LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

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-BF121417.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	4.993	491	494	512	rBV	94216	196286	7.29%	0.752%
2	5.398	559	563	590	rBV	1665306	2691538	100.00%	10.318%
3	6.345	720	724	732	rVB2	26441	32644	1.21%	0.125%
4	6.422	733	737	755	rBV	1888546	2650156	98.46%	10.160%
5	6.545	755	758	764	rVV	2330087	2490280	92.52%	9.547%
6	6.587	764	765	776	rVB2	41979	48042	1.78%	0.184%
7	6.769	793	796	806	rBV	735245	739398	27.47%	2.835%
8	6.922	819	822	837	rBV	1859567	1995238	74.13%	7.649%
9	7.269	877	881	890	rBV2	23488	49475	1.84%	0.190%
10	7.345	890	894	916	rVV	1175952	1571966	58.40%	6.026%
11	7.663	944	948	955	rBV	82571	77028	2.86%	0.295%
12	8.051	1011	1014	1029	rBV	820830	881056	32.73%	3.378%
13	8.622	1107	1111	1116	rBV2	41627	56599	2.10%	0.217%
14	9.122	1192	1196	1204	rBV	2570077	2366400	87.92%	9.072%
15	9.192	1204	1208	1212	rVB	55479	56175	2.09%	0.215%
16	9.522	1258	1264	1270	rBV	145745	192726	7.16%	0.739%
17	9.716	1293	1297	1302	rVB	70706	72121	2.68%	0.276%
18	9.804	1309	1312	1317	rBV	840578	794357	29.51%	3.045%
19	10.216	1379	1382	1385	rVB	87918	64110	2.38%	0.246%
20	10.433	1414	1419	1424	rBV	39920	55263	2.05%	0.212%
21	10.522	1431	1434	1437	rBV	87672	72820	2.71%	0.279%
22	10.604	1444	1448	1460	rBV	1167836	1244654	46.24%	4.772%
23	10.692	1460	1463	1472	rVB2	82776	125663	4.67%	0.482%
24	11.139	1536	1539	1541	rBV	47295	41935	1.56%	0.161%
25	11.163	1541	1543	1548	rVB	31527	30698	1.14%	0.118%
26	11.298	1563	1566	1569	rBV	837171	798984	29.69%	3.063%
27	11.327	1569	1571	1576	rVB	113954	118552	4.40%	0.454%
28	11.516	1599	1603	1606	rBV4	21102	28611	1.06%	0.110%
29	11.563	1608	1611	1614	rVB	45079	41725	1.55%	0.160%
30	11.669	1626	1629	1632	rVB	322404	243411	9.04%	0.933%
31	11.810	1650	1653	1656	rBV2	79237	82279	3.06%	0.315%
32	12.351	1742	1745	1747	rBV	1097091	990811	36.81%	3.798%
33	12.374	1747	1749	1756	rVV2	847398	739997	27.49%	2.837%
34	12.457	1760	1763	1768	rVB	192290	164676	6.12%	0.631%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.522	1768	1774	1781	rBV	194593	236729	8.80%	0.908%
36	12.680	1798	1801	1803	rBV2	36472	41218	1.53%	0.158%
37	12.733	1807	1810	1811	rBV2	53111	49091	1.82%	0.188%
38	12.751	1811	1813	1817	rVB	155283	149429	5.55%	0.573%
39	12.880	1831	1835	1838	rBV	2293923	2088146	77.58%	8.005%
40	13.063	1861	1866	1868	rBV6	26749	49281	1.83%	0.189%
41	13.086	1868	1870	1875	rVB	42682	45432	1.69%	0.174%
42	13.186	1884	1887	1889	rBV4	26093	29244	1.09%	0.112%
43	13.427	1925	1928	1930	rBV	31726	29005	1.08%	0.111%
44	13.757	1981	1984	1990	rBV3	177997	209172	7.77%	0.802%
45	13.892	2005	2007	2010	rVB	48155	43687	1.62%	0.167%
46	13.951	2013	2017	2021	rBV	765347	821466	30.52%	3.149%
47	15.421	2263	2267	2274	rVB	385809	487217	18.10%	1.868%

