LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

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-BF012218.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	3.134	173	178	189	rVB	27675	55635	1.25%	0.170%
2	4.263	352	370	374	rBV3	33949	140465	3.15%	0.429%
3	4.899	475	478	488	rBV	80318	96664	2.17%	0.296%
4	5.087	488	510	516	rBV2	81811	358556	8.05%	1.096%
5	5.198	516	529	532	rVV2	56758	159743	3.59%	0.488%
6	5.322	546	550	567	rBV	1599538	1721761	38.66%	5.264%
7	5.516	575	583	592	rBV2	51780	130576	2.93%	0.399%
8	6.157	677	692	701	rBV2	132344	386366	8.68%	1.181%
9	6.357	722	726	743	rBV	978449	1181044	26.52%	3.611%
10	6.481	743	747	758	rBV	3280570	3123450	70.14%	9.549%
11	6.710	782	786	794	rBV	1029420	925653	20.79%	2.830%
12	6.863	808	812	816	rBV	3305617	3143620	70.59%	9.610%
13	7.140	855	859	871	rBV	272765	406198	9.12%	1.242%
14	7.281	878	883	886	rBV	2617318	2579036	57.91%	7.884%
15	7.763	962	965	969	rBV	46309	76112	1.71%	0.233%
16	7.992	1000	1004	1020	rBV	1364600	1323740	29.72%	4.047%
17	8.287	1049	1054	1059	rBV	185104	285342	6.41%	0.872%
18	8.645	1112	1115	1124	rBV	326935	334104	7.50%	1.021%
19	8.804	1138	1142	1153	rBV	131060	219274	4.92%	0.670%
20	9.069	1182	1187	1190	rBV	4655914	4453449	100.00%	13.615%
21	9.463	1251	1254	1262	rVB	118462	130621	2.93%	0.399%
22	9.669	1286	1289	1291	rBV	78014	73199	1.64%	0.224%
23	9.745	1298	1302	1310	rVB	1470839	1347732	30.26%	4.120%
24	10.169	1371	1374	1377	rVB	100177	81911	1.84%	0.250%
25	10.375	1407	1409	1414	rVB2	86170	83914	1.88%	0.257%
26	10.539	1433	1437	1447	rBV	2287282	2335458	52.44%	7.140%
27	10.639	1451	1454	1456	rBV	84421	71989	1.62%	0.220%
28	11.233	1551	1555	1562	rBV	1337335	1279834	28.74%	3.913%
29	12.498	1767	1770	1774	rVB	135535	112169	2.52%	0.343%
30	12.822	1819	1825	1828	rBV	3869644	3962216	88.97%	12.113%
31	13.710	1973	1976	1980	rBV	101567	111056	2.49%	0.340%
32	13.874	2000	2004	2014	rVB	1081209	1109040	24.90%	3.390%
33	15.304	2242	2247	2255	rVB	572751	789335	17.72%	2.413%
34	18.656	2813	2817	2829	rVB10	40381	121180	2.72%	0.370%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

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-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 32710442

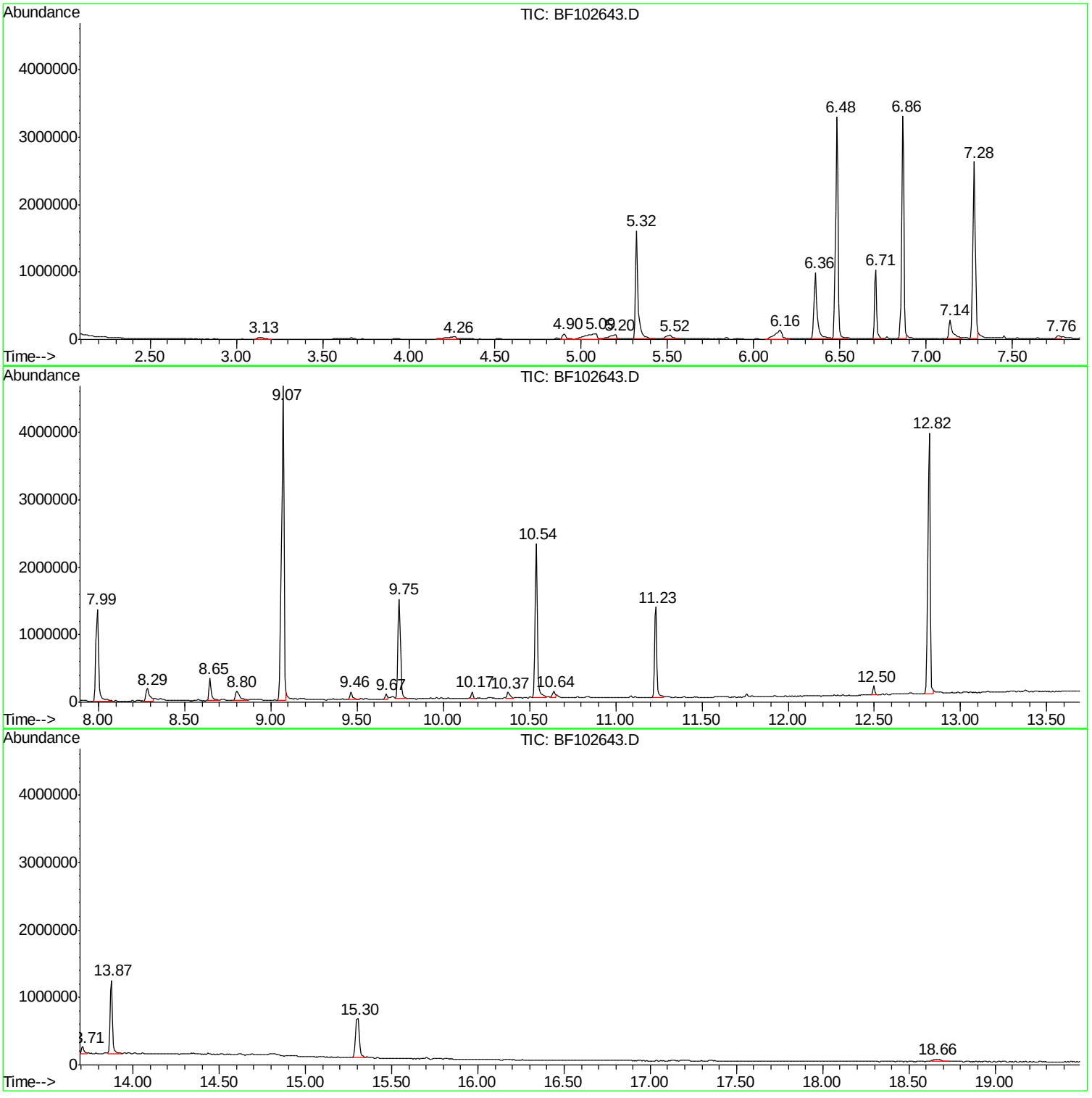
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

