LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106350.D
Acq On : 12 Jun 2018 17:47
Operator : JU/SJ
Sample : J3415-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-33COMP

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	5.207	484	488	493	rVB	228680	256837	8.75%	0.839%
2	5.595	549	554	558	rBV	2783126	2778738	94.70%	9.081%
3	6.595	719	724	727	rBV	2784212	2718884	92.66%	8.886%
4	6.742	745	749	752	rBV	3040509	2726331	92.91%	8.910%
5	6.972	785	788	792	rVB	1132671	895505	30.52%	2.927%
6	7.131	811	815	818	rBV	2602944	2177699	74.22%	7.117%
7	7.531	879	883	886	rBV	1798219	1697276	57.84%	5.547%
8	7.601	890	895	898	rBV	41285	41552	1.42%	0.136%
9	8.254	1002	1006	1009	rBV	1278733	1003048	34.18%	3.278%
10	9.330	1185	1189	1192	rVB	3027381	2551234	86.94%	8.338%
11	9.719	1252	1255	1258	rBV	513915	364040	12.41%	1.190%
12	9.930	1286	1291	1294	rBV	46857	39836	1.36%	0.130%
13	10.013	1301	1305	1309	rVB2	1145116	942077	32.11%	3.079%
14	10.430	1374	1376	1379	rVB	75541	54672	1.86%	0.179%
15	10.801	1435	1439	1443	rBV	1825108	1574959	53.67%	5.147%
16	10.901	1453	1456	1461	rBV	73018	70688	2.41%	0.231%
17	11.354	1527	1533	1535	rBV	36548	33680	1.15%	0.110%
18	11.507	1555	1559	1562	rBV	1094649	988313	33.68%	3.230%
19	11.883	1620	1623	1626	rVB	501012	402522	13.72%	1.315%
20	12.571	1736	1740	1741	rBV	1545031	1251067	42.64%	4.089%
21	12.589	1741	1743	1751	rVV	1930089	1986363	67.69%	6.492%
22	12.677	1754	1758	1761	rVB	236915	215662	7.35%	0.705%
23	12.913	1793	1798	1802	rBV5	23192	39278	1.34%	0.128%
24	13.089	1824	1828	1831	rBV	3322075	2934311	100.00%	9.590%
25	13.277	1855	1860	1863	rBV5	31364	41881	1.43%	0.137%
26	13.324	1866	1868	1873	rVB3	46355	41448	1.41%	0.135%
27	13.977	1975	1979	1984	rBV	271385	296483	10.10%	0.969%
28	14.077	1994	1996	1999	rBV3	31698	33386	1.14%	0.109%
29	14.160	2006	2010	2014	rBV	1384587	1230547	41.94%	4.022%
30	14.636	2089	2091	2095	rVB4	51185	41315	1.41%	0.135%
31	15.036	2156	2159	2163	rVB	223917	233728	7.97%	0.764%
32	15.712	2269	2274	2281	rVB	719127	935116	31.87%	3.056%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106350.D
Acq On : 12 Jun 2018 17:47
Operator : JU/SJ
Sample : J3415-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-33COMP

