LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118612.D
Acq On : 21 Jan 2020 1:03
Operator : CG/JU
Sample : L1164-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

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-BF012020.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	2.152	6	11	18	rVB	1516232	2054907	21.92%	2.044%
2	5.092	503	511	519	rVB	1452717	1787625	19.07%	1.778%
3	5.498	574	580	583	rBV	8417203	8287518	88.39%	8.245%
4	6.504	745	751	754	rBV	8507369	8863296	94.53%	8.818%
5	6.651	771	776	779	rBV	9250687	9012633	96.13%	8.966%
6	6.881	811	815	818	rBV	3469517	2693577	28.73%	2.680%
7	7.039	838	842	845	rBV	8357455	7137693	76.13%	7.101%
8	7.439	902	910	913	rBV	5868088	5408161	57.68%	5.380%
9	8.163	1029	1033	1036	rBV	3969482	3218907	34.33%	3.202%
10	8.875	1149	1154	1157	rVB	125025	118451	1.26%	0.118%
11	9.239	1211	1216	1219	rBV	11188432	9375811	100.00%	9.327%
12	9.328	1227	1231	1235	rBV2	131127	190024	2.03%	0.189%
13	9.627	1279	1282	1285	rBV	635004	507611	5.41%	0.505%
14	9.775	1304	1307	1310	rBV	179247	162106	1.73%	0.161%
15	9.916	1325	1331	1335	rBV	3733051	3237846	34.53%	3.221%
16	9.951	1335	1337	1340	rVB	142494	117150	1.25%	0.117%
17	10.122	1363	1366	1369	rVB	175992	161510	1.72%	0.161%
18	10.463	1421	1424	1430	rBV	200990	192352	2.05%	0.191%
19	10.704	1460	1465	1468	rBV	5940266	5213728	55.61%	5.187%
20	10.827	1483	1486	1487	rBV	208205	174891	1.87%	0.174%
21	11.298	1564	1566	1572	rVB2	130411	176069	1.88%	0.175%
22	11.404	1580	1584	1586	rBV	3201561	2928052	31.23%	2.913%
23	11.427	1586	1588	1591	rVV	1466742	1171962	12.50%	1.166%
24	11.474	1591	1596	1599	rVB	569714	520349	5.55%	0.518%
25	11.627	1619	1622	1625	rVB	136420	122064	1.30%	0.121%
26	11.698	1632	1634	1637	rBV	122544	112195	1.20%	0.112%
27	11.798	1648	1651	1654	rBV	496060	392376	4.18%	0.390%
28	11.904	1666	1669	1671	rBV	163365	150952	1.61%	0.150%
29	11.927	1671	1673	1678	rVB	983132	861736	9.19%	0.857%
30	12.016	1685	1688	1690	rBV2	325995	331750	3.54%	0.330%
31	12.198	1717	1719	1721	rBV	130102	119336	1.27%	0.119%
32	12.451	1760	1762	1765	rBV	156117	148573	1.58%	0.148%
33	12.486	1765	1768	1770	rBV	1602179	1497299	15.97%	1.490%
34	12.504	1770	1771	1774	rVV2	1016685	819945	8.75%	0.816%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
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Acq On : 21 Jan 2020 1:03
Operator : CG/JU
Sample : L1164-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

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-BF012020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.533	1774	1776	1782	rVB2	154542	139601	1.49%	0.139%
36	12.592	1783	1786	1787	rVV2	216285	203195	2.17%	0.202%
37	12.616	1787	1790	1793	rVB	2784913	2304063	24.57%	2.292%
38	12.716	1804	1807	1810	rBV3	294770	342532	3.65%	0.341%
39	12.845	1823	1829	1832	rBV	2266971	2570223	27.41%	2.557%
40	12.986	1850	1853	1857	rBV	8740548	8578489	91.50%	8.534%
41	13.174	1883	1885	1888	rVB	321815	258002	2.75%	0.257%
42	13.274	1900	1902	1905	rBV2	290180	289062	3.08%	0.288%
43	13.439	1928	1930	1933	rVB	359228	311212	3.32%	0.310%
44	13.886	2003	2006	2010	rBV	1360840	1470275	15.68%	1.463%
45	14.039	2028	2032	2035	rBV2	3285212	4308310	45.95%	4.286%
46	14.068	2035	2037	2043	rVB	1062144	941858	10.05%	0.937%
47	15.521	2282	2284	2288	rVB	1403614	1533236	16.35%	1.525%

