LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103023.D
Acq On : 15 Feb 2018 17:48
Operator : SJ/JU
Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-021418

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-BF020318.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	2.122	3	6	24	rVB	536350	832244	12.74%	2.121%
2	5.493	575	579	588	rBV	2339759	2135861	32.70%	5.443%
3	6.498	746	750	762	rBV	2117093	2141505	32.79%	5.457%
4	6.645	771	775	778	rBV	2409187	2143628	32.82%	5.463%
5	6.875	810	814	818	rBV	1336952	1071598	16.41%	2.731%
6	7.034	837	841	844	rBV	1737400	1569279	24.03%	3.999%
7	7.434	905	909	913	rBV	1370997	1309532	20.05%	3.337%
8	8.157	1029	1032	1036	rBV	1589107	1378744	21.11%	3.513%
9	9.234	1211	1215	1218	rBV	2236882	1965739	30.09%	5.009%
10	9.622	1278	1281	1288	rVB	187879	173045	2.65%	0.441%
11	9.834	1312	1317	1320	rBV	102189	85127	1.30%	0.217%
12	9.916	1327	1331	1335	rBV	1597653	1403912	21.49%	3.578%
13	10.333	1399	1402	1405	rVB	118787	92109	1.41%	0.235%
14	10.704	1461	1465	1474	rVB	1141846	1077253	16.49%	2.745%
15	10.804	1480	1482	1492	rVB	82866	109178	1.67%	0.278%
16	11.404	1580	1584	1586	rBV	1312892	1134631	17.37%	2.891%
17	11.428	1586	1588	1593	rVB2	114458	106797	1.64%	0.272%
18	11.786	1645	1649	1652	rBV	3565487	2996485	45.88%	7.636%
19	12.475	1761	1766	1768	rBV	5440395	6531813	100.00%	16.645%
20	12.498	1768	1770	1776	rVV2	5655608	5482817	83.94%	13.972%
21	12.575	1780	1783	1787	rVB	1632230	1404388	21.50%	3.579%
22	12.616	1787	1790	1794	rBV	189498	165162	2.53%	0.421%
23	12.845	1826	1829	1831	rBV	135823	112663	1.72%	0.287%
24	12.986	1849	1853	1856	rBV	1464630	1272482	19.48%	3.243%
25	13.222	1891	1893	1898	rVB3	111558	126826	1.94%	0.323%
26	13.298	1904	1906	1908	rBV	131439	106534	1.63%	0.271%
27	13.363	1915	1917	1922	rBV5	65883	75860	1.16%	0.193%
28	13.733	1976	1980	1985	rVB4	93537	137910	2.11%	0.351%
29	13.869	2000	2003	2007	rBV	213987	222691	3.41%	0.567%
30	13.969	2017	2020	2024	rBV	142688	156349	2.39%	0.398%
31	14.045	2029	2033	2036	rBV	1023427	940388	14.40%	2.396%
32	15.527	2281	2285	2293	rVB	632322	779329	11.93%	1.986%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103023.D
Acq On : 15 Feb 2018 17:48
Operator : SJ/JU
Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-021418