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

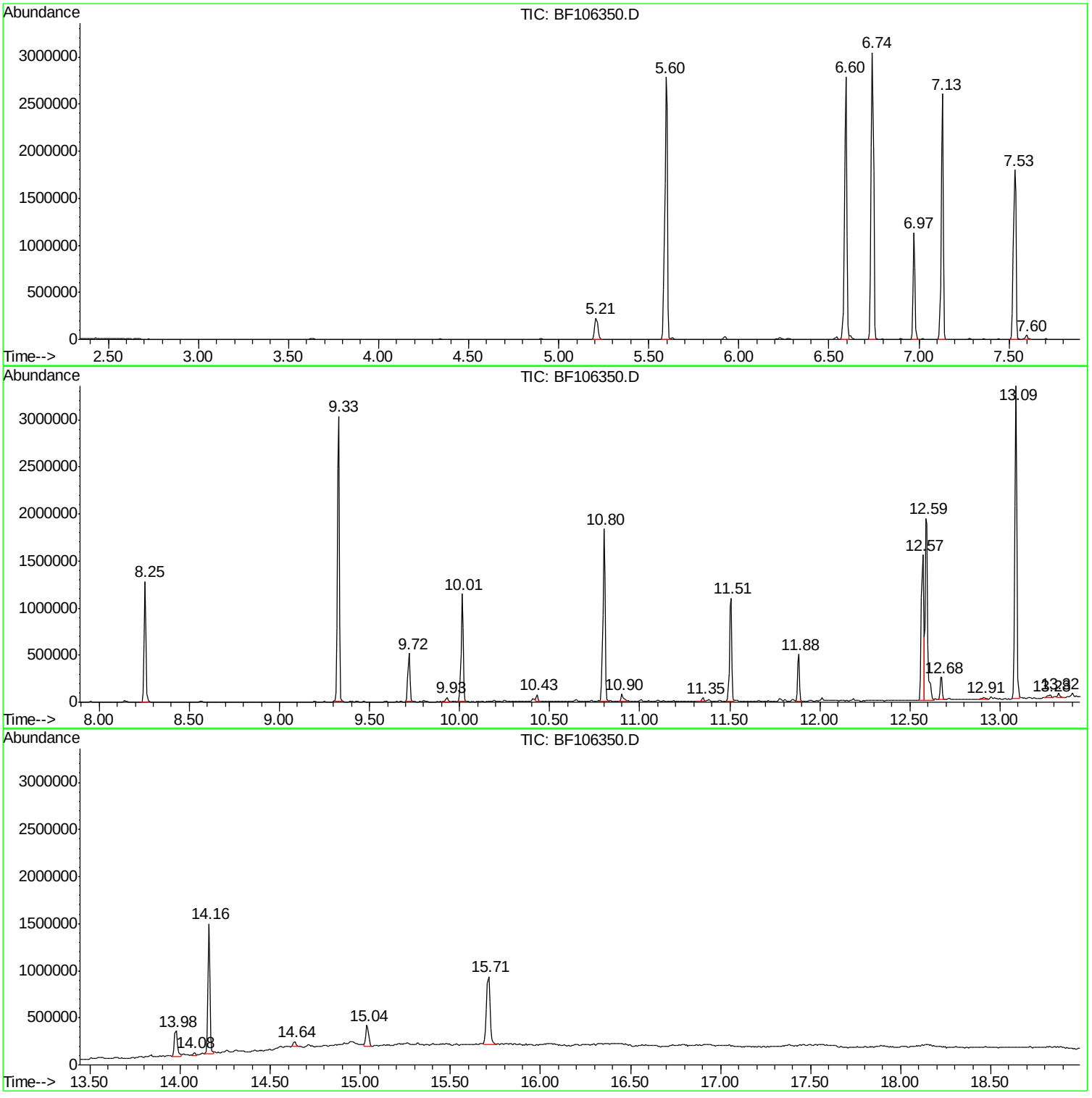
Sum of corrected areas: 30598476

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106350.D
Acq On : 12 Jun 2018 17:47
Operator : JU/SJ
Sample : J3415-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-33COMP

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106350.D
Acq On : 12 Jun 2018 17:47
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ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

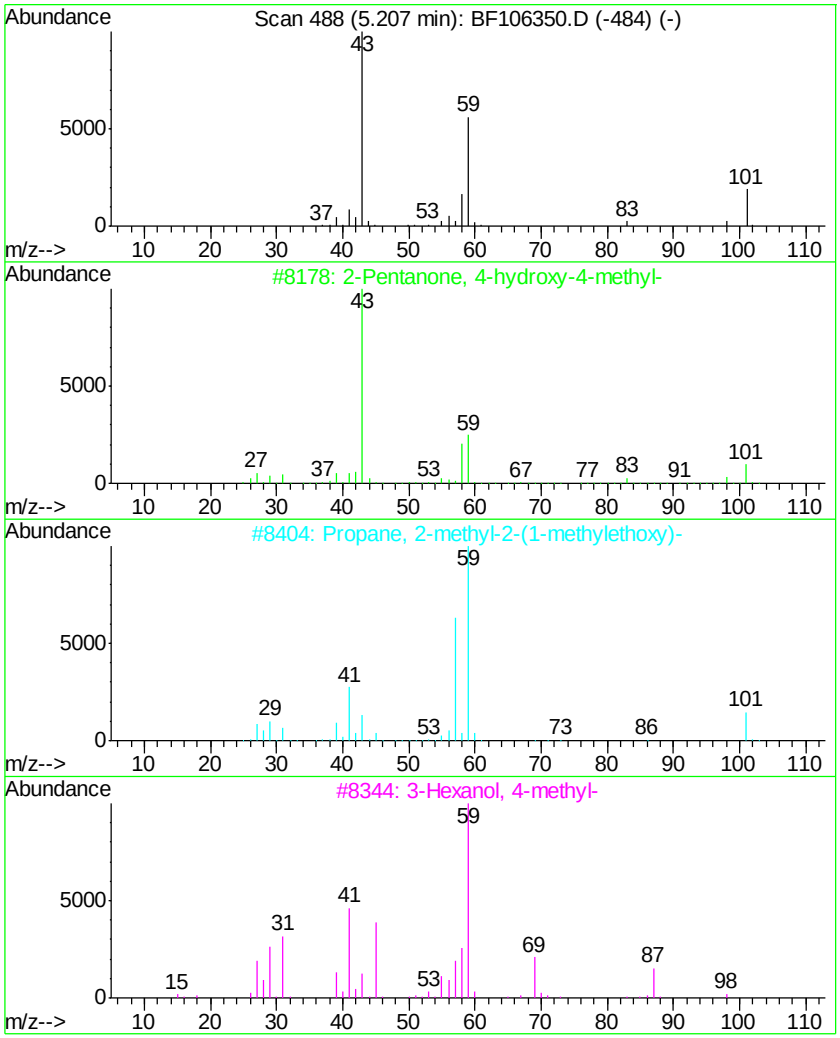
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