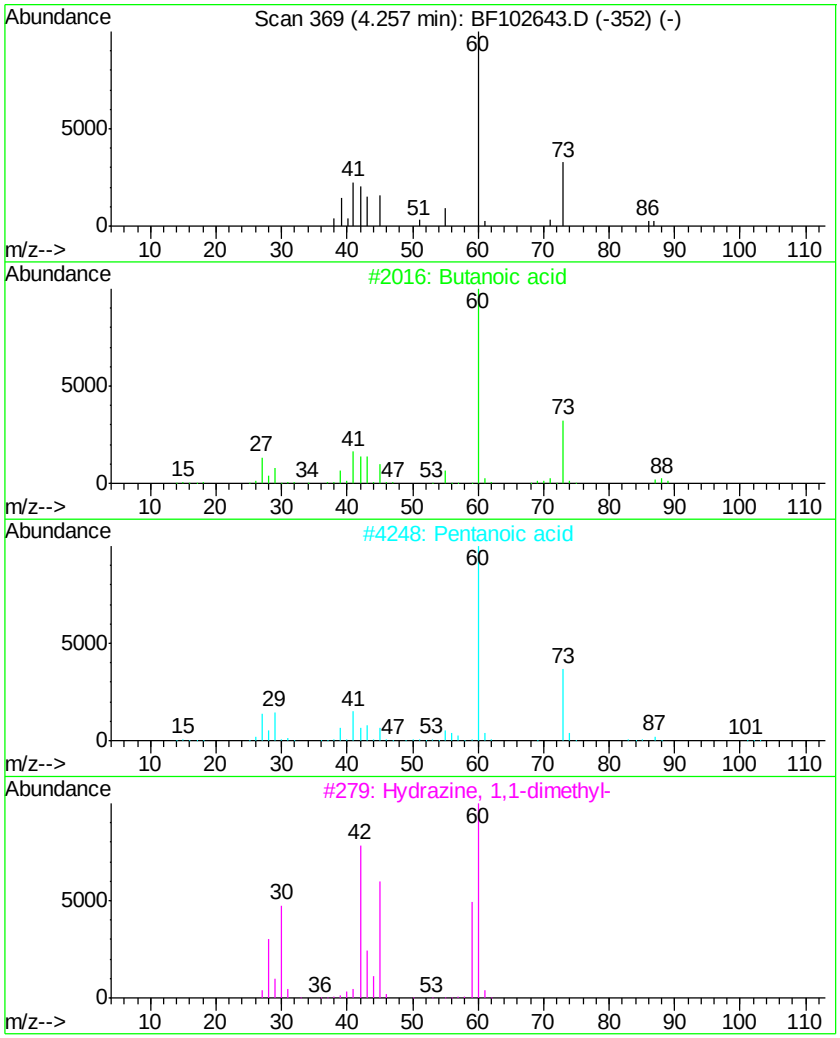
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

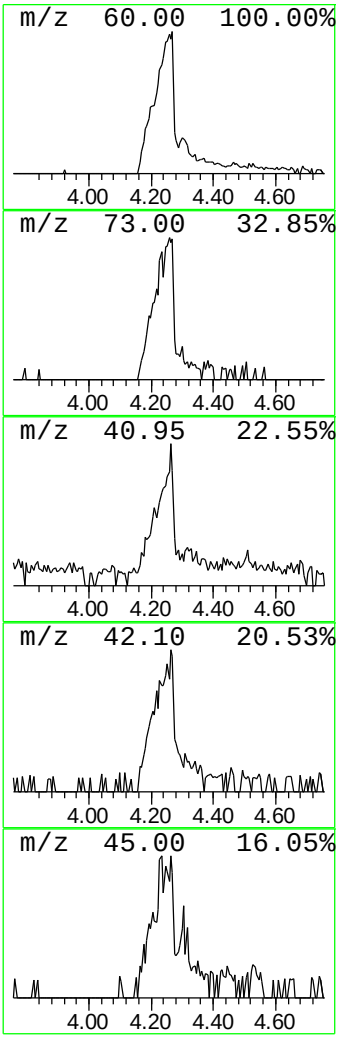
****

Peak Number 1 unknown4.26 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.26	3.03 ng	140465	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	9
2	Pentanoic acid	102	C5H10O2	000109-52-4	9
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	7
4	Urea	60	CH4N2O	000057-13-6	5
5	Formic acid hydrazide	60	CH4N2O	000624-84-0	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

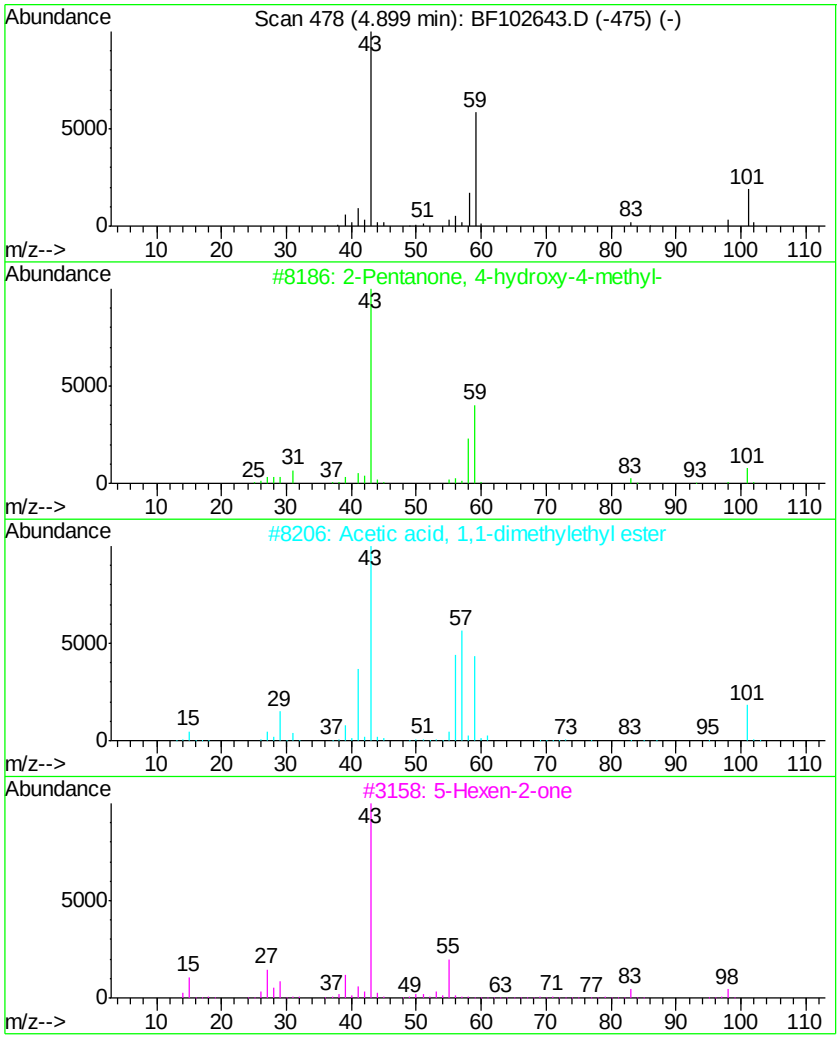
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

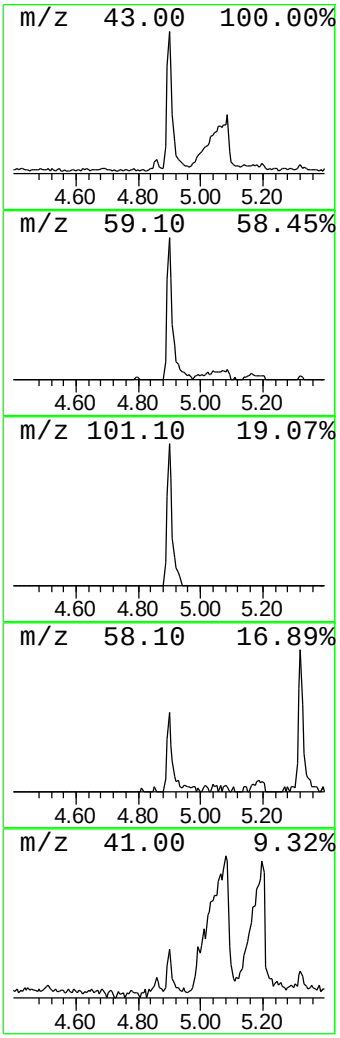
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.09 ng	96664	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	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Hexanol	102	C6H14O	000623-37-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