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

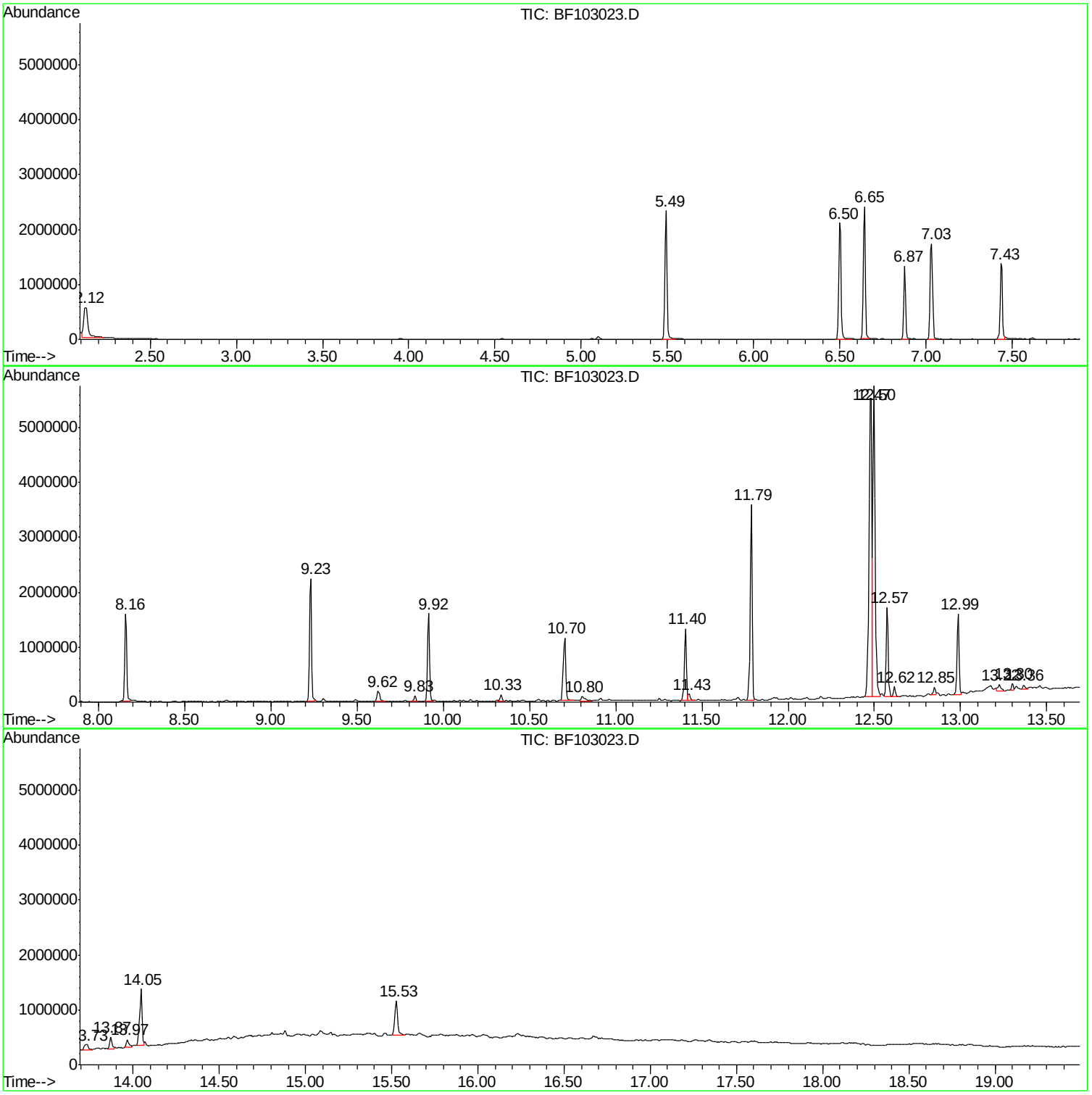
Sum of corrected areas: 39241879

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103023.D
Acq On : 15 Feb 2018 17:48
Operator : SJ/JU
Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-021418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103023.D
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

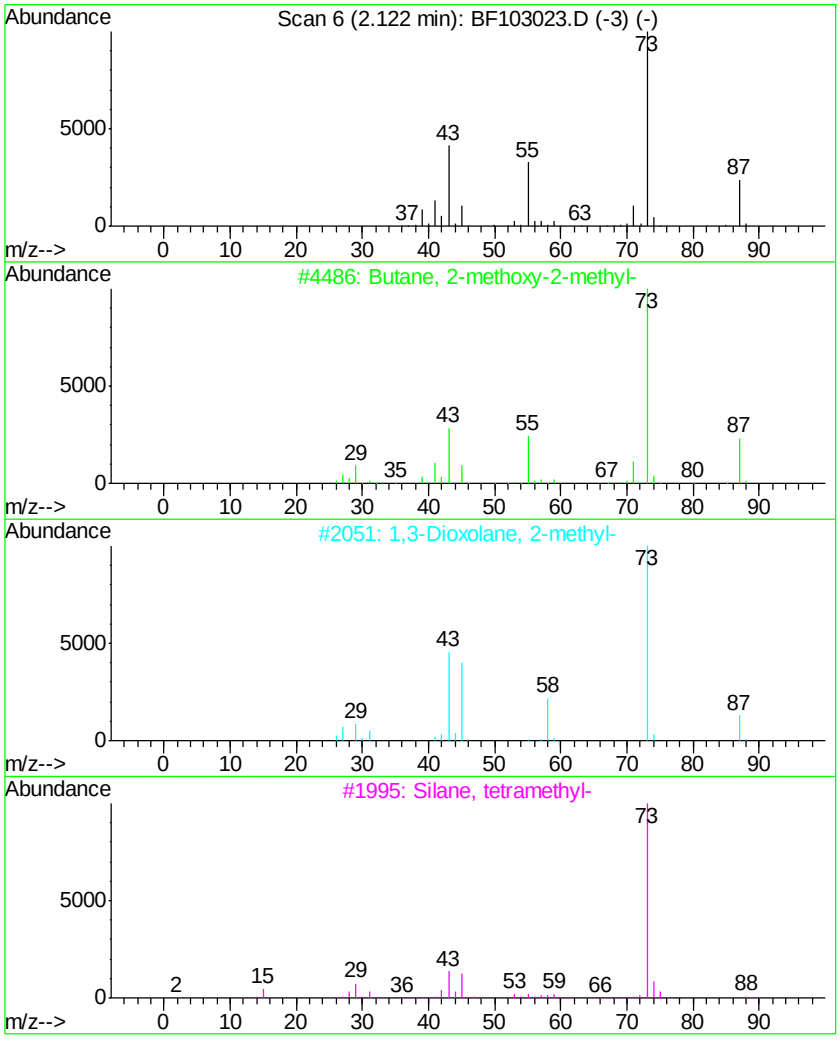
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

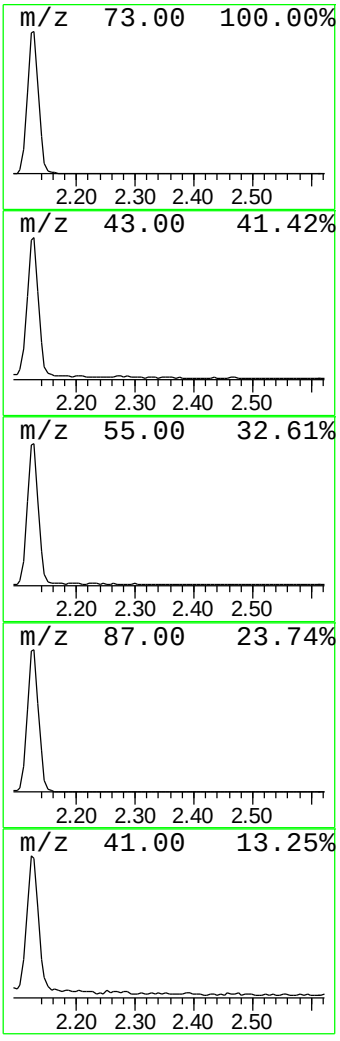
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	15.53 ng	832244	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103023.D
Acq On : 15 Feb 2018 17:48
Operator : SJ/JU
Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-021418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

