339	63481	2.14%	0.181%
25	12.724	1764	1766	1769	rBV	70252	61277	2.07%	0.175%
26	12.954	1802	1805	1812	rVB3	137639	195990	6.62%	0.559%
27	13.089	1825	1828	1836	rVB	2455388	2175131	73.44%	6.209%
28	13.307	1863	1865	1867	rBV	108804	81416	2.75%	0.232%
29	13.648	1921	1923	1927	rBV	145206	123369	4.17%	0.352%
30	13.977	1976	1979	1982	rBV	273270	250466	8.46%	0.715%
31	14.159	2006	2010	2014	rBV	2006999	2010119	67.87%	5.738%
32	14.601	2083	2085	2090	rVB	319643	312487	10.55%	0.892%
33	15.283	2199	2201	2206	rVB	424936	413819	13.97%	1.181%
34	15.695	2267	2271	2278	rVB2	1502266	2110828	71.27%	6.026%

LSC Area Percent Report

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Data File : BF107545.D
Acq On : 21 Jul 2018 00:56
Operator : JU/SJ
Sample : J3828-11 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-071818-C

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-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 35030392

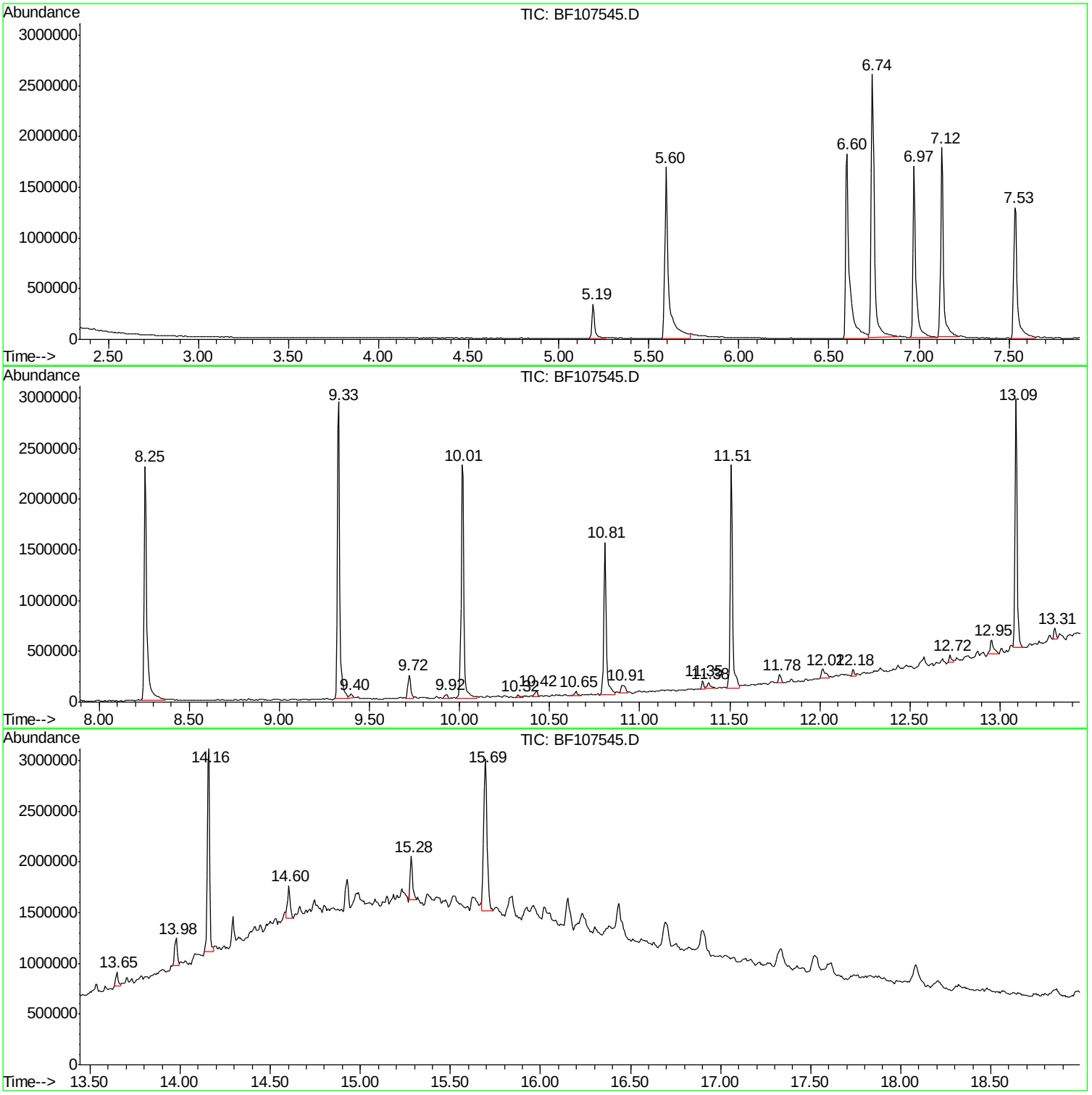
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107545.D
Acq On : 21 Jul 2018 00:56
Operator : JU/SJ
Sample : J3828-11 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-02-071818-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107545.D
Acq On : 21 Jul 2018 00:56
Operator : JU/SJ
Sample : J3828-11 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-071818-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