Sum of corrected areas: 26084791

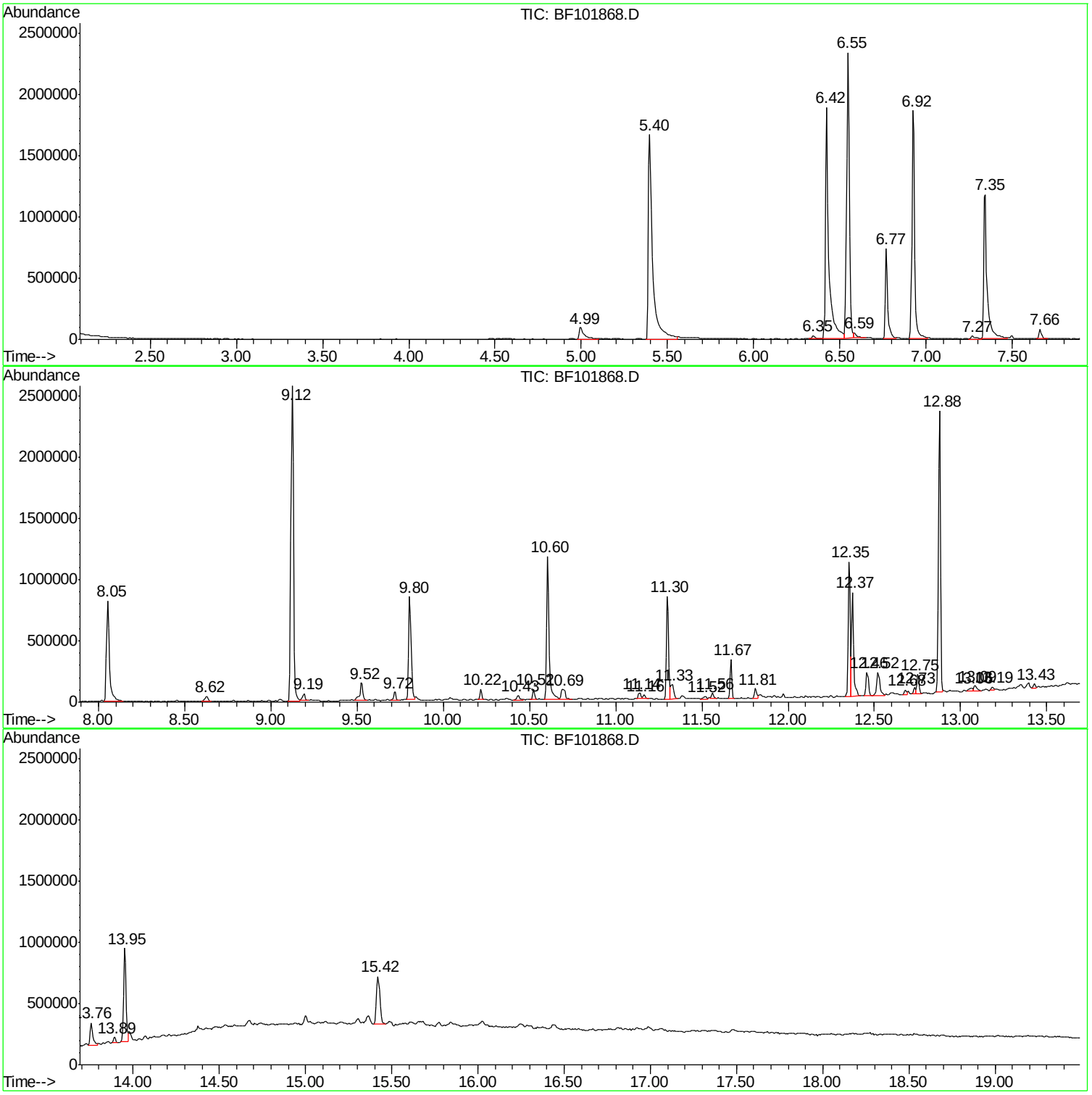
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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\BF010318\
Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

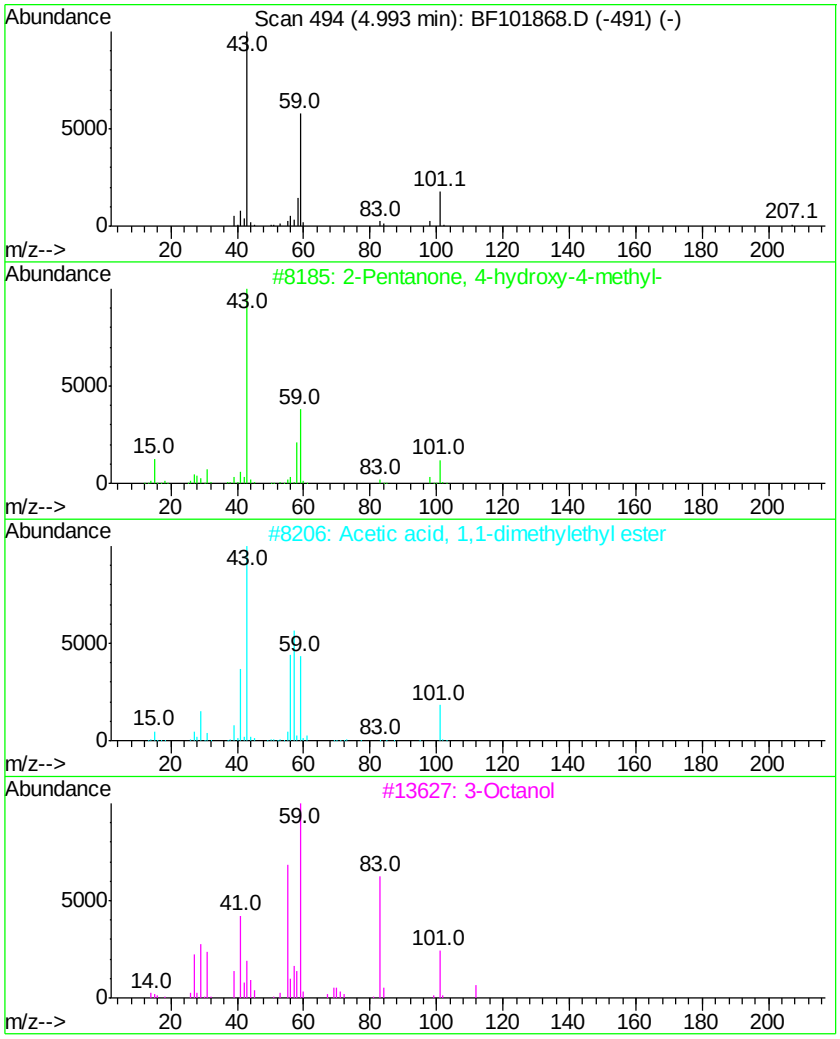
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

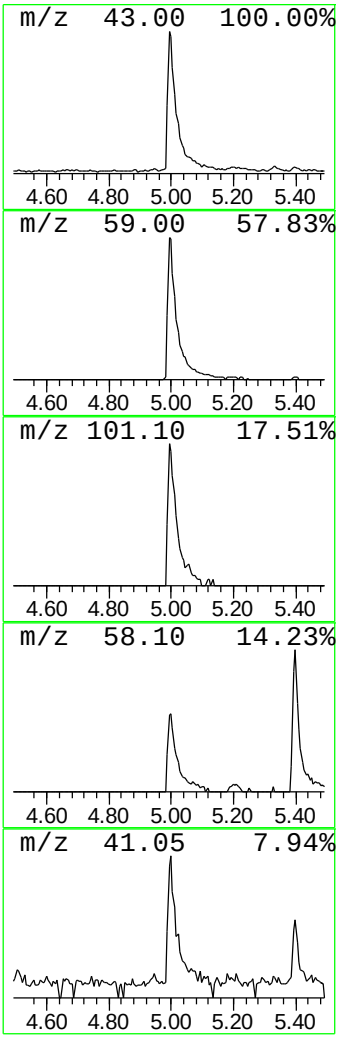
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	5.31 ng	196286	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Octanol	130	C8H18O	000589-98-0	33
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