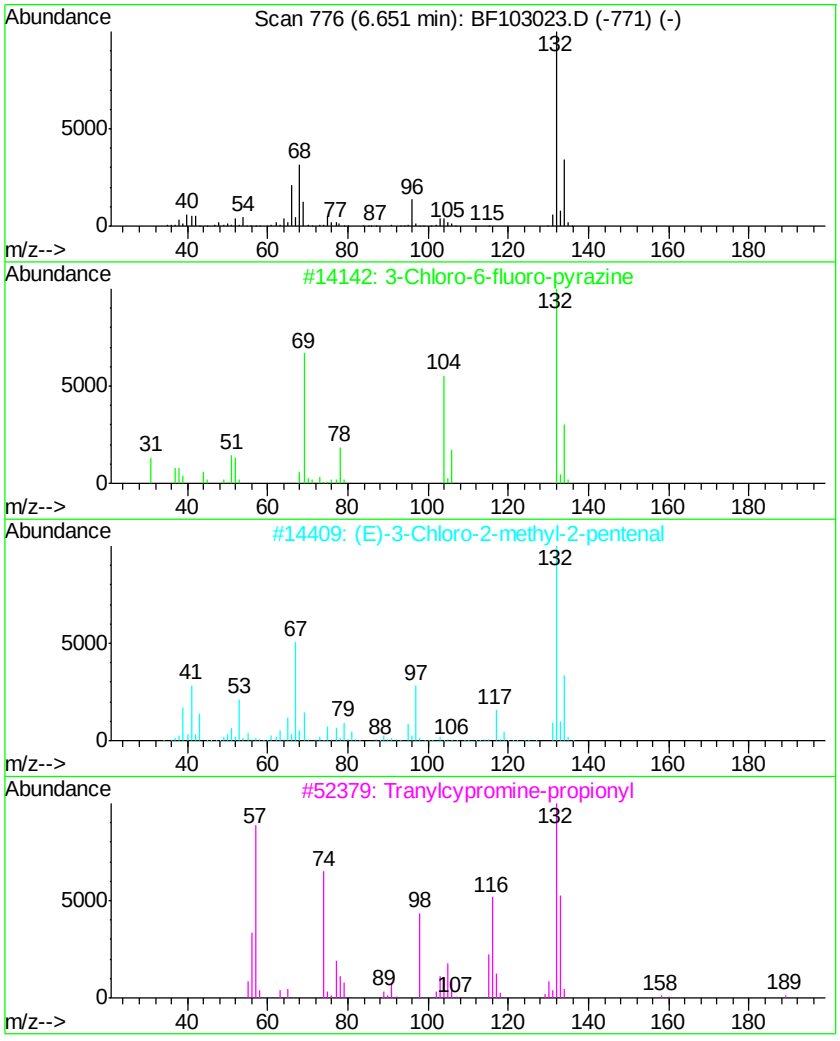
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

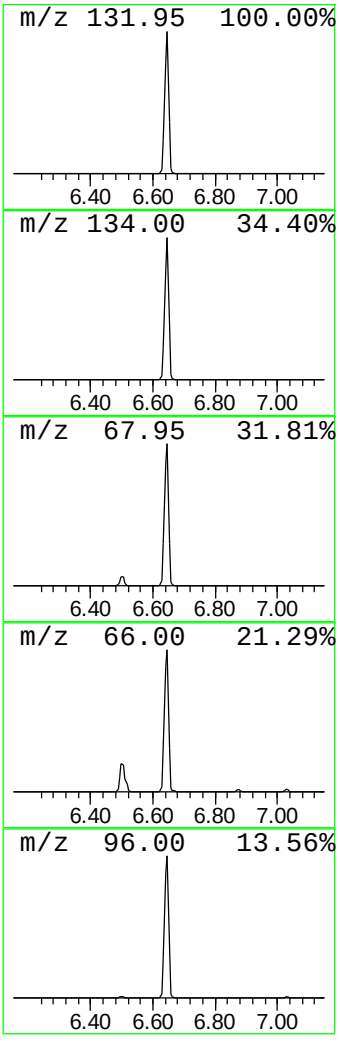
****

Peak Number 2 unknown6.65 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	40.01 ng	2143630	1,4-Dichlorobenzene-d4	6.87

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	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Data File : BF103023.D
Acq On : 15 Feb 2018 17:48
Operator : SJ/JU
Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-021418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

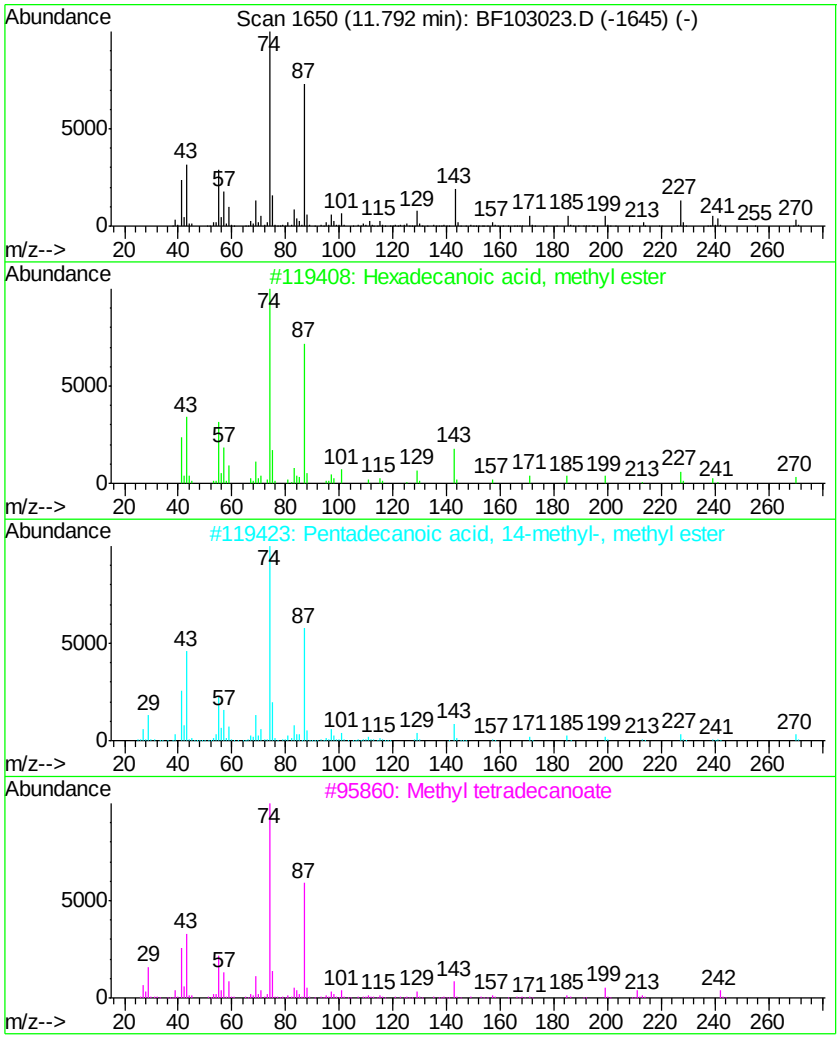
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