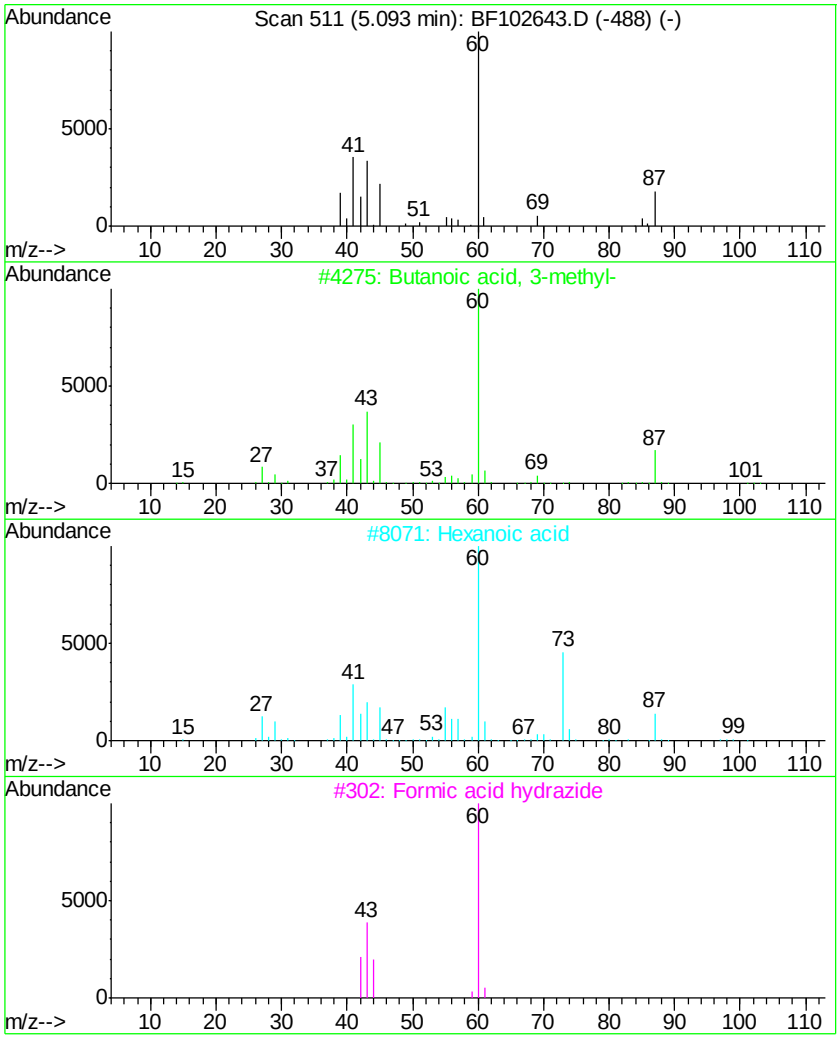
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

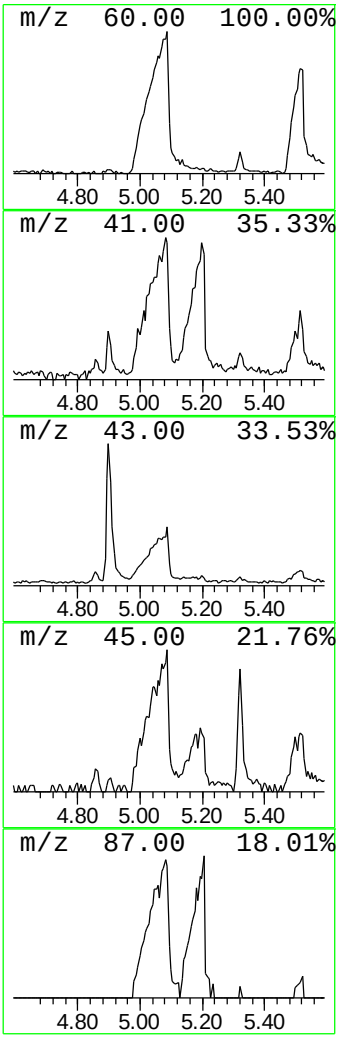
****

Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	7.75 ng	358556	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	74
2	Hexanoic acid	116	C6H12O2	000142-62-1	40
3	Formic acid hydrazide	60	CH4N2O	000624-84-0	9
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	Pentanoic acid	102	C5H10O2	000109-52-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

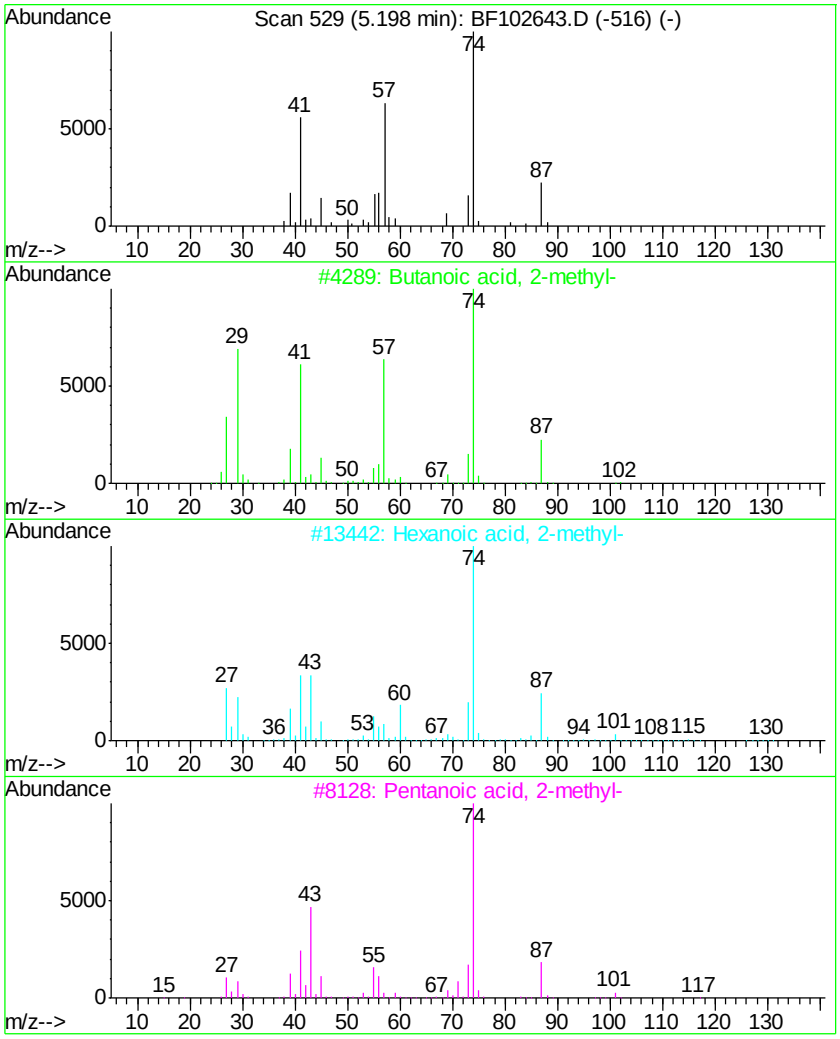
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