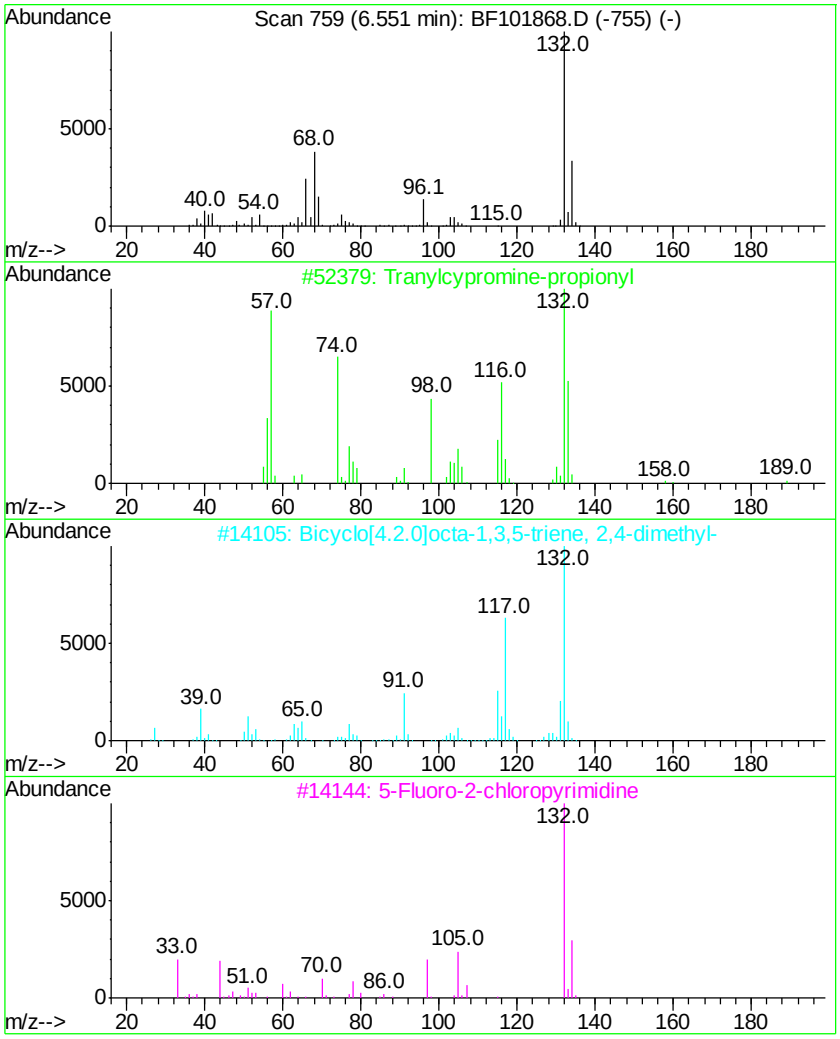
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