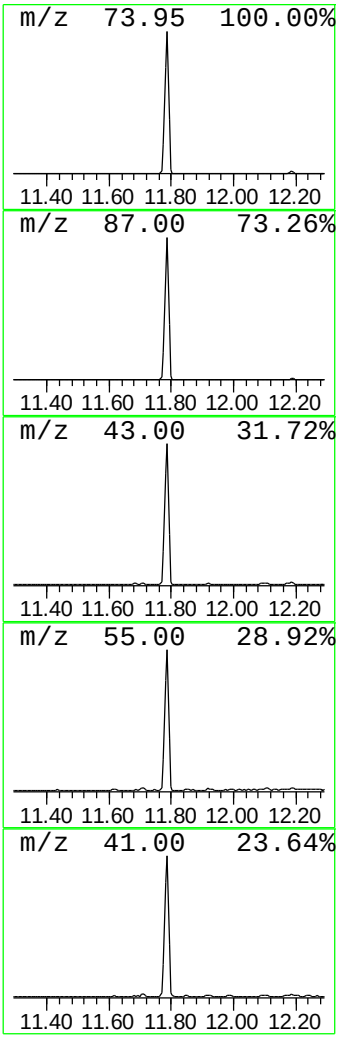
****

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	52.82 ng	2996490	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87





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Data File : BF103023.D
Acq On : 15 Feb 2018 17:48
Operator : SJ/JU
Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-021418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

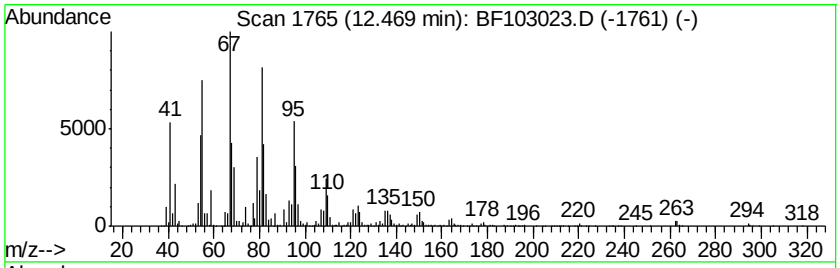
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

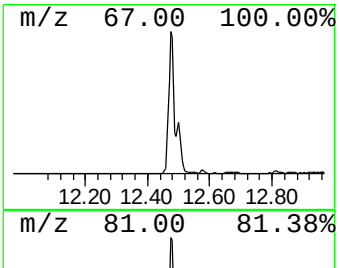
****

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	115.14 ng	6531810	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103023.D
Acq On : 15 Feb 2018 17:48
Operator : SJ/JU
Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-021418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

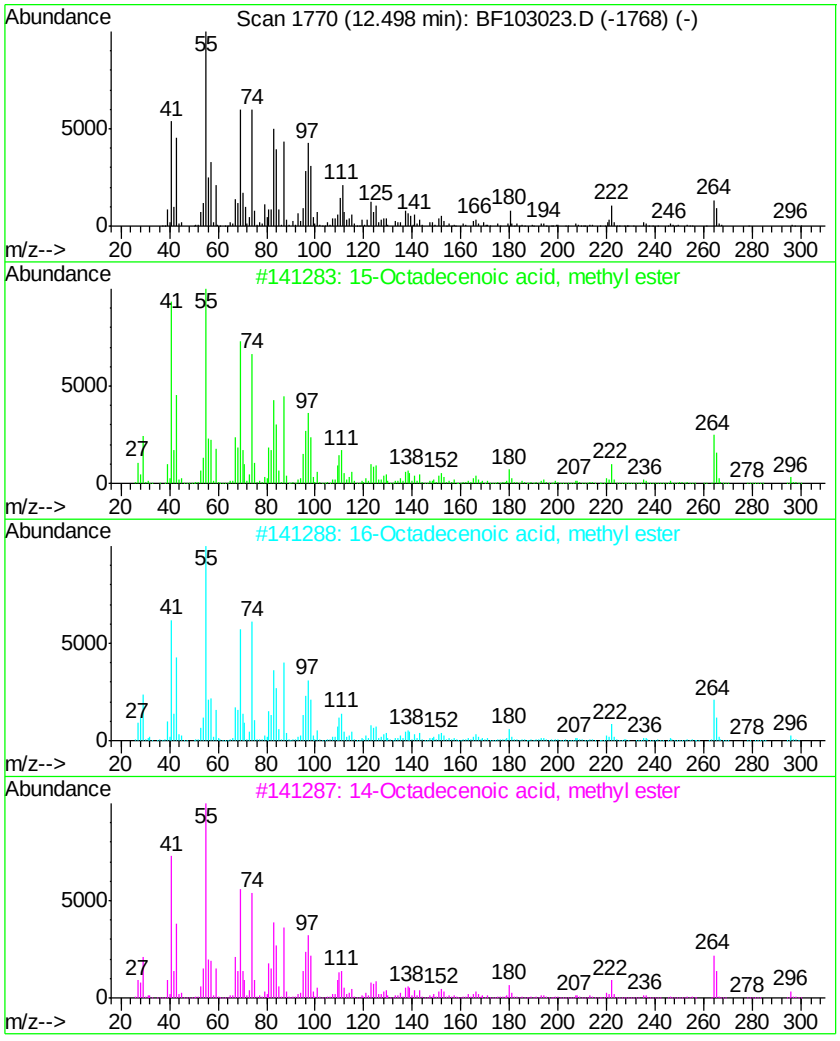
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