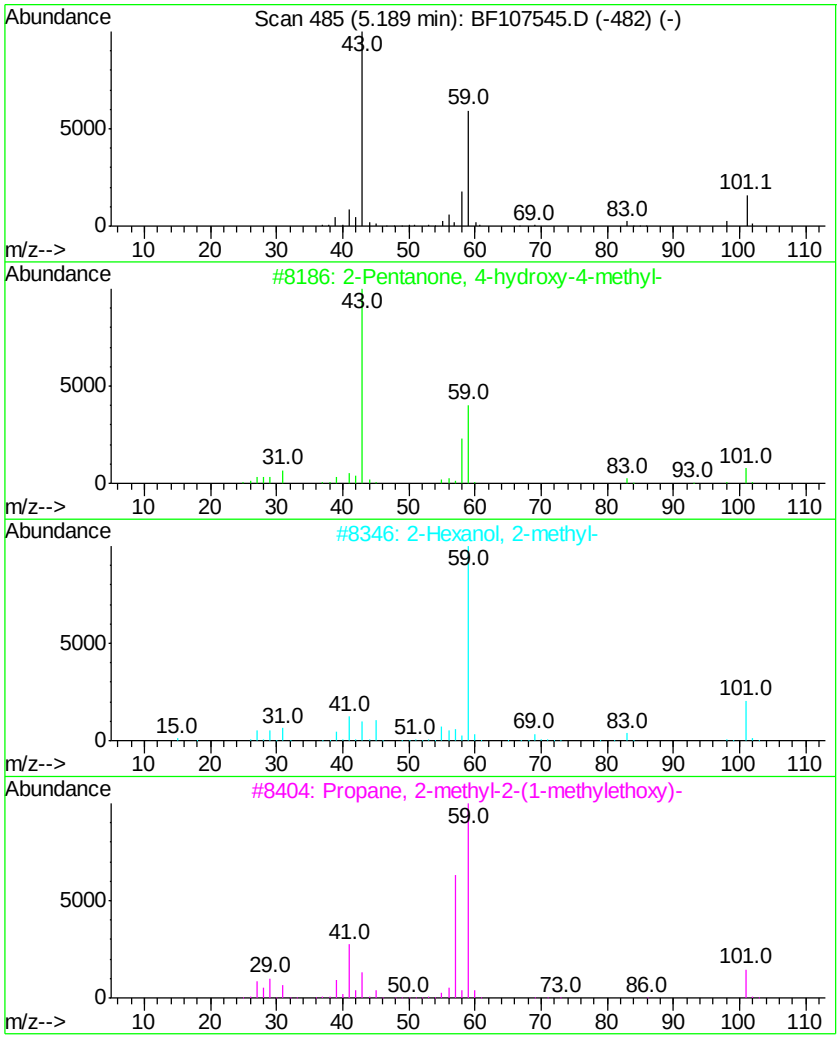
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