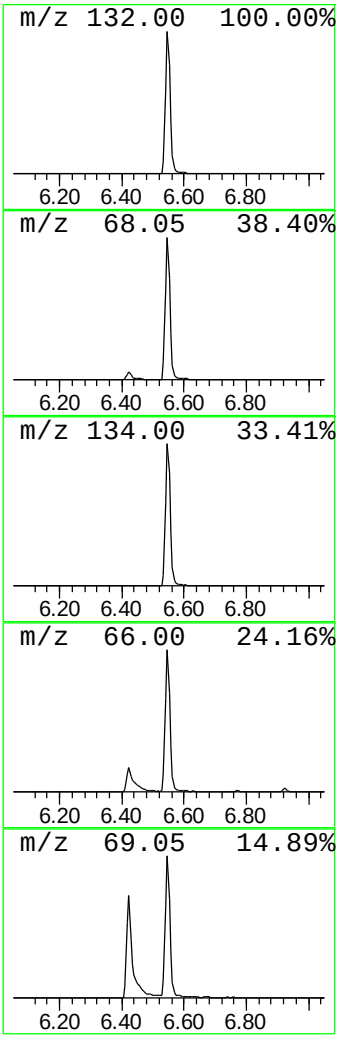
****

Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	67.36 ng	2490280	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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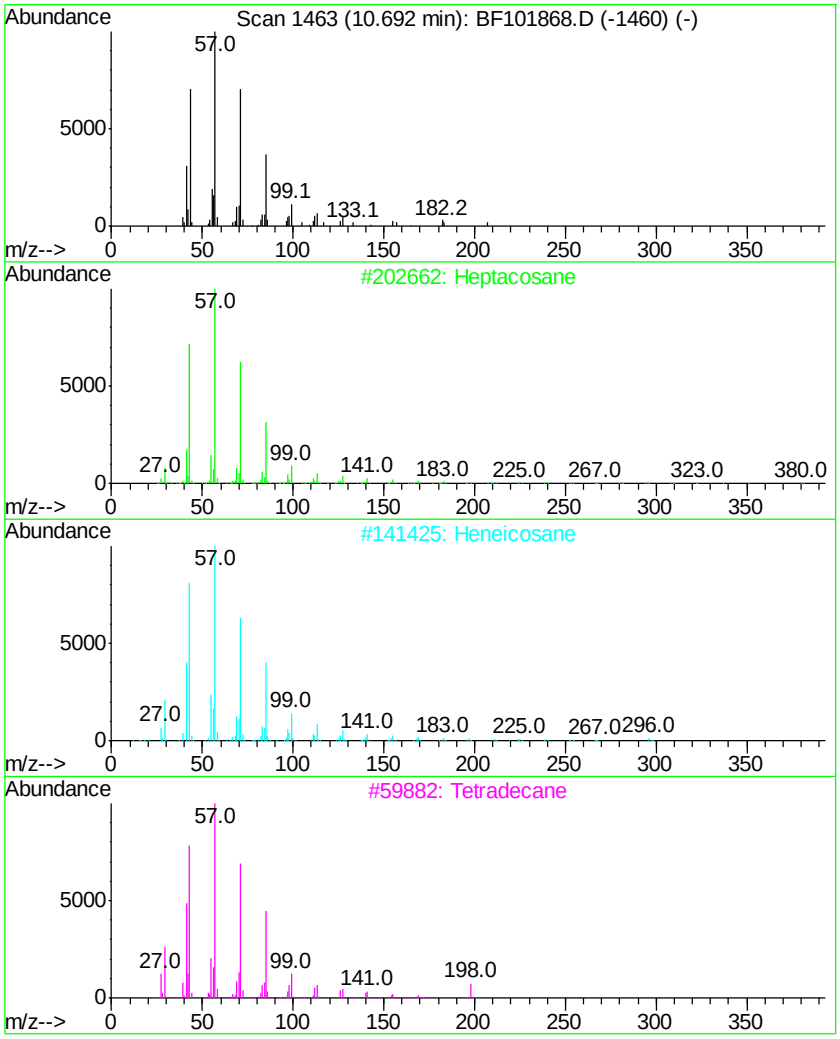
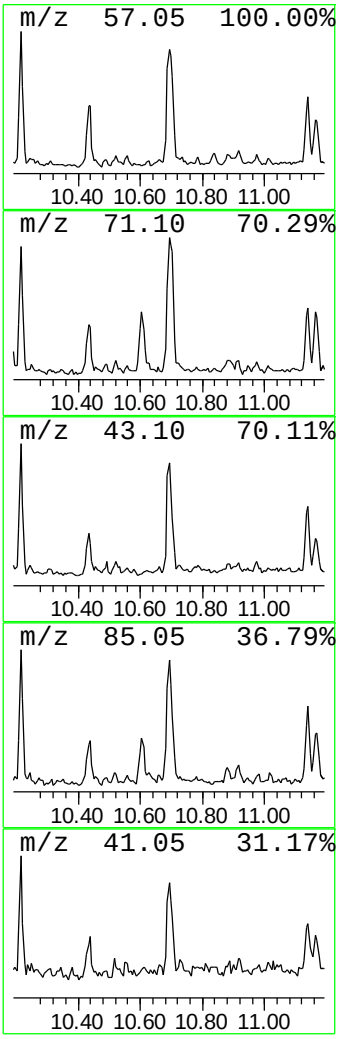
Peak Number 4 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	3.15 ng	125663	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetradecane	198	C14H30	000629-59-4	91
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
5	Pentadecane	212	C15H32	000629-62-9	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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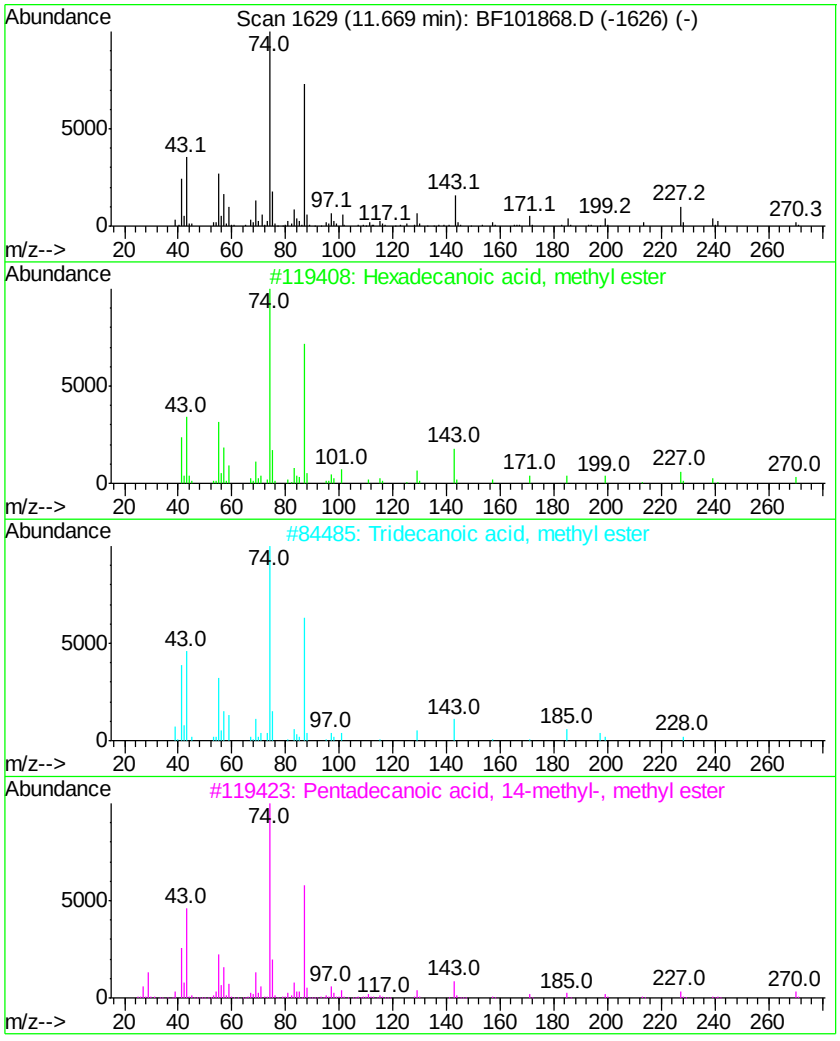
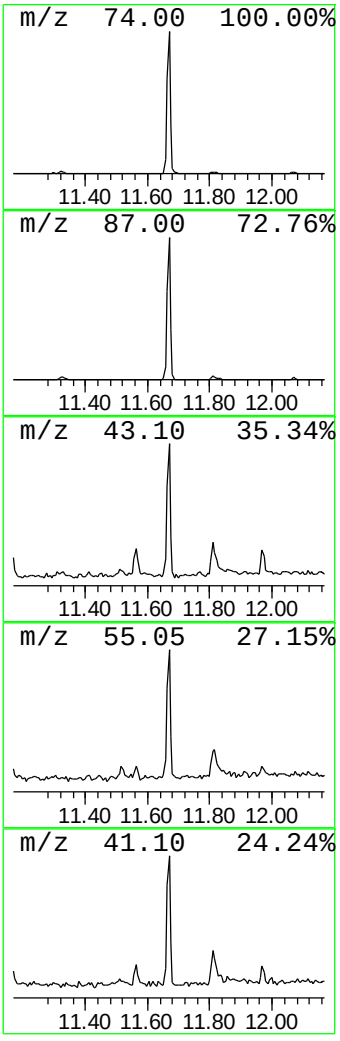