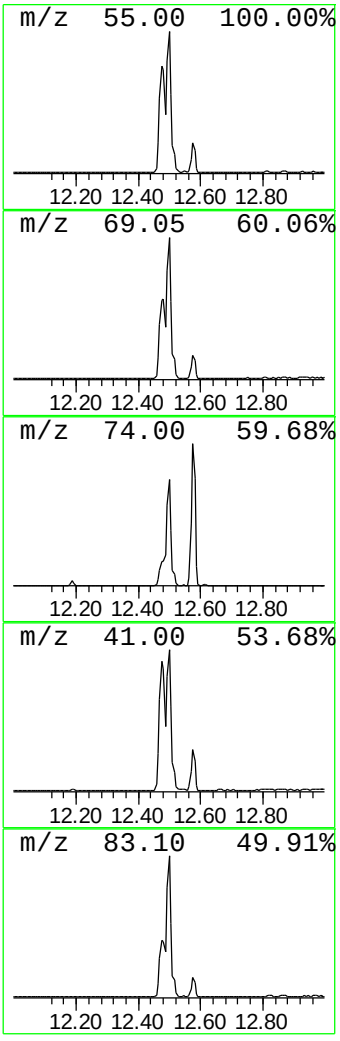
****

Peak Number 6 15-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	96.64 ng	5482820	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	96
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	96
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	96
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	94
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	94





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Data File : BF103023.D
Acq On : 15 Feb 2018 17:48
Operator : SJ/JU
Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-021418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

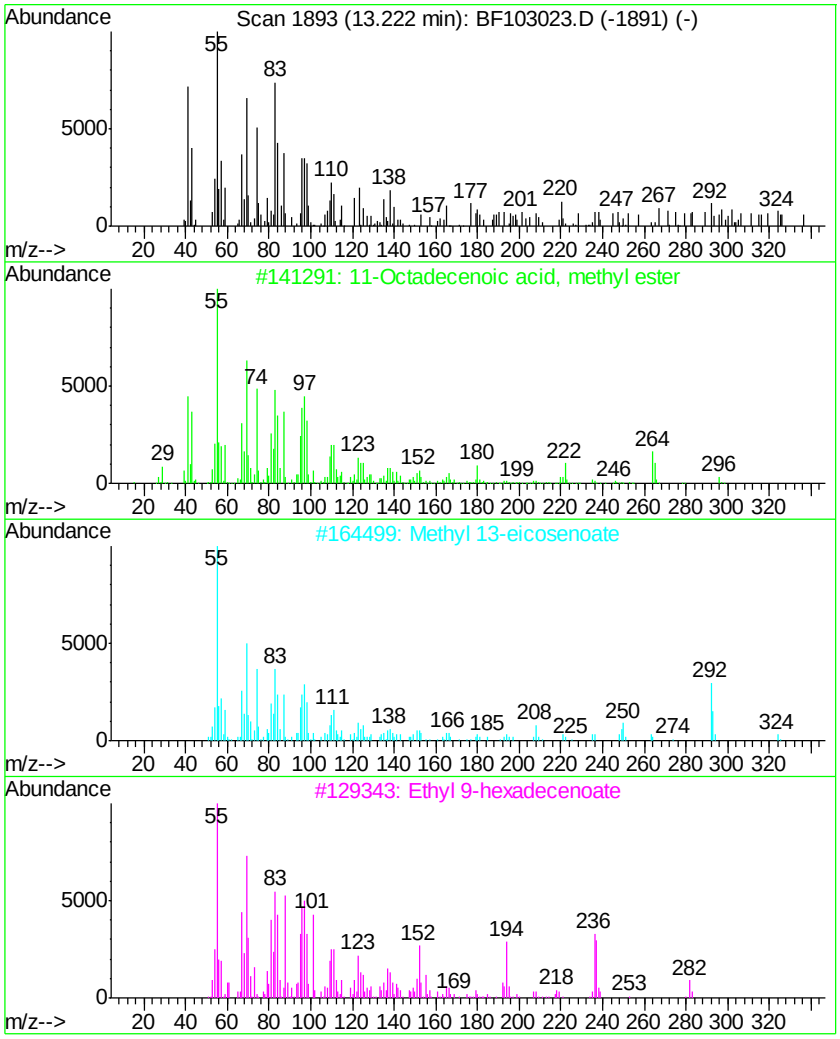
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

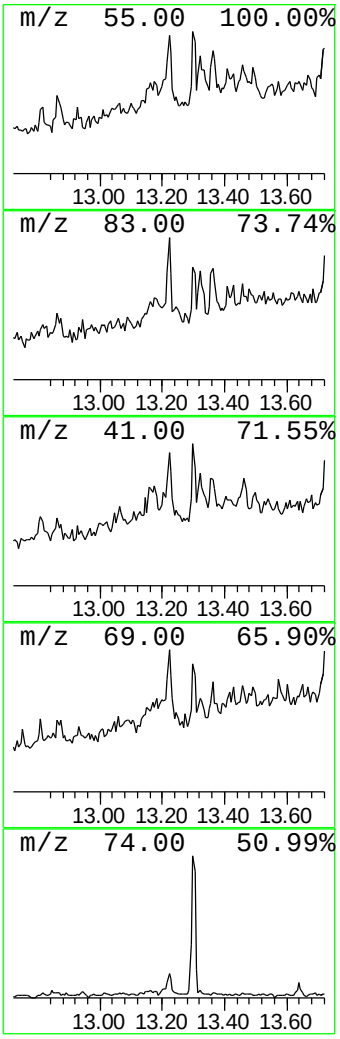
****

Peak Number 7 11-Octadecenoic acid, methy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.22	2.70 ng	126826	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	89
2	Methyl 13-eicosenoate	324	C21H40O2	1000336-48-4	86
3	Ethyl 9-hexadecenoate	282	C18H34O2	054546-22-4	78
4	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	78
5	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	78





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Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-021418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