Sum of corrected areas: 100518513

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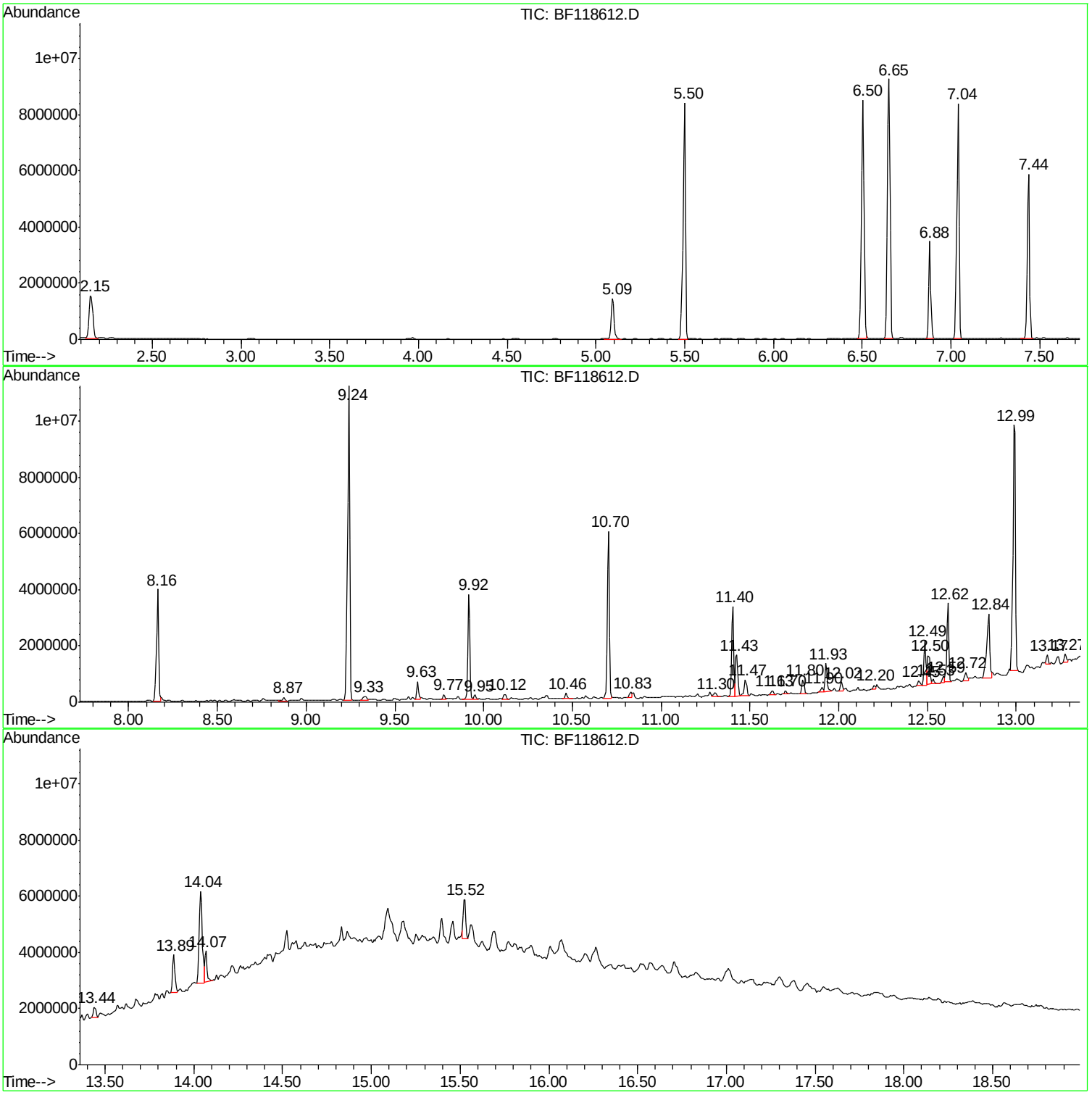
Instrument :
BNA_F
ClientSampleId :
QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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\BF012020\
Data File : BF118612.D
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Operator : CG/JU
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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