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	6.09 ng	243411	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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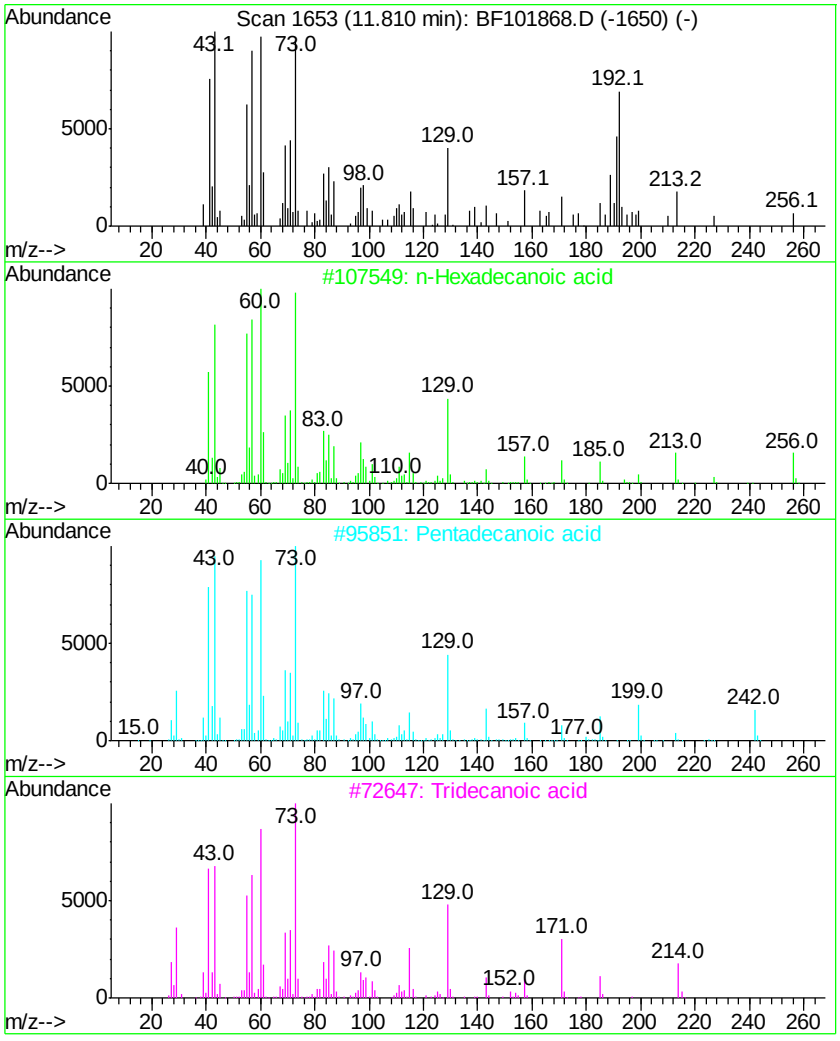
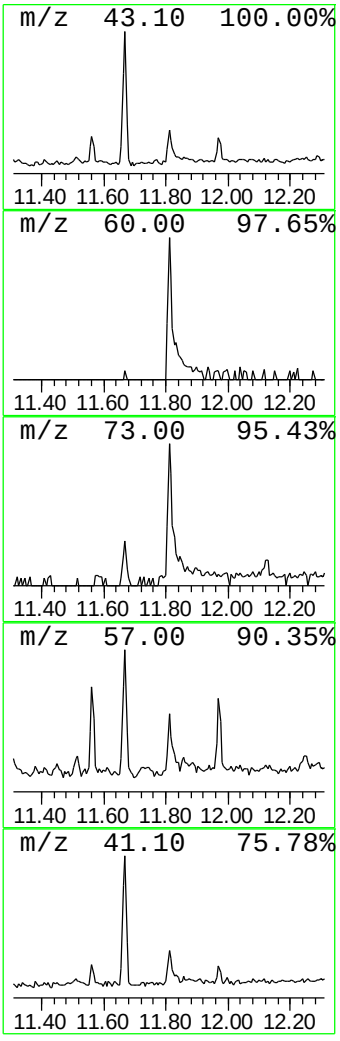
Peak Number 6 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	2.06 ng	82279	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3	Tridecanoic acid	214	C13H26O2	000638-53-9	49
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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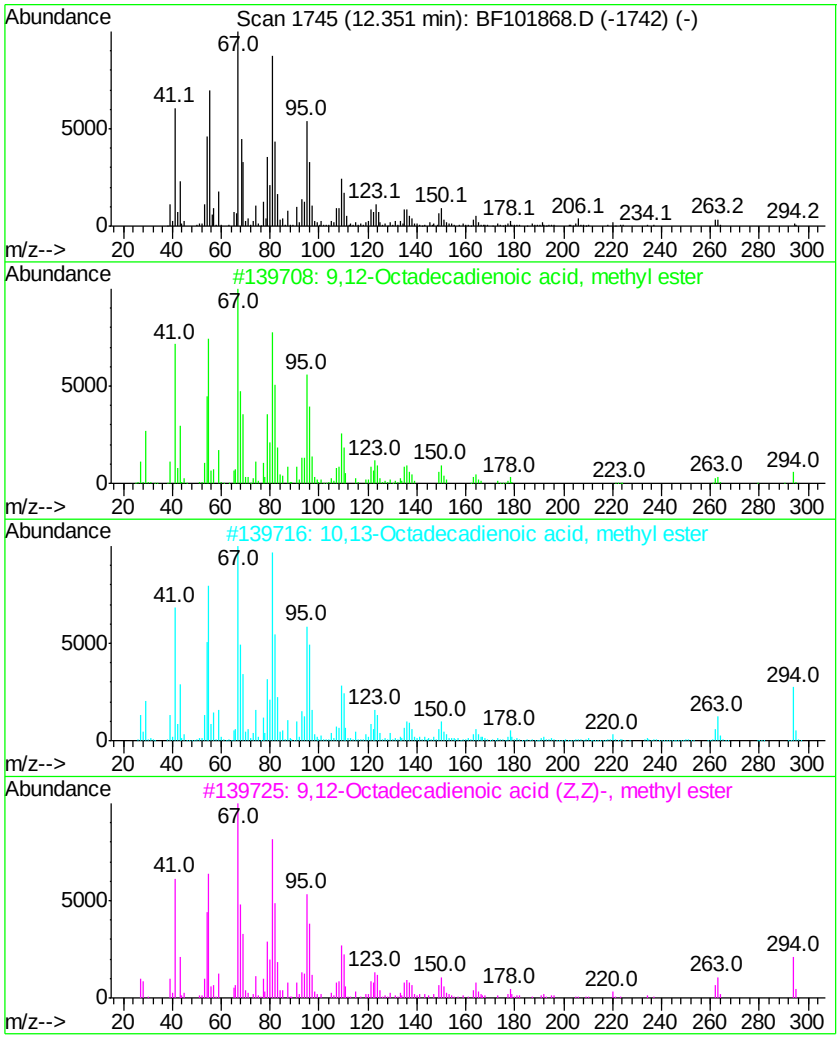
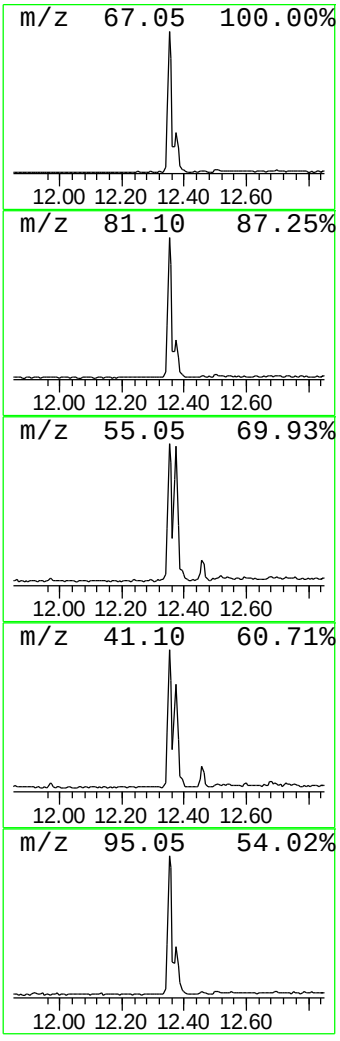
Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	24.80 ng	990811	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	96
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95