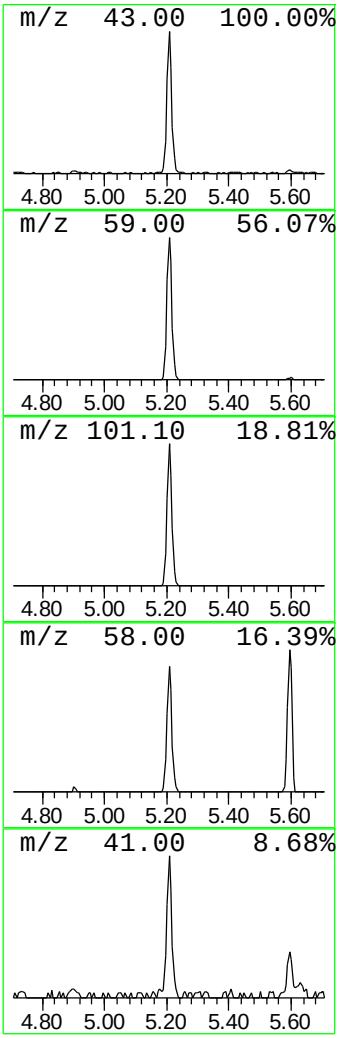
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	5.74 ng	256837	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	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106350.D
Acq On : 12 Jun 2018 17:47
Operator : JU/SJ
Sample : J3415-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-33COMP

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
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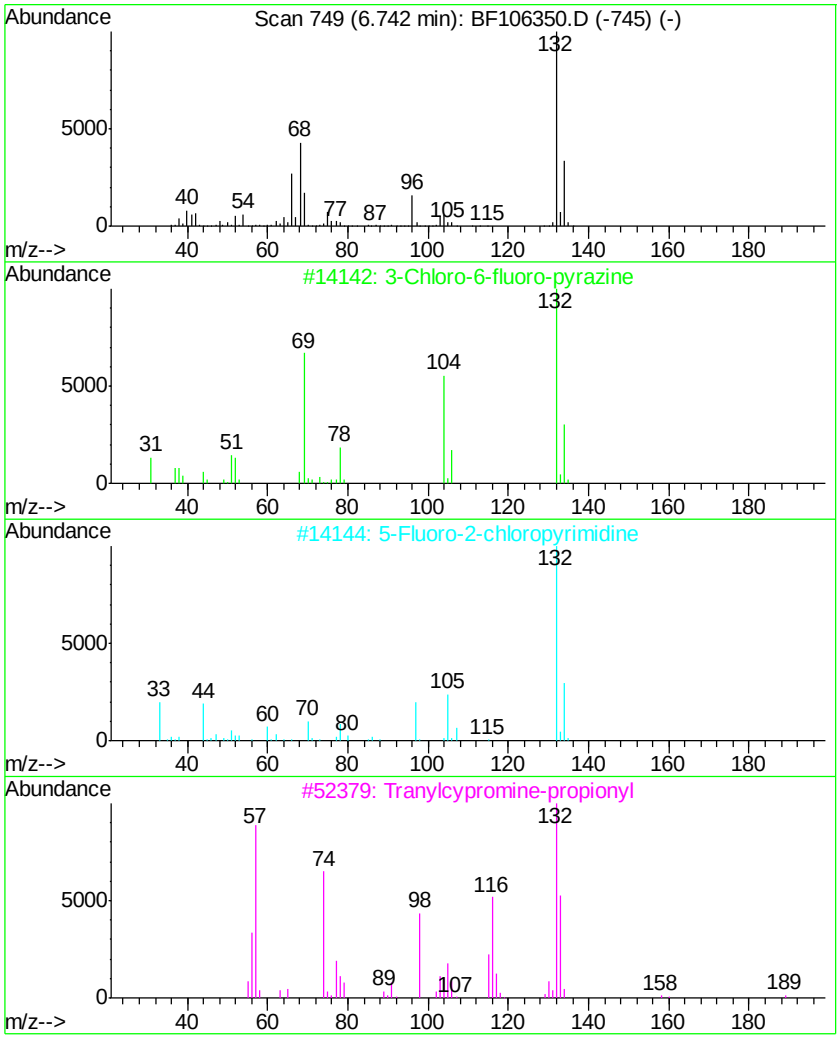
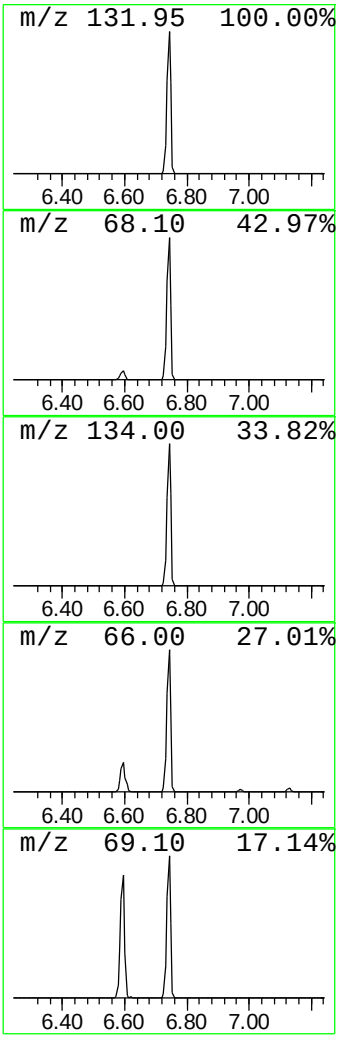
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	60.89 ng	2726330	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106350.D
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Operator : JU/SJ
Sample : J3415-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-33COMP