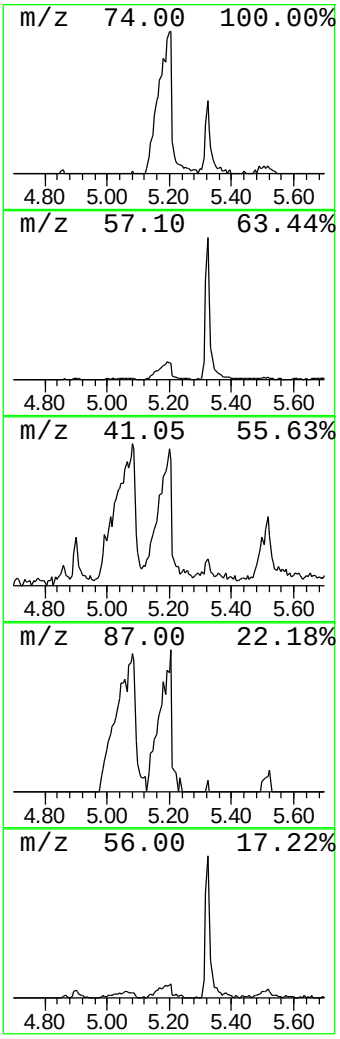
****

Peak Number 4 Butanoic acid, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.45 ng	159743	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
2	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	78
3	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	39
4	Morpholine	87	C4H9NO	000110-91-8	9
5	1-Pentanamine	87	C5H13N	000110-58-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

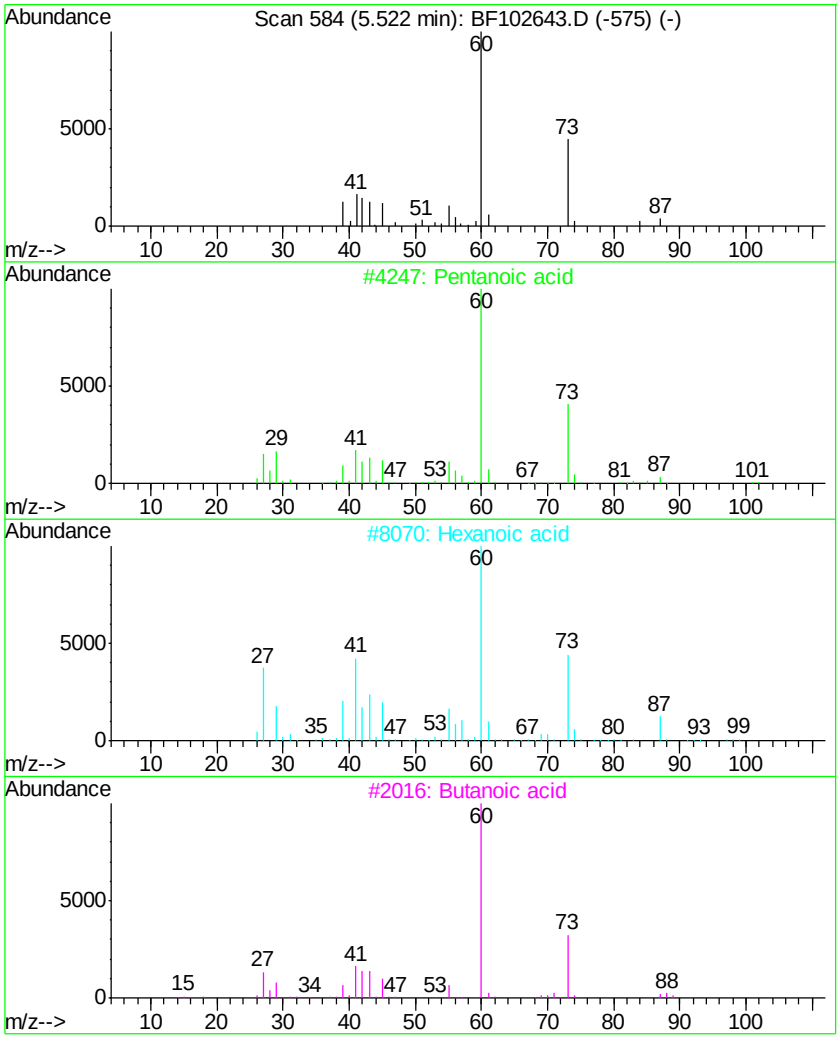
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

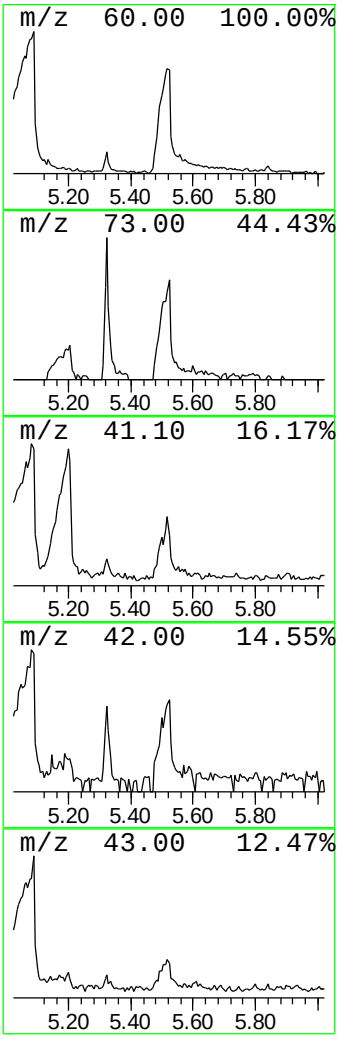
****

Peak Number 5 Pentanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	2.82 ng	130576	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	83
2	Hexanoic acid	116	C6H12O2	000142-62-1	78
3	Butanoic acid	88	C4H8O2	000107-92-6	78
4	.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	40
5	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

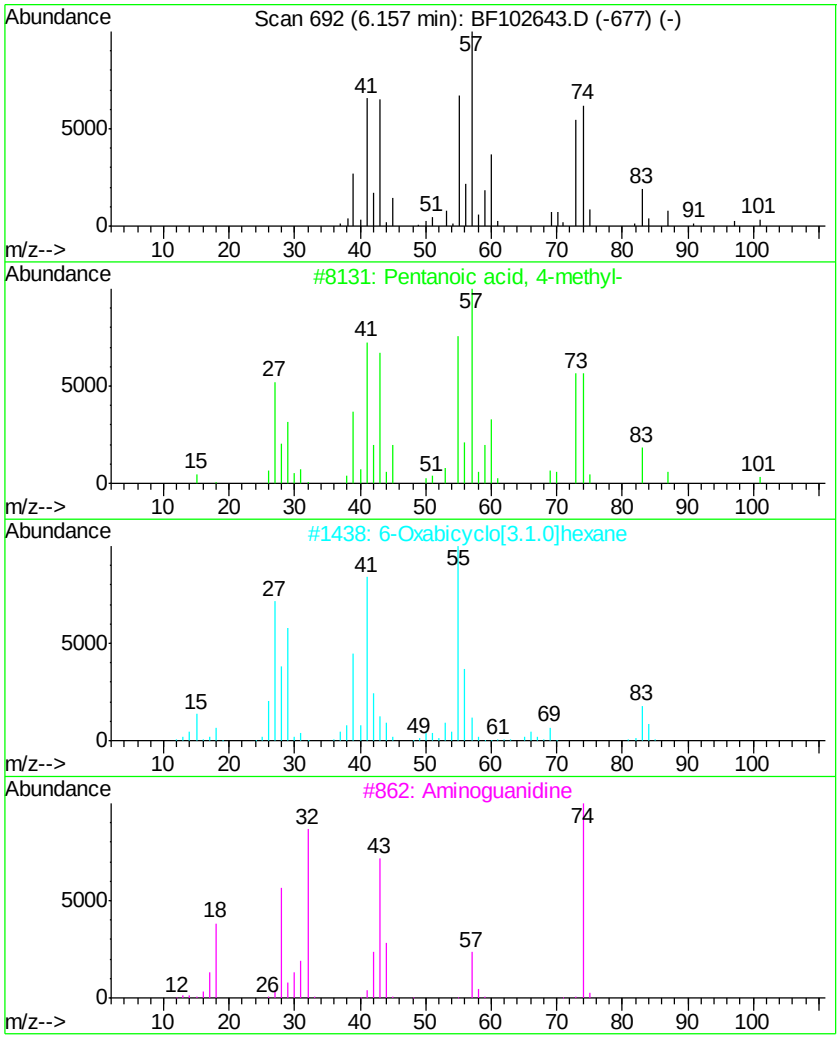
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