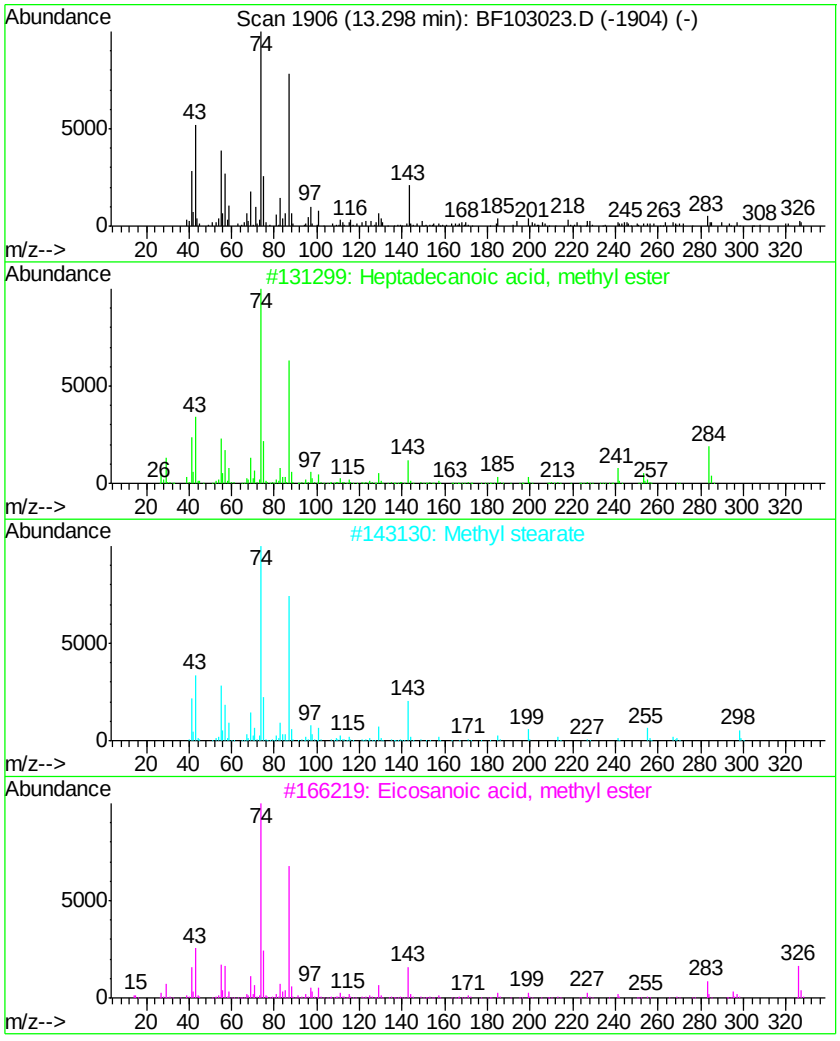
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

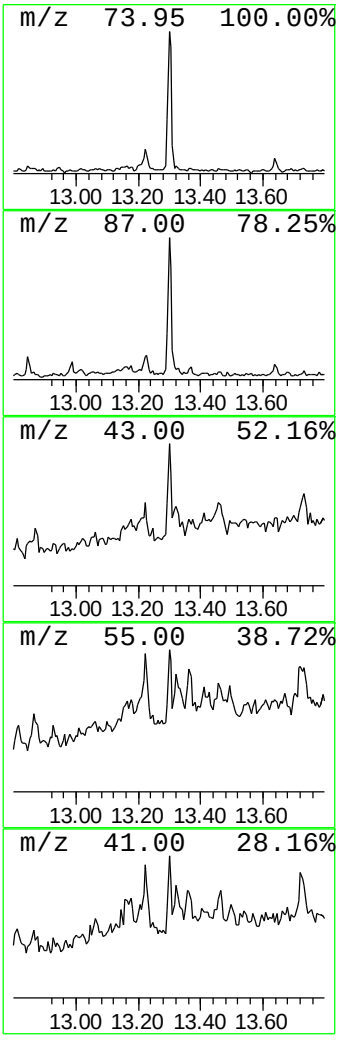
****

Peak Number 8 Heptadecanoic acid, methyl ... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	2.27 ng	106534	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	97
2	Methyl stearate	298	C19H38O2	000112-61-8	95
3	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	93
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-021418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

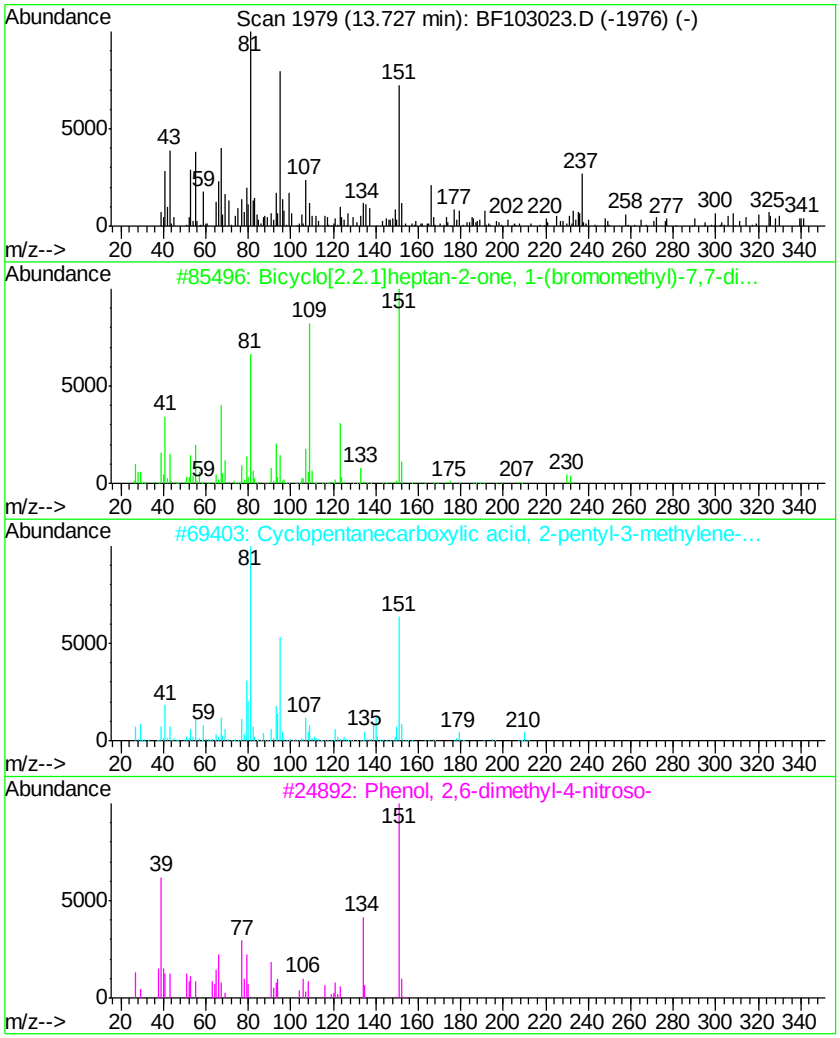
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