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

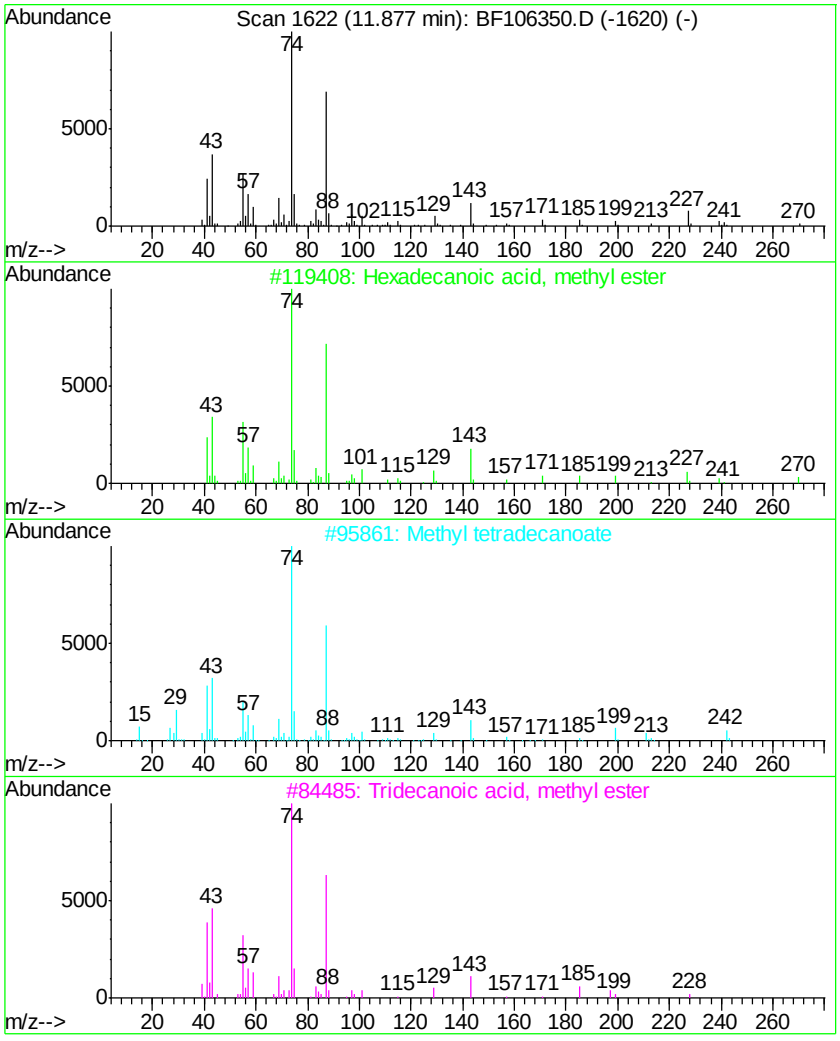
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

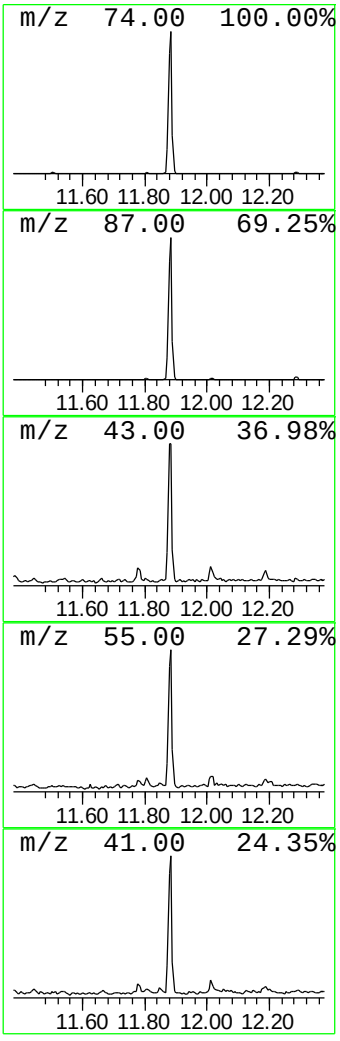
****

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	8.15 ng	402522	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	87
5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
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Sample : J3415-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-33COMP