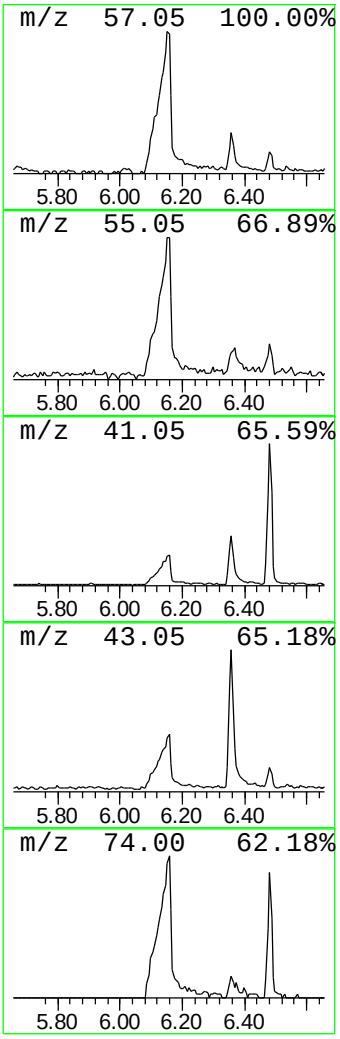
****

Peak Number 6 Pentanoic acid, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	8.35 ng	386366	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	83
2	6-Oxabicyclo[3.1.0]hexane	84	C5H8O	000285-67-6	11
3	Aminoguanidine	74	CH6N4	000079-17-4	9
4	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	9
5	Homoserine	119	C4H9NO3	000498-19-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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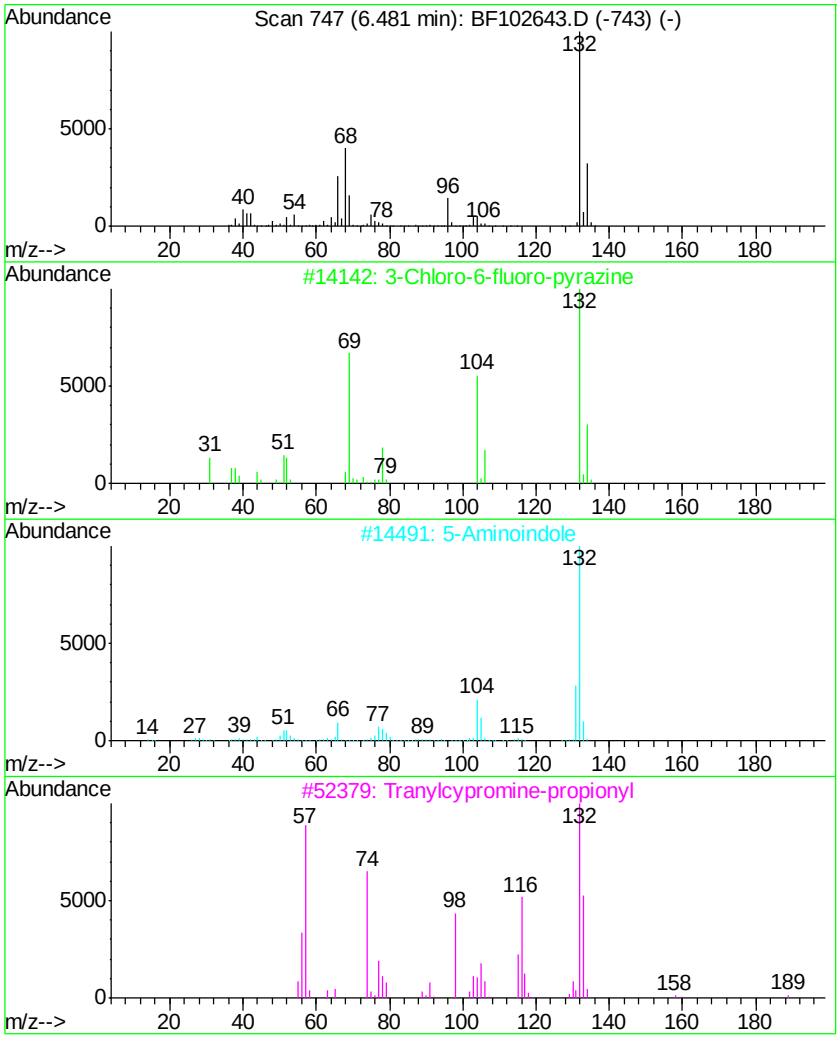
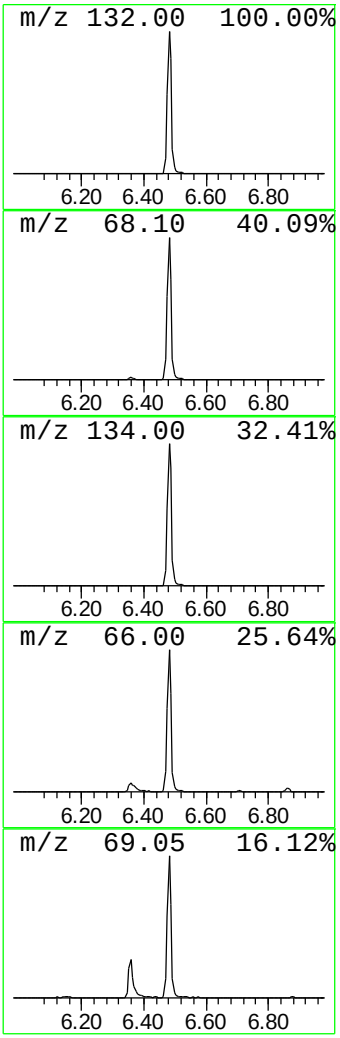
Peak Number 7 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	67.49 ng	3123450	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
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Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