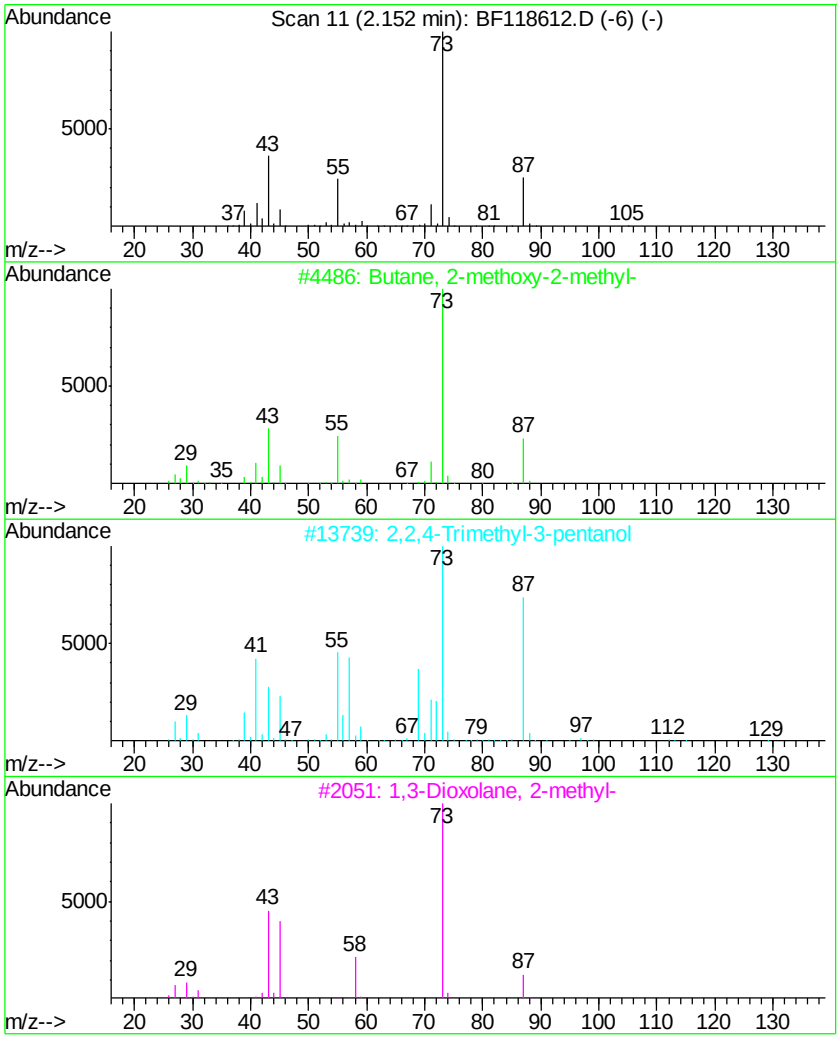
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

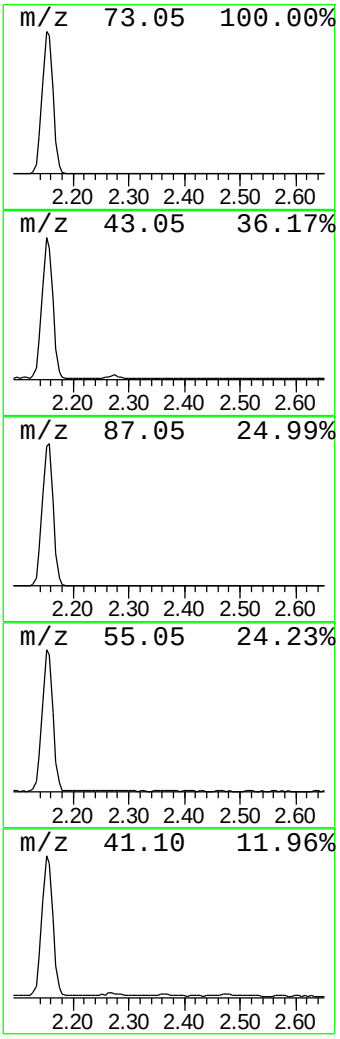
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	15.26 ng	2054910	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





Library Search Compound Report

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Data File : BF118612.D
Acq On : 21 Jan 2020 1:03
Operator : CG/JU
Sample : L1164-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