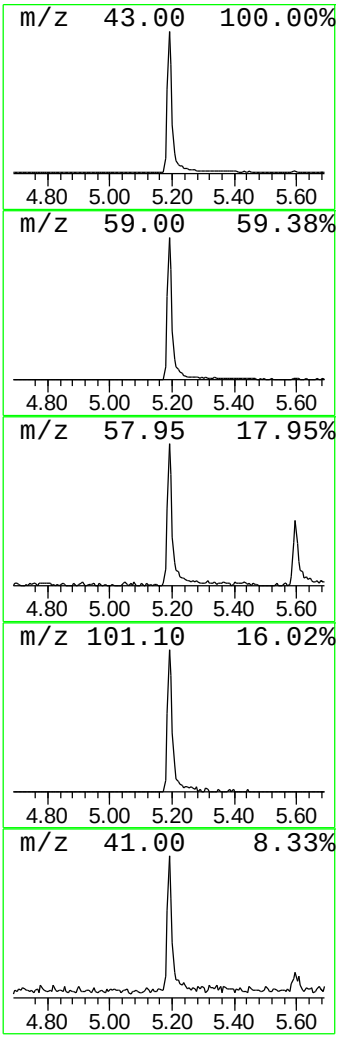
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.96 ng	389939	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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	3-Octanol	130	C8H18O	000589-98-0	33





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107545.D
Acq On : 21 Jul 2018 00:56
Operator : JU/SJ
Sample : J3828-11 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-071818-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

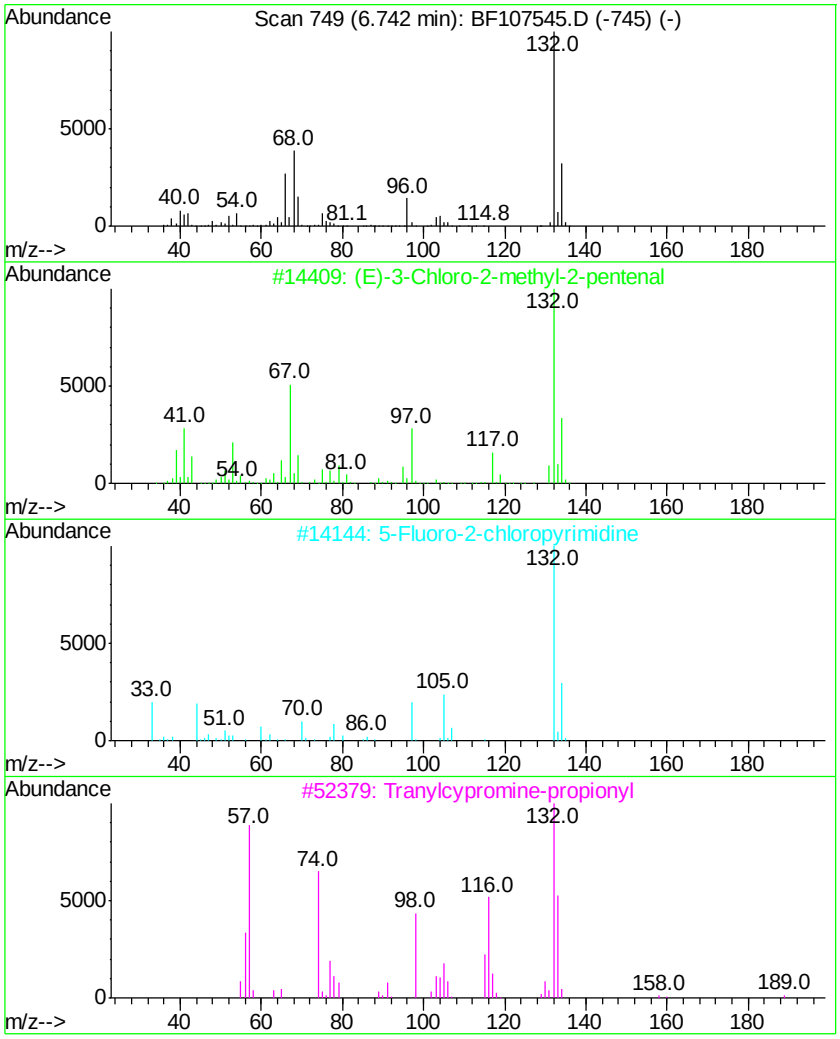
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