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

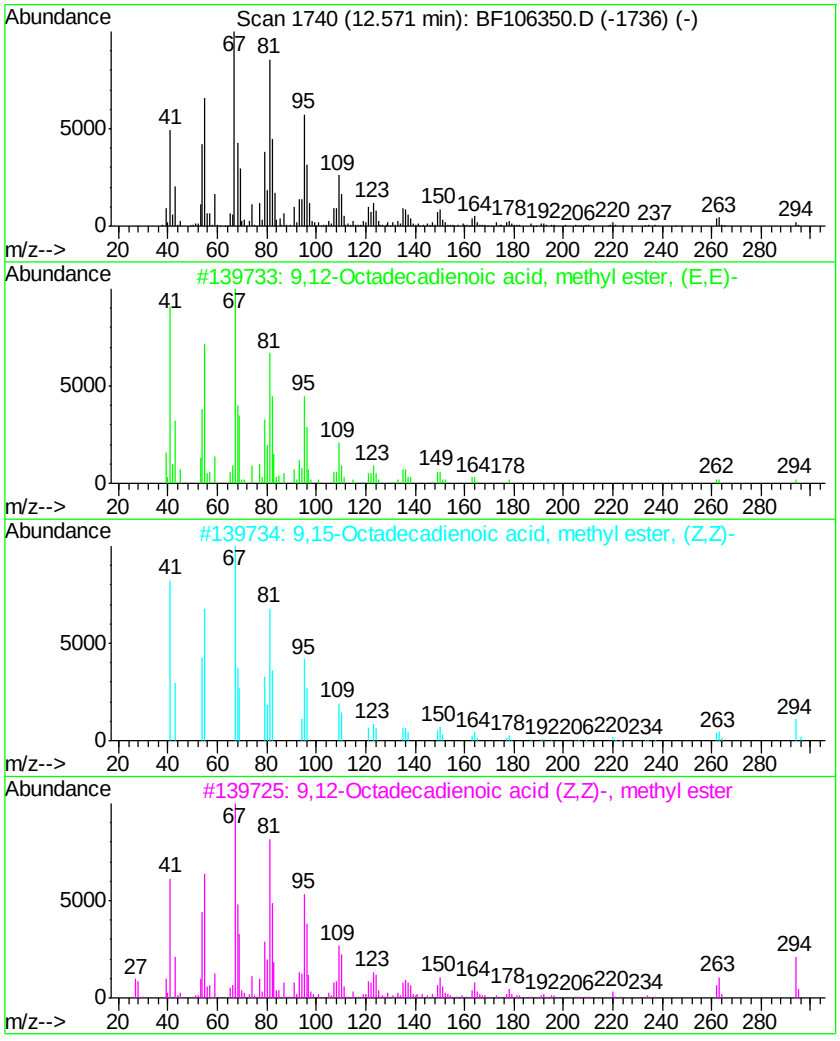
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

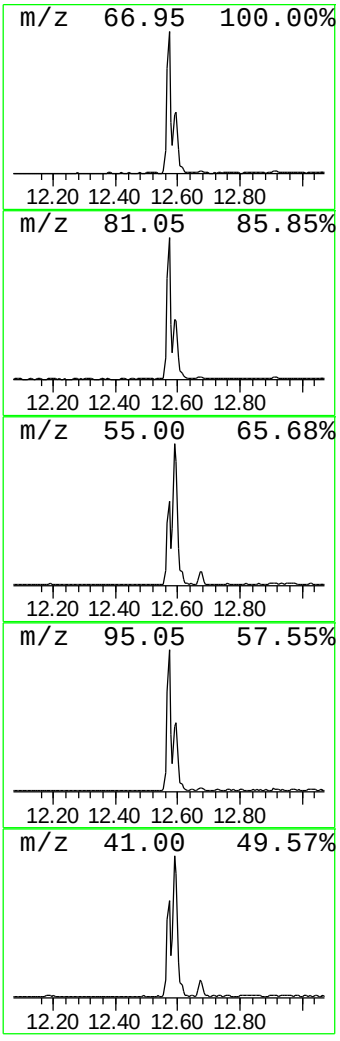
****

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	25.32 ng	1251070	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
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Sample : J3415-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-33COMP

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

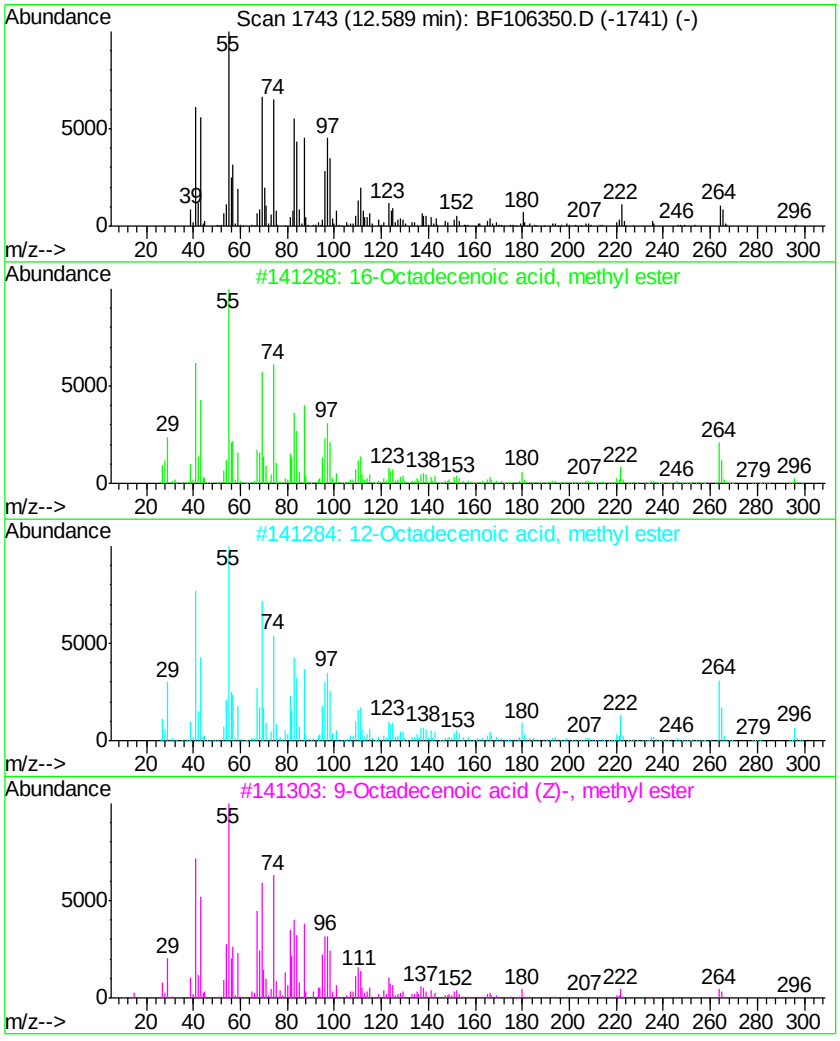
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