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Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

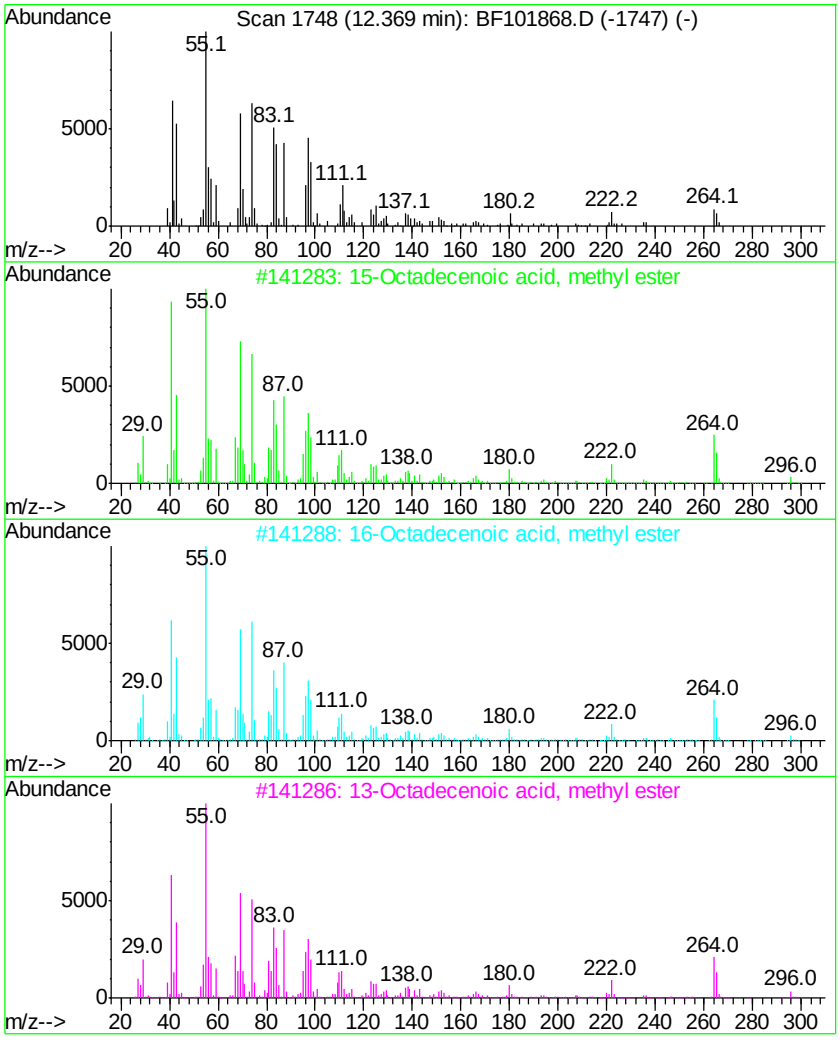
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