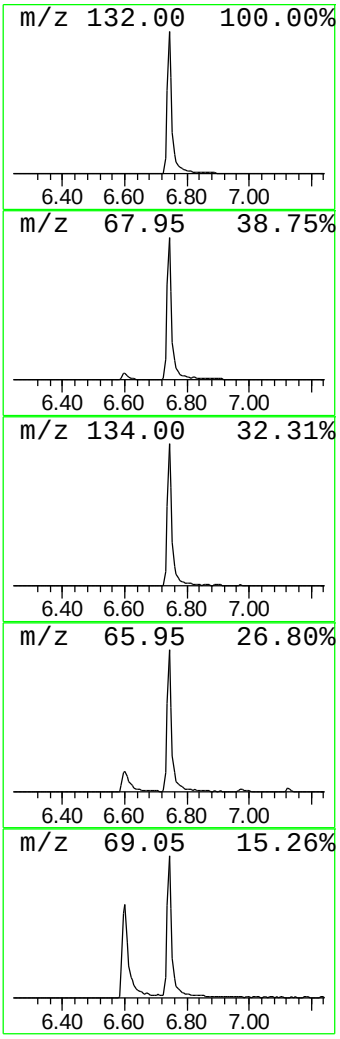
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	30.06 ng	2961750	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107545.D
Acq On : 21 Jul 2018 00:56
Operator : JU/SJ
Sample : J3828-11 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-071818-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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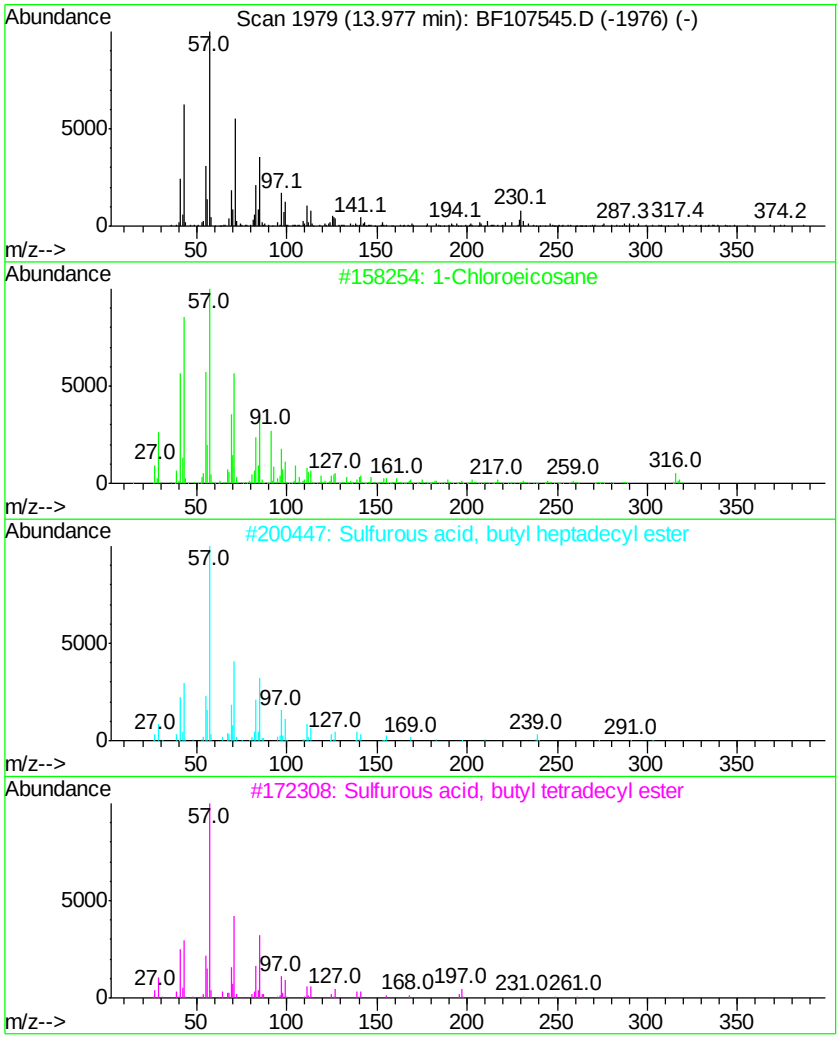