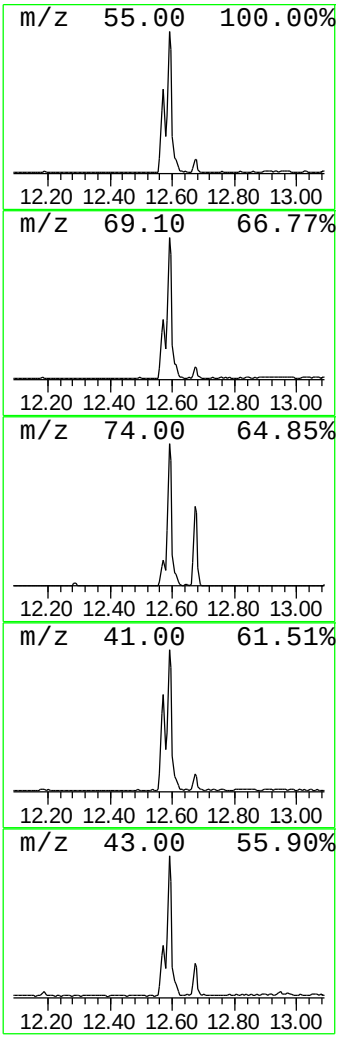
****

Peak Number 6 16-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	40.20 ng	1986360	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	93
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	93
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	90
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	89
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	89





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Data File : BF106350.D
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Operator : JU/SJ
Sample : J3415-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-33COMP

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

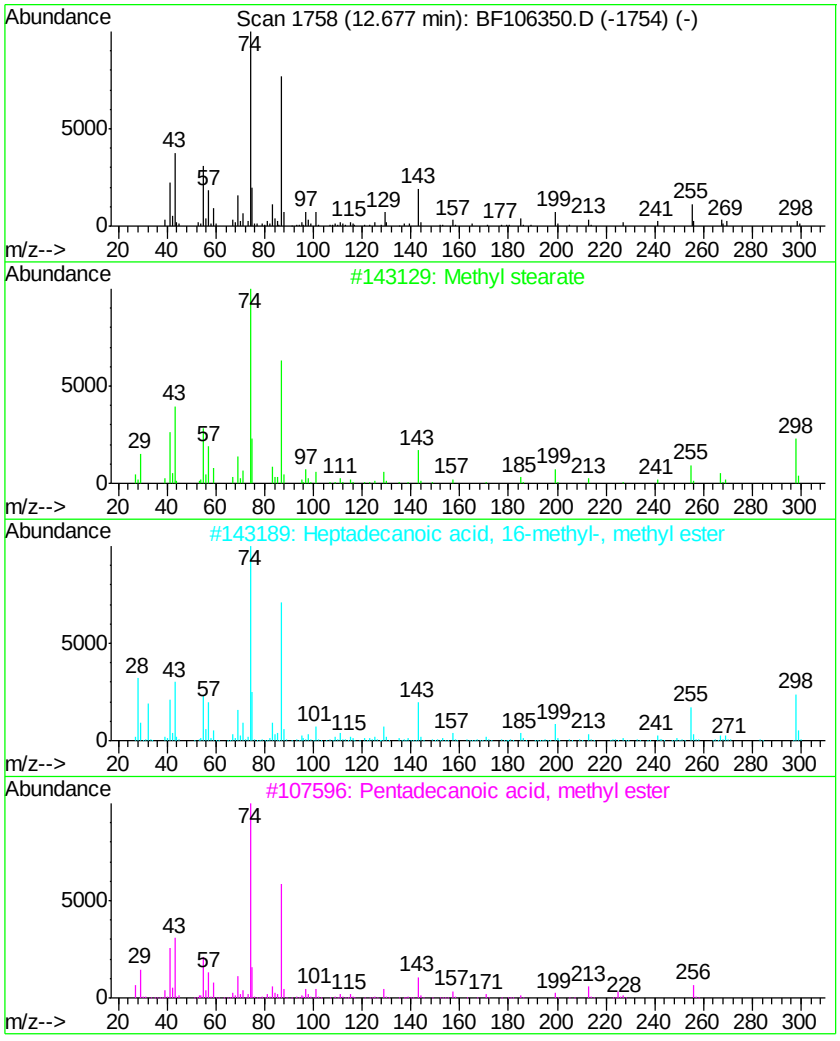
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