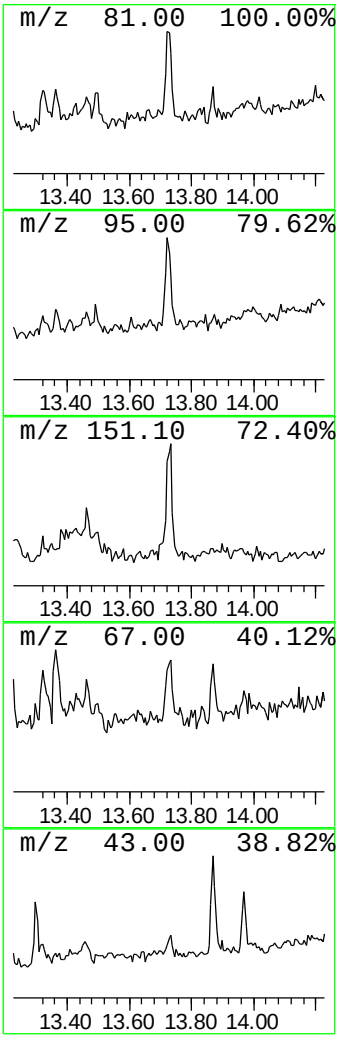
****

Peak Number 9 unknown13.73 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.93 ng	137910	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1-(b...	230	C10H15BrO	064161-50-8	46
2	Cyclopentanecarboxylic acid, 2-p...	210	C13H22O2	1000154-24-8	45
3	Phenol, 2,6-dimethyl-4-nitroso-	151	C8H9NO2	013331-93-6	30
4	Methyl 2-octylcyclopropene-1-oct...	308	C20H36O2	003220-60-8	27
5	3-Methyl-6-(4-phenyl-4H-[1,2,4]t...	327	C15H13N5S2	1000297-22-6	15