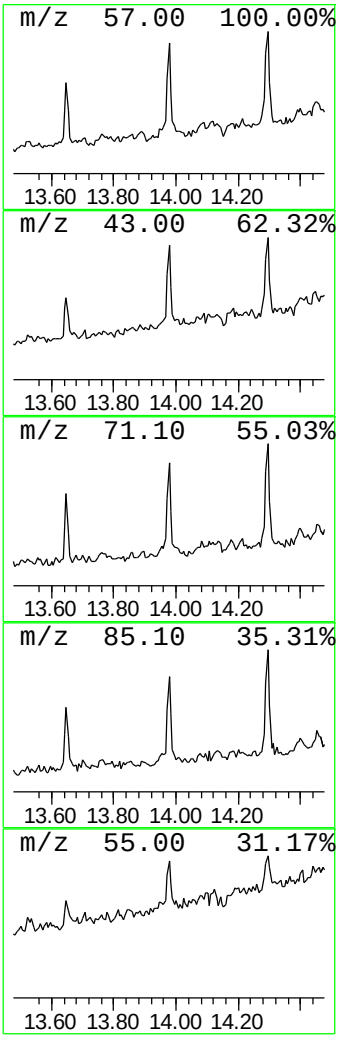
Peak Number 4 1-Chloroeicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	2.49 ng	250466	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Chloroeicosane	316	C20H41Cl	042217-02-7	91
2	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	87
3	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	86