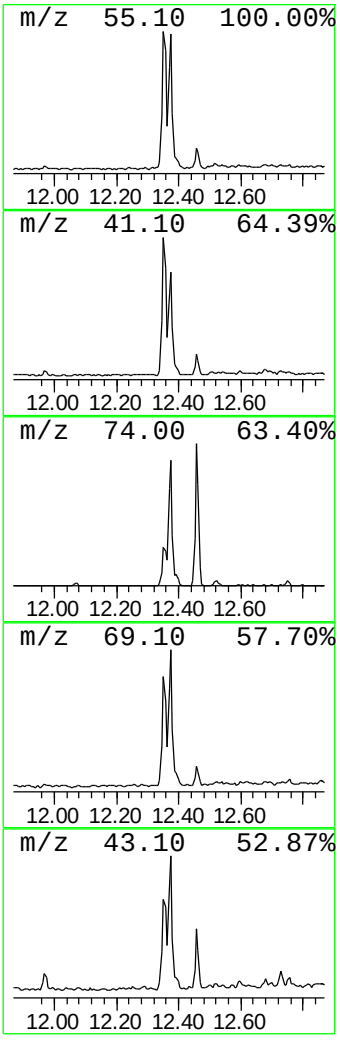
****

Peak Number 8 15-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	18.52 ng	739997	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	98
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	98
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	94
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	94
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	91





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Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

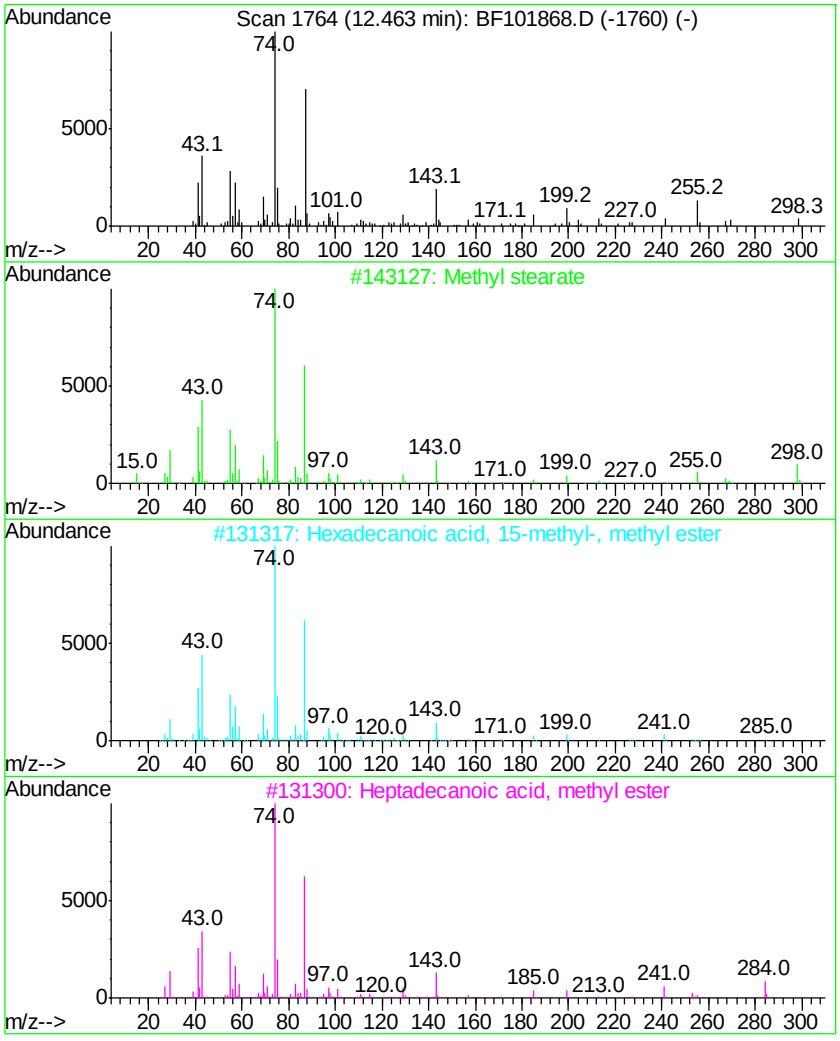
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

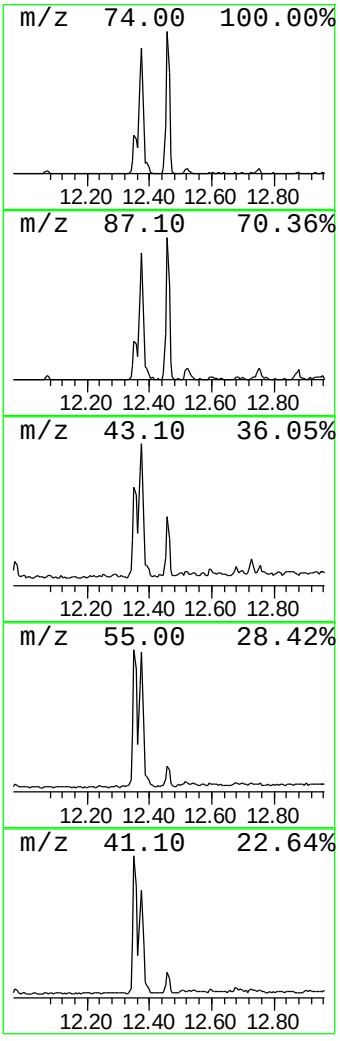
****

Peak Number 9 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	4.12 ng	164676	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90