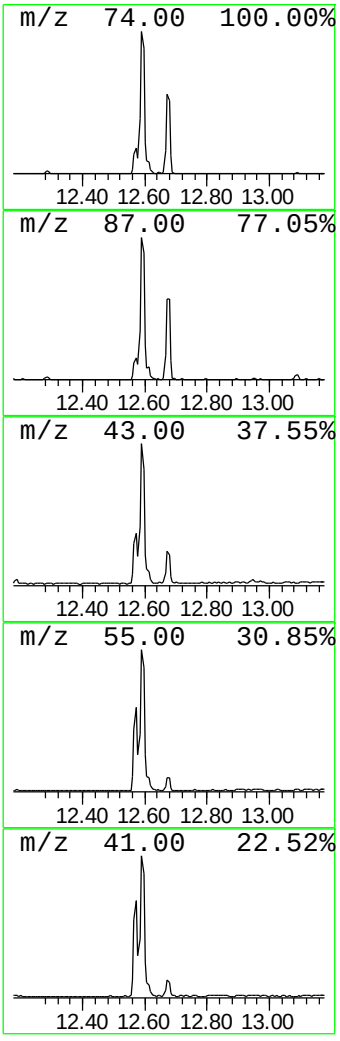
****

Peak Number 7 Methyl stearate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	4.36 ng	215662	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106350.D
Acq On : 12 Jun 2018 17:47
Operator : JU/SJ
Sample : J3415-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-33COMP

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

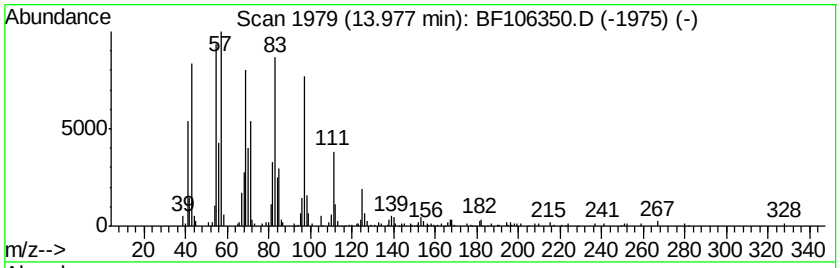
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

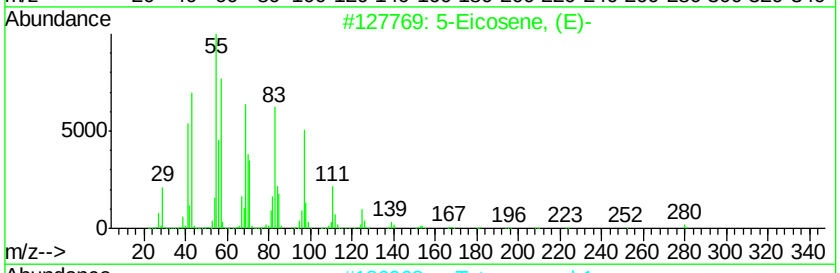
****

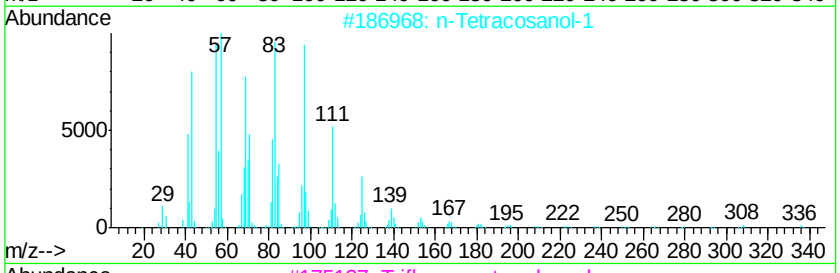
Peak Number 8 5-Eicosene, (E)- Concentration Rank 8

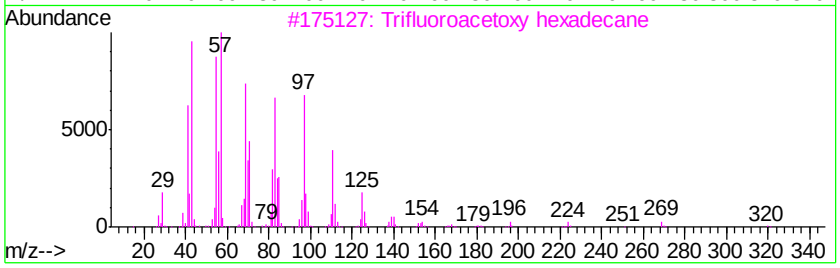
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	4.82 ng	296483	Chrysene-d12	14.16

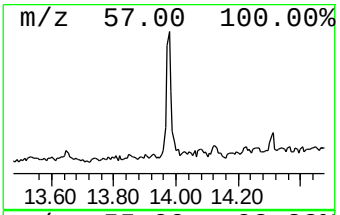
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Cyclopentadecane	210	C15H30	000295-48-7	93
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91