4	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	86
5	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107545.D
Acq On : 21 Jul 2018 00:56
Operator : JU/SJ
Sample : J3828-11 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-071818-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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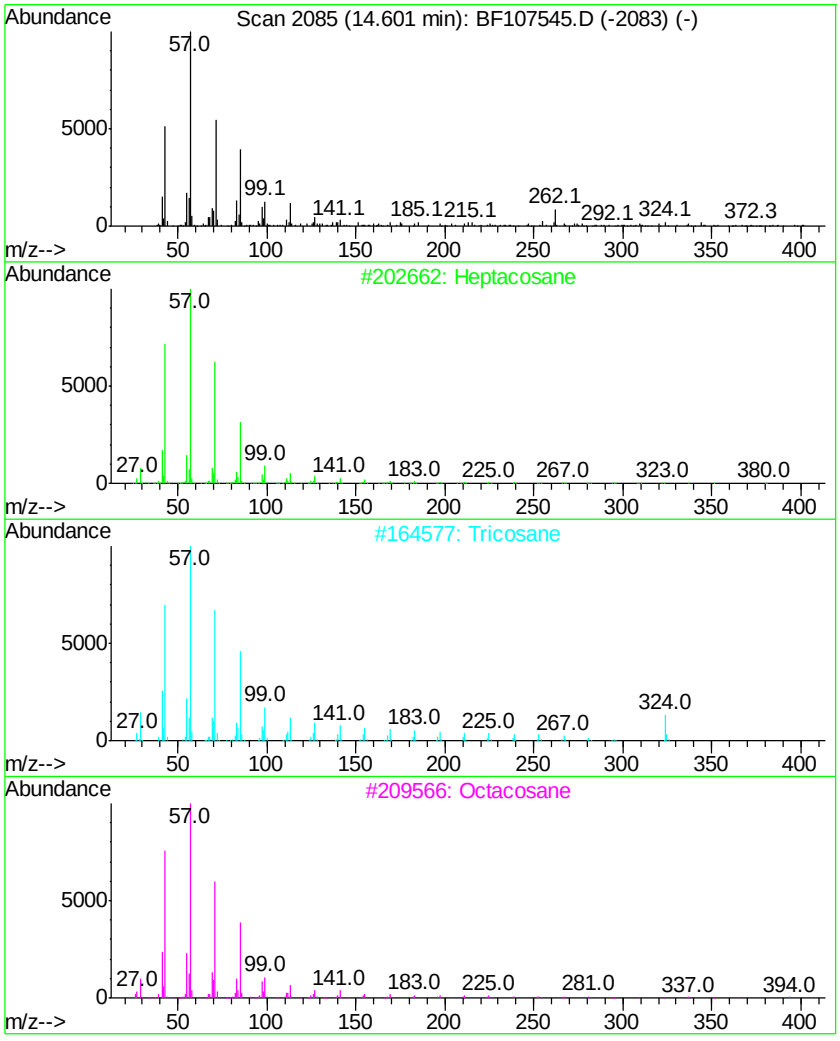
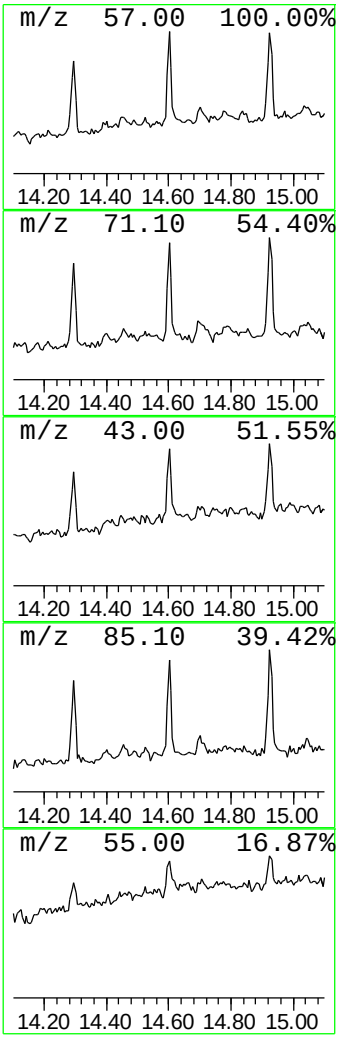
****

Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	3.11 ng	312487	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	97
2	Tricosane	324	C23H48	000638-67-5	91
3	Octacosane	394	C28H58	000630-02-4	87
4	Docosane	310	C22H46	000629-97-0	87
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	87





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Data File : BF107545.D
Acq On : 21 Jul 2018 00:56
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Sample : J3828-11 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-071818-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

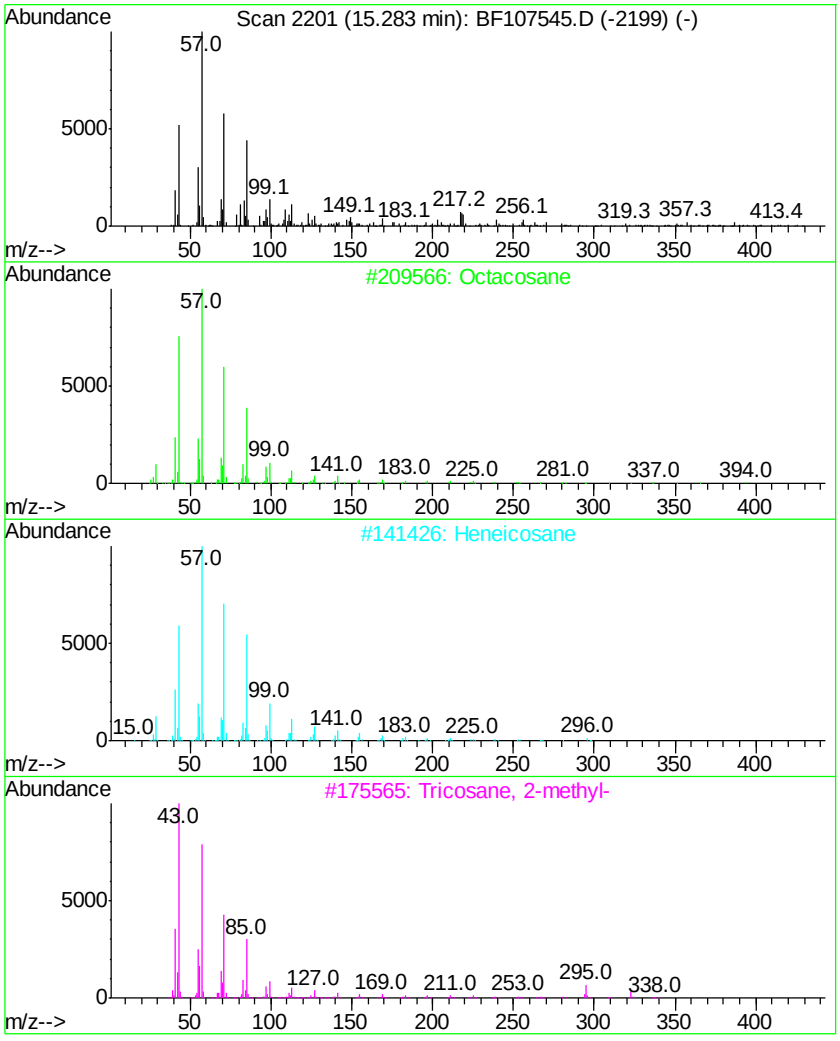
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

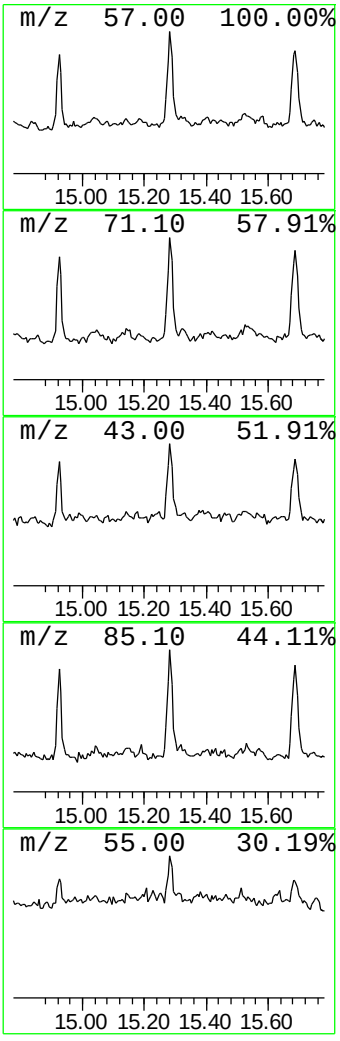
****

Peak Number 6 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	3.92 ng	413819	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
5	1-Iodoundecane	282	C11H23I	004282-44-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072018\
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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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...	5.19	4.0	ng	389939	1	6.97	1970530	20.0
unknown6.74	6.74	30.1	ng	2961750	1	6.97	1970530	20.0
1-Chloroeicosane	13.98	2.5	ng	250466	5	14.16	2010120	20.0
Heptacosane	14.60	3.1	ng	312487	5	14.16	2010120	20.0
Octacosane	15.28	3.9	ng	413819	6	15.69	2110830	20.0