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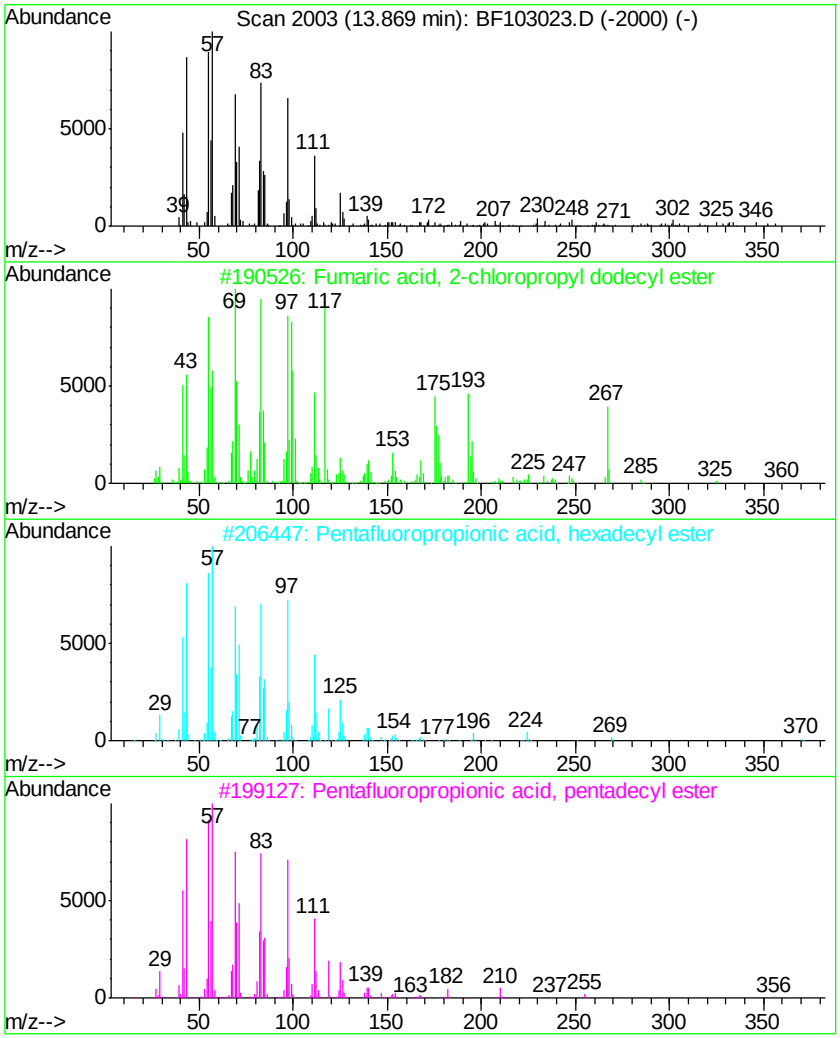
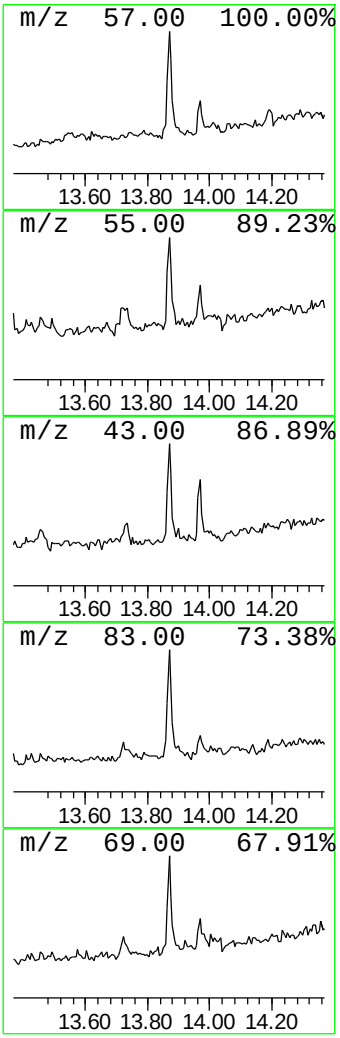
Peak Number 10 Fumaric acid, 2-chloropropy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	4.74 ng	222691	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloropropyl dod...	360	C19H33ClO4	1000348-57-0	98
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103023.D
Acq On : 15 Feb 2018 17:48
Operator : SJ/JU
Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-021418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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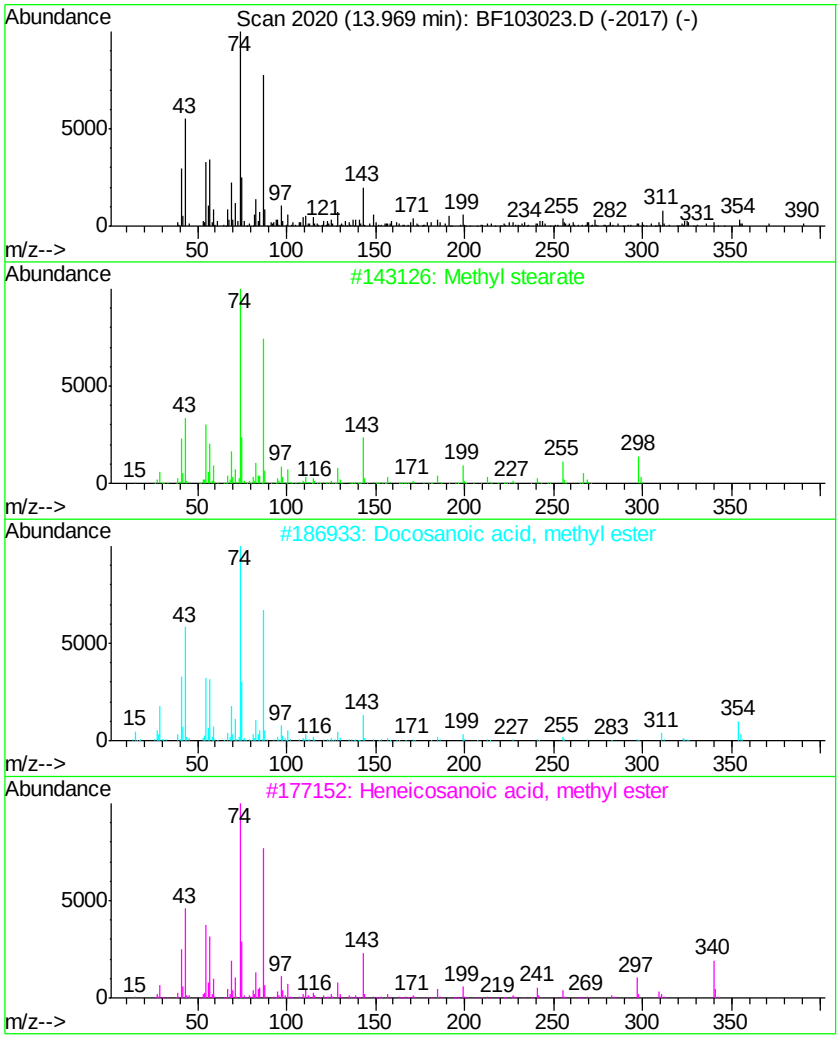
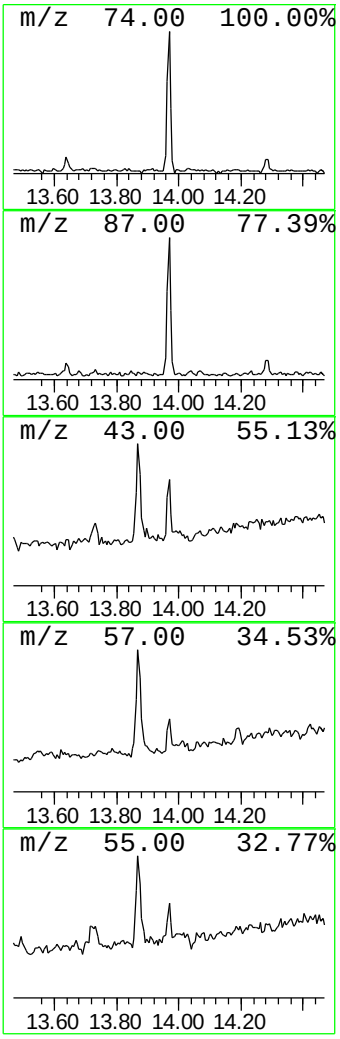
Peak Number 11 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.33 ng	156349	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	95
3	Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	93
4	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	90
5	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	90





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103023.D
Acq On : 15 Feb 2018 17:48
Operator : SJ/JU
Sample : J1404-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-021418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.12	15.5	ng	832244	1	6.87	1071600	20.0
unknown6.65	6.65	40.0	ng	2143630	1	6.87	1071600	20.0
Hexadecanoic acid...	11.79	52.8	ng	2996490	4	11.40	1134630	20.0
9,12-Octadecadien...	12.47	115.1	ng	6531810	4	11.40	1134630	20.0
15-Octadecenoic a...	12.50	96.6	ng	5482820	4	11.40	1134630	20.0
11-Octadecenoic a...	13.22	2.7	ng	126826	5	14.05	940388	20.0
Heptadecanoic aci...	13.30	2.3	ng	106534	5	14.05	940388	20.0
unknown13.73	13.73	2.9	ng	137910	5	14.05	940388	20.0
Fumaric acid, 2-c...	13.87	4.7	ng	222691	5	14.05	940388	20.0
Methyl stearate	13.97	3.3	ng	156349	5	14.05	940388	20.0