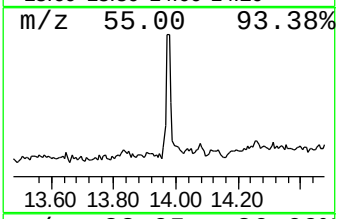


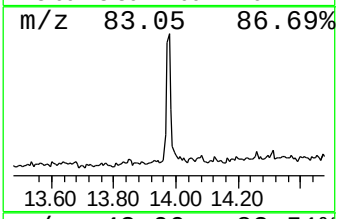


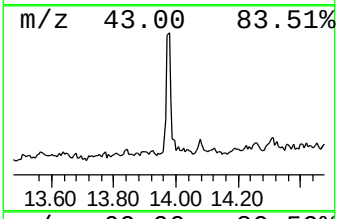


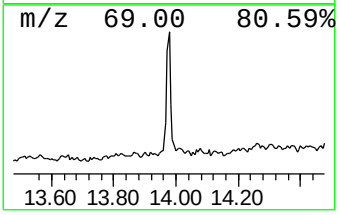












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Data File : BF106350.D
Acq On : 12 Jun 2018 17:47
Operator : JU/SJ
Sample : J3415-02
Misc :
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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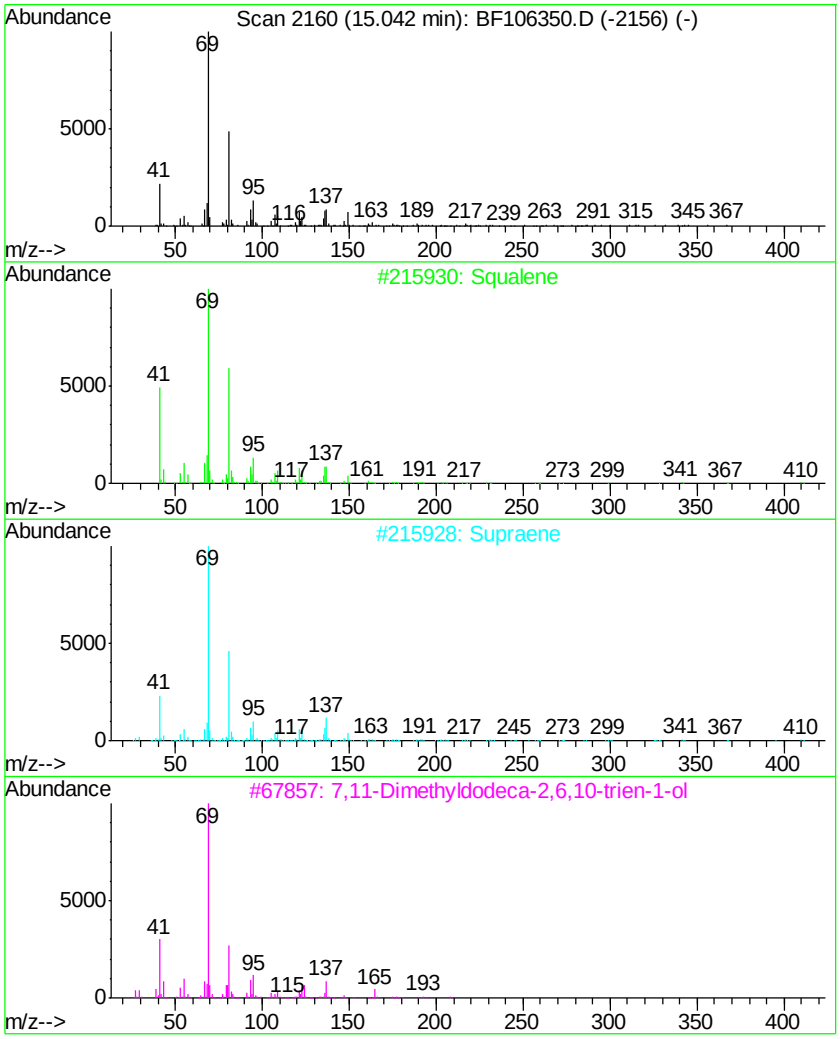
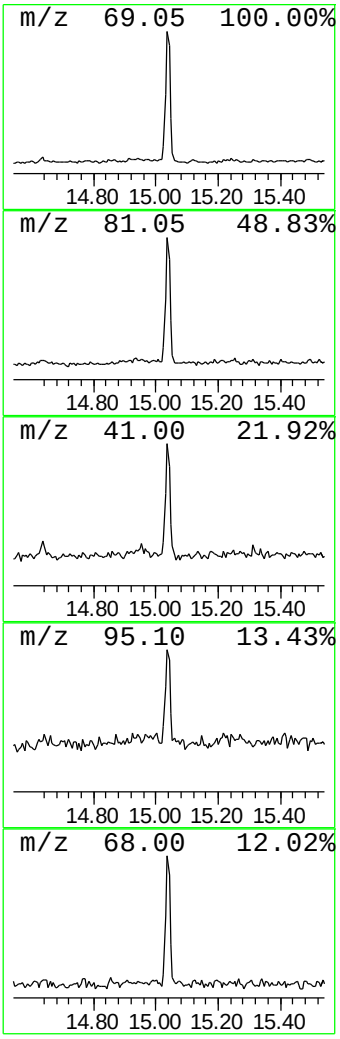
Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	5.00 ng	233728	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	72
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061218\
Data File : BF106350.D
Acq On : 12 Jun 2018 17:47
Operator : JU/SJ
Sample : J3415-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-33COMP

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...	5.21	5.7	ng	256837	1	6.97	895505	20.0
unknown6.74	6.74	60.9	ng	2726330	1	6.97	895505	20.0
Hexadecanoic acid...	11.88	8.2	ng	402522	4	11.51	988313	20.0
9,12-Octadecadien...	12.57	25.3	ng	1251070	4	11.51	988313	20.0
16-Octadecenoic a...	12.59	40.2	ng	1986360	4	11.51	988313	20.0
Methyl stearate	12.68	4.4	ng	215662	4	11.51	988313	20.0
5-Eicosene, (E)-	13.98	4.8	ng	296483	5	14.16	1230550	20.0
Squalene	15.04	5.0	ng	233728	6	15.71	935116	20.0