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Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

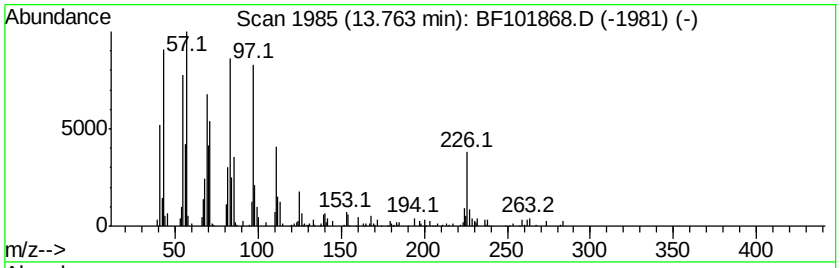
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

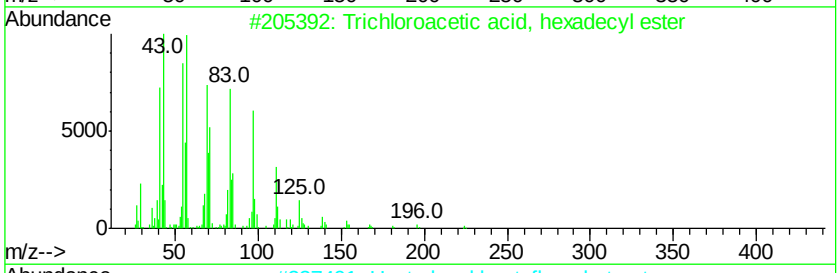
****

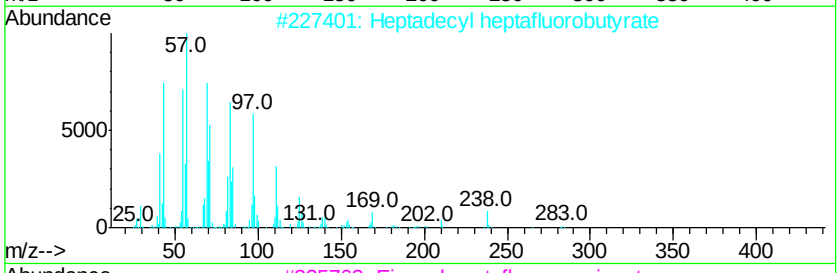
Peak Number 10 Trichloroacetic acid, hexad... Concentration Rank 7

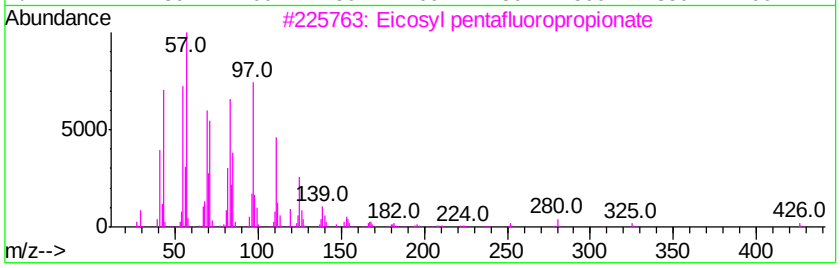
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	5.09 ng	209172	Chrysene-d12	13.95

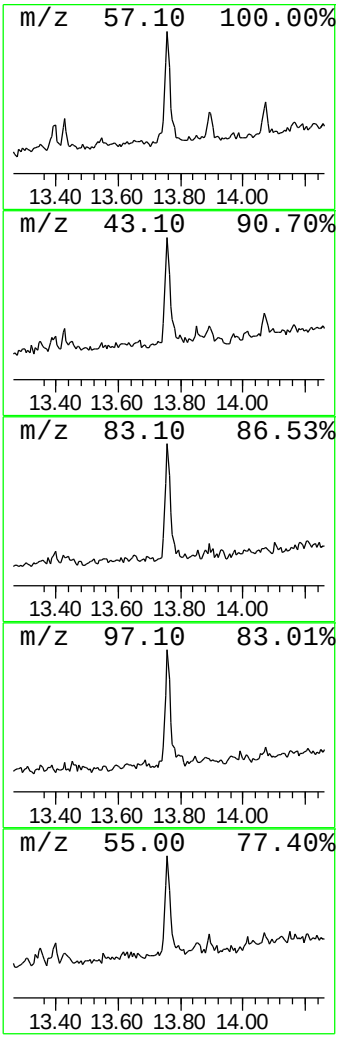
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
4	Z-8-Hexadecene	224	C16H32	1000130-87-5	91
5	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91











Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010318\
Data File : BF101868.D
Acq On : 3 Jan 2018 18:58
Operator : SJ/JU
Sample : I7105-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT1500

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	4.99	5.3	ng	196286	1	6.77	739398	20.0
unknown6.55	6.55	67.4	ng	2490280	1	6.77	739398	20.0
Heptacosane	10.69	3.1	ng	125663	4	11.30	798984	20.0
Hexadecanoic acid...	11.67	6.1	ng	243411	4	11.30	798984	20.0
n-Hexadecanoic acid	11.81	2.1	ng	82279	4	11.30	798984	20.0
9,12-Octadecadien...	12.35	24.8	ng	990811	4	11.30	798984	20.0
15-Octadecenoic a...	12.37	18.5	ng	739997	4	11.30	798984	20.0
Methyl stearate	12.46	4.1	ng	164676	4	11.30	798984	20.0
Trichloroacetic a...	13.76	5.1	ng	209172	5	13.95	821466	20.0