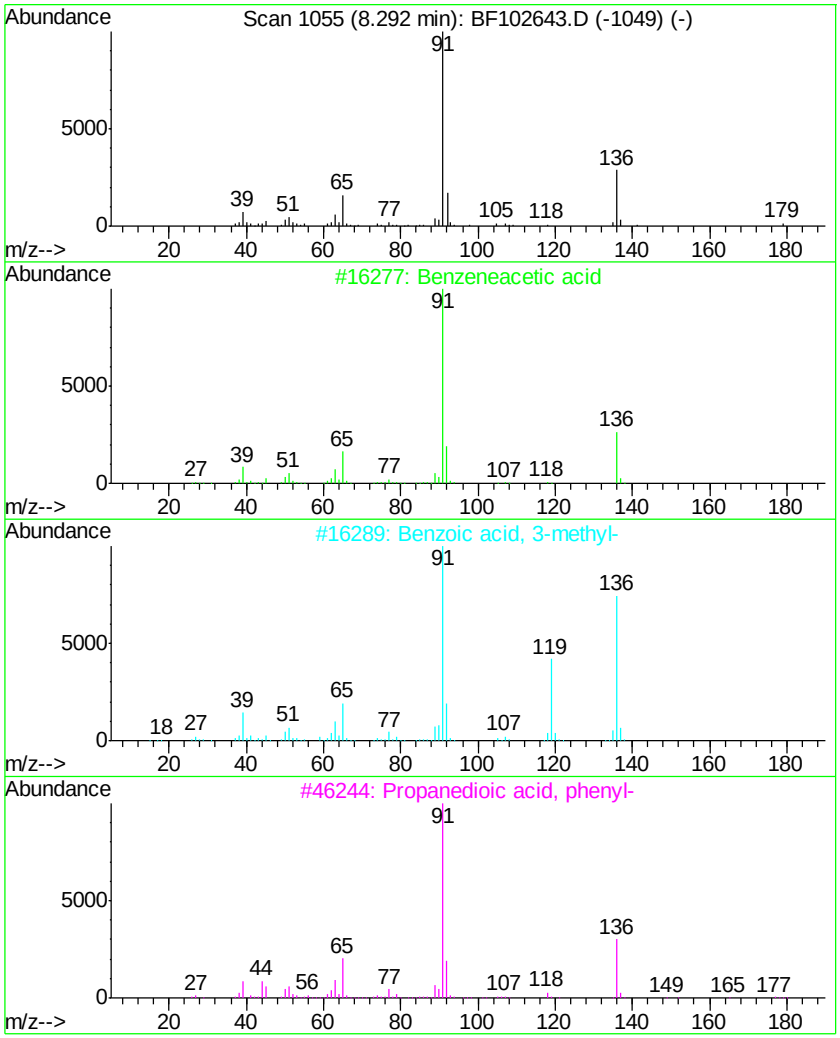
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

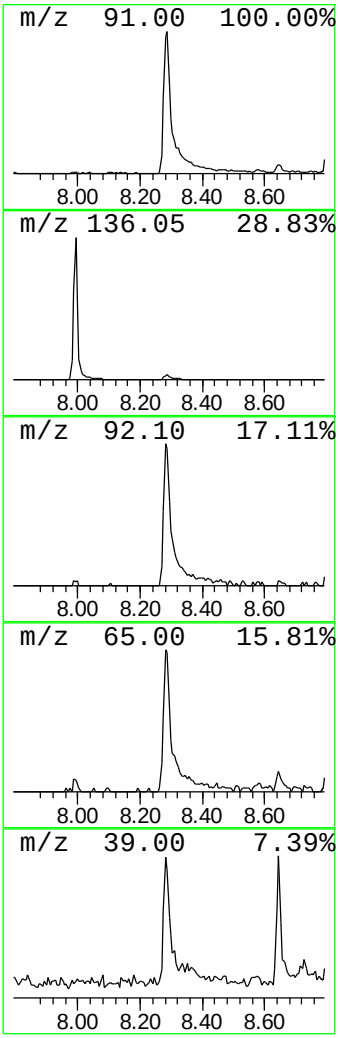
****

Peak Number 9 Benzeneacetic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.29	4.31 ng	285342	Naphthalene-d8	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	94
2	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	64
3	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	50
4	Benzene, (bromomethyl)-	170	C7H7Br	000100-39-0	47
5	Benzyl 2-chloroethyl sulfone	218	C9H11ClO2S	066998-67-2	46





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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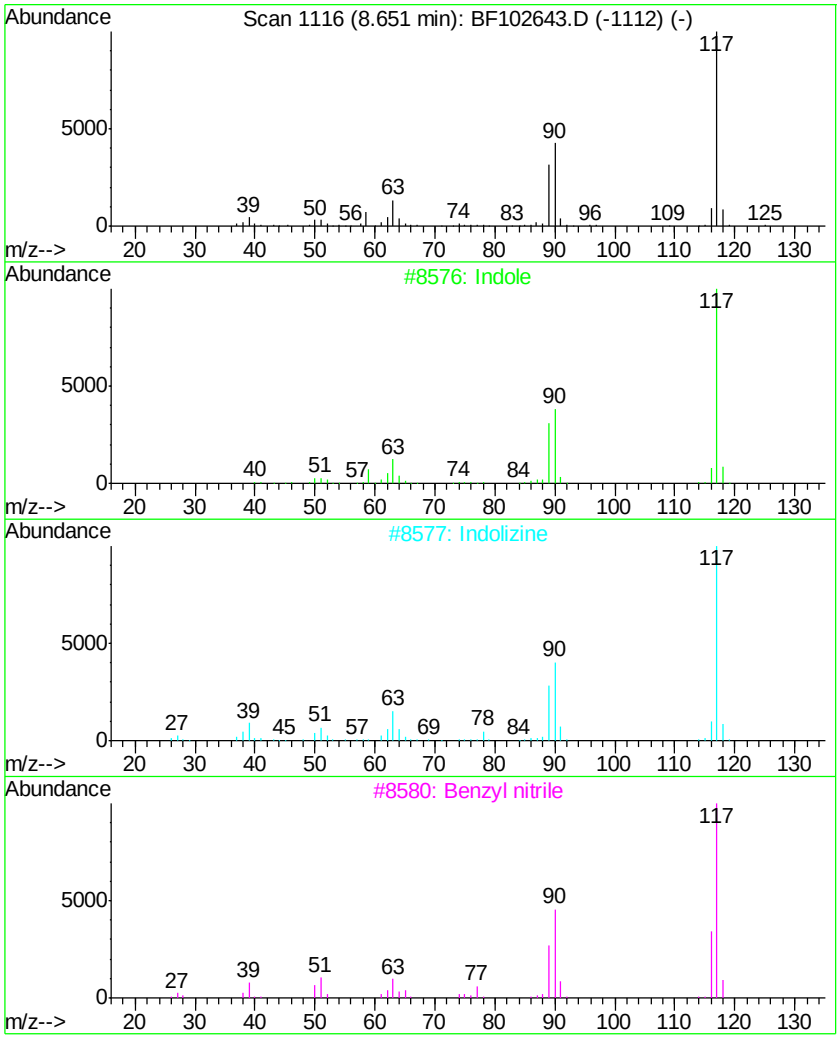
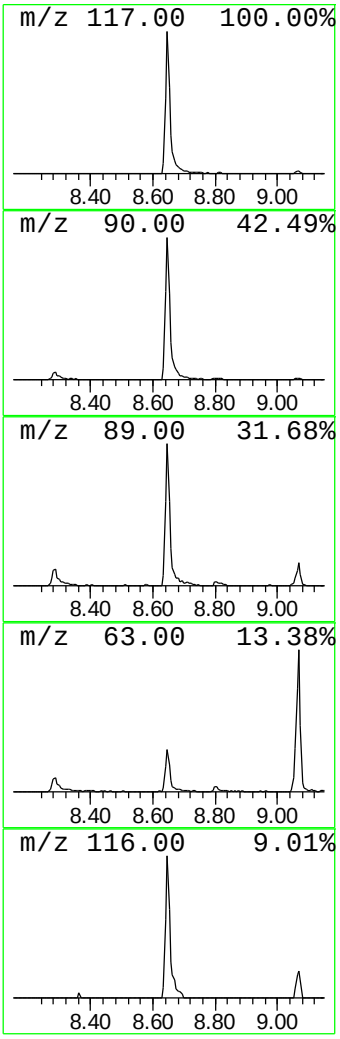
Peak Number 10 Indole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	5.05 ng	334104	Naphthalene-d8	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole	117	C8H7N	000120-72-9	97
2	Indolizine	117	C8H7N	000274-40-8	91
3	Benzyl nitrile	117	C8H7N	000140-29-4	91
4	Benzene, 1-isocyano-2-methyl-	117	C8H7N	010468-64-1	91
5	m-Aminophenylacetylene	117	C8H7N	054060-30-9	87





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Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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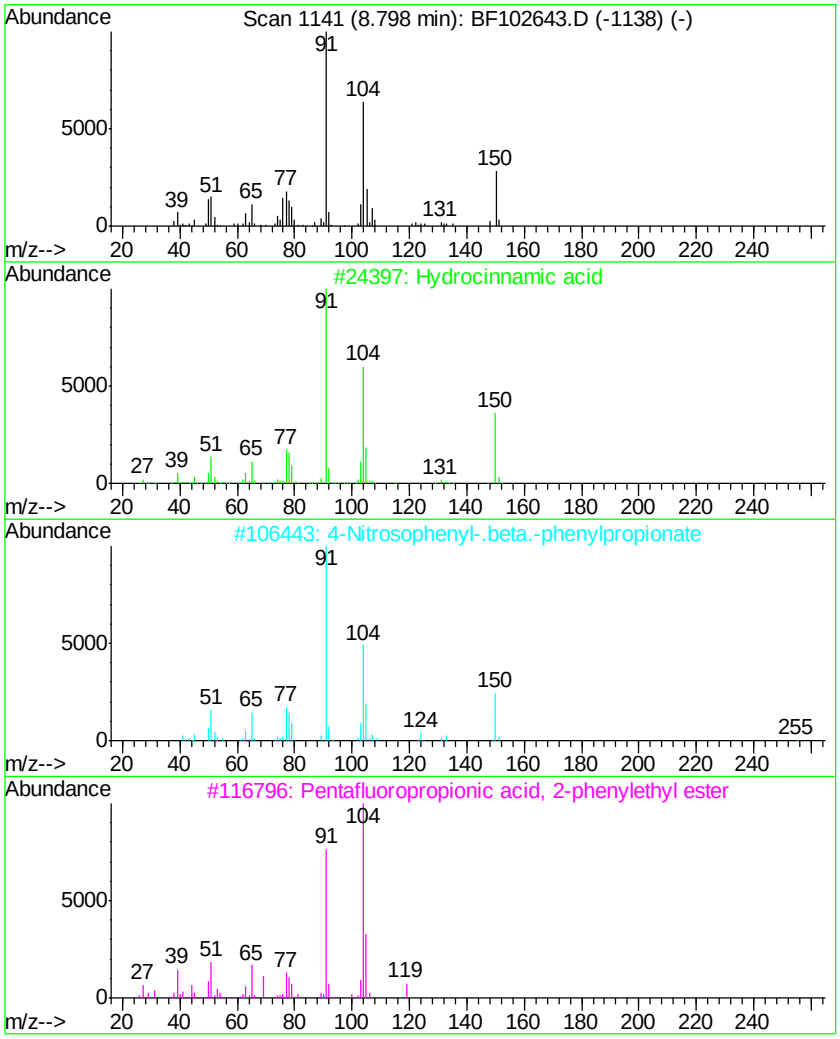
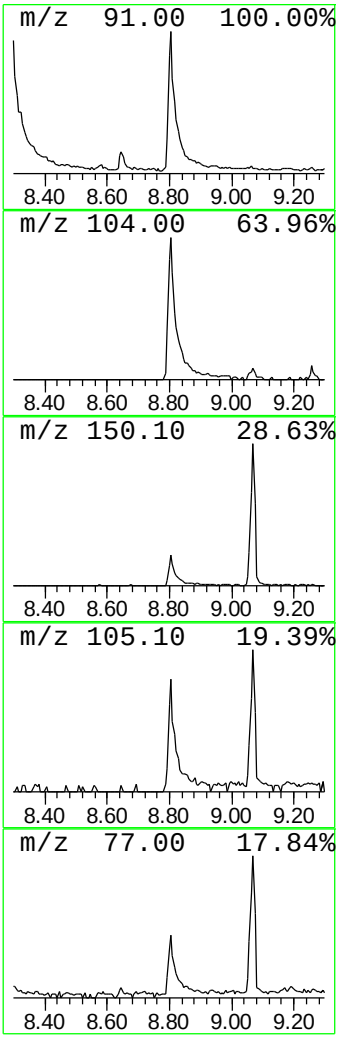
Peak Number 11 Hydrocinnamic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	3.31 ng	219274	Naphthalene-d8	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrocinnamic acid	150	C9H10O2	000501-52-0	96
2	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
3	Pentafluoropropionic acid, 2-phe...	268	C11H9F5O2	081089-48-7	50
4	2-Butenoic acid, 3-methyl-, 2-ph...	204	C13H16O2	042078-65-9	43
5	Acetic acid, trifluoro-, 2-pheny...	218	C10H9F3O2	055419-66-4	38





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Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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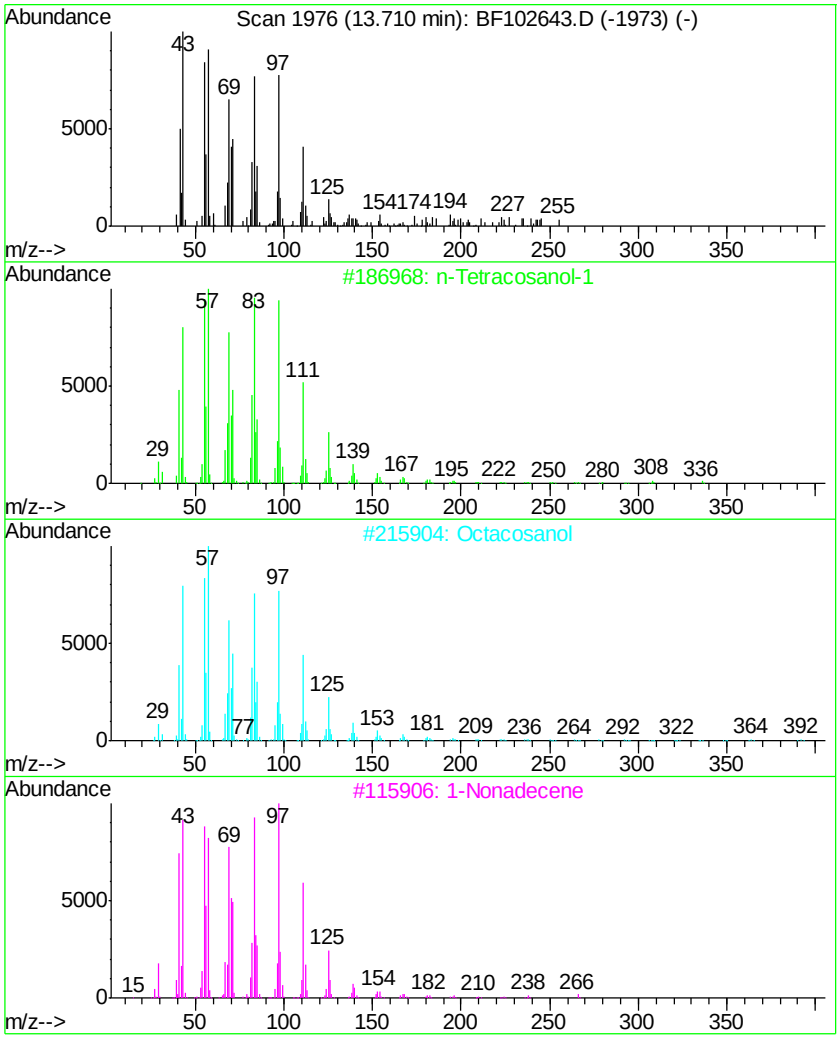
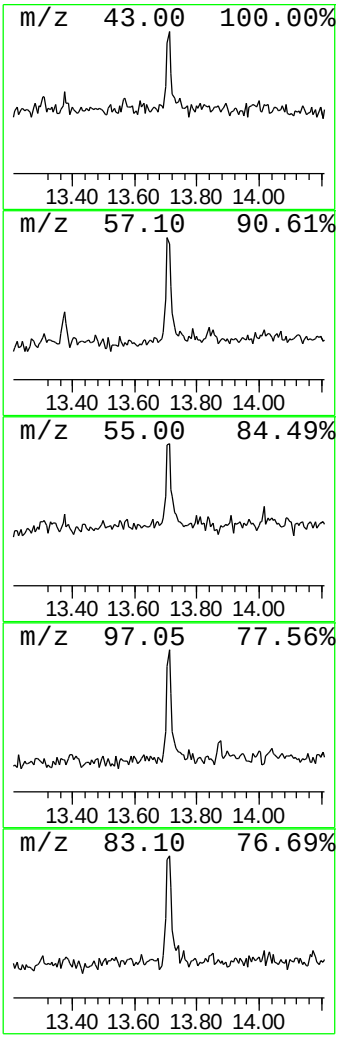
Peak Number 12 n-Tetracosanol-1 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	2.00 ng	111056	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Octacosanol	410	C28H58O	000557-61-9	87
3	1-Nonadecene	266	C19H38	018435-45-5	80
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	64
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	60





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Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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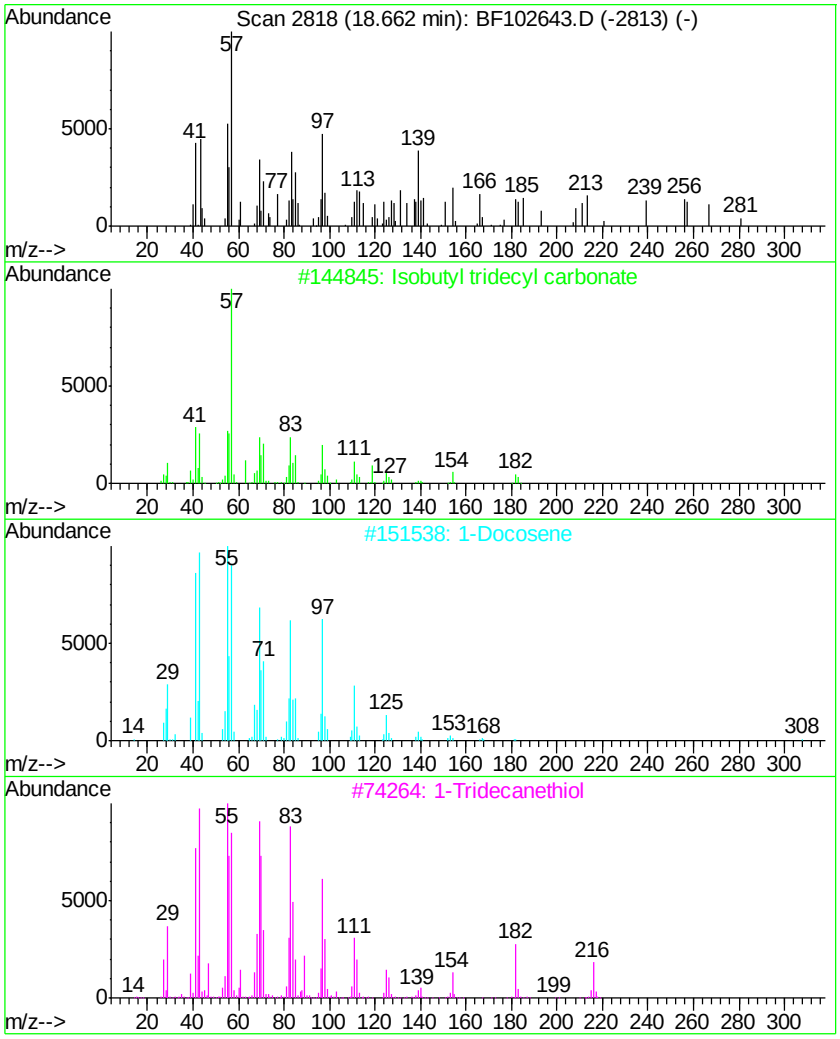
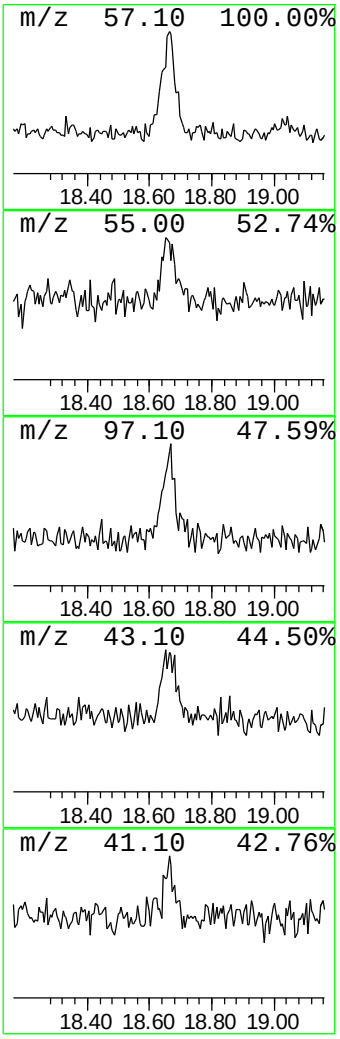
Peak Number 13 unknown18.66 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.66	3.07 ng	121180	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl tridecyl carbonate	300	C18H36O3	959275-44-6	38
2	1-Docosene	308	C22H44	001599-67-3	27
3	1-Tridecanethiol	216	C13H28S	019484-26-5	22
4	1-Tridecene	182	C13H26	002437-56-1	22
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013018\
Data File : BF102643.D
Acq On : 30 Jan 2018 16:58
Operator : SJ/JU
Sample : J1364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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
unknown4.26	4.26	3.0	ng	140465	1	6.71	925653	20.0
2-Pentanone, 4-hy...	4.90	2.1	ng	96664	1	6.71	925653	20.0
Butanoic acid, 3-...	5.09	7.8	ng	358556	1	6.71	925653	20.0
Butanoic acid, 2-...	5.20	3.5	ng	159743	1	6.71	925653	20.0
Pentanoic acid	5.52	2.8	ng	130576	1	6.71	925653	20.0
Pentanoic acid, 4...	6.16	8.3	ng	386366	1	6.71	925653	20.0
unknown6.48	6.48	67.5	ng	3123450	1	6.71	925653	20.0
Benzeneacetic acid	8.29	4.3	ng	285342	2	7.99	1323740	20.0
Indole	8.65	5.0	ng	334104	2	7.99	1323740	20.0
Hydrocinnamic acid	8.80	3.3	ng	219274	2	7.99	1323740	20.0
n-Tetracosanol-1	13.71	2.0	ng	111056	5	13.87	1109040	20.0
unknown18.66	18.66	3.1	ng	121180	6	15.30	789335	20.0