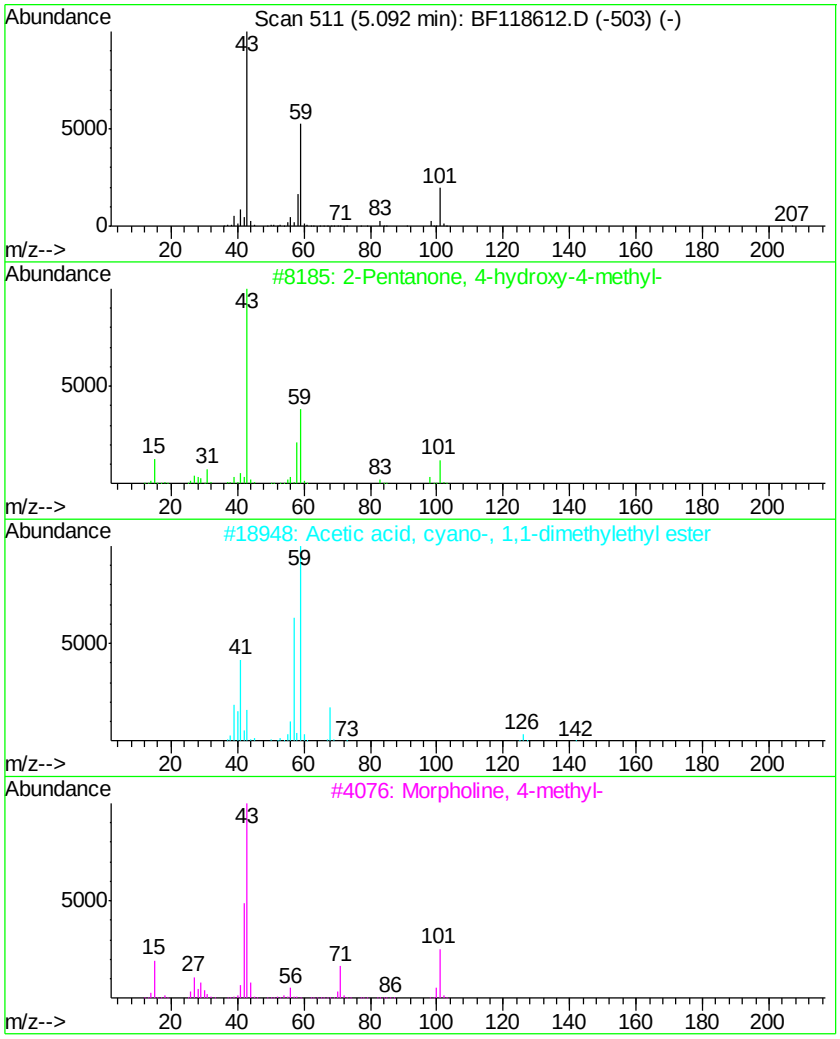
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

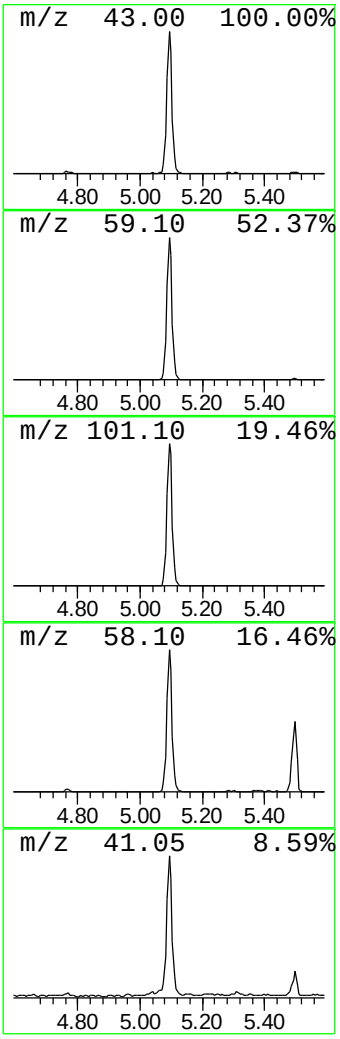
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	13.27 ng	1787630	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118612.D
Acq On : 21 Jan 2020 1:03
Operator : CG/JU
Sample : L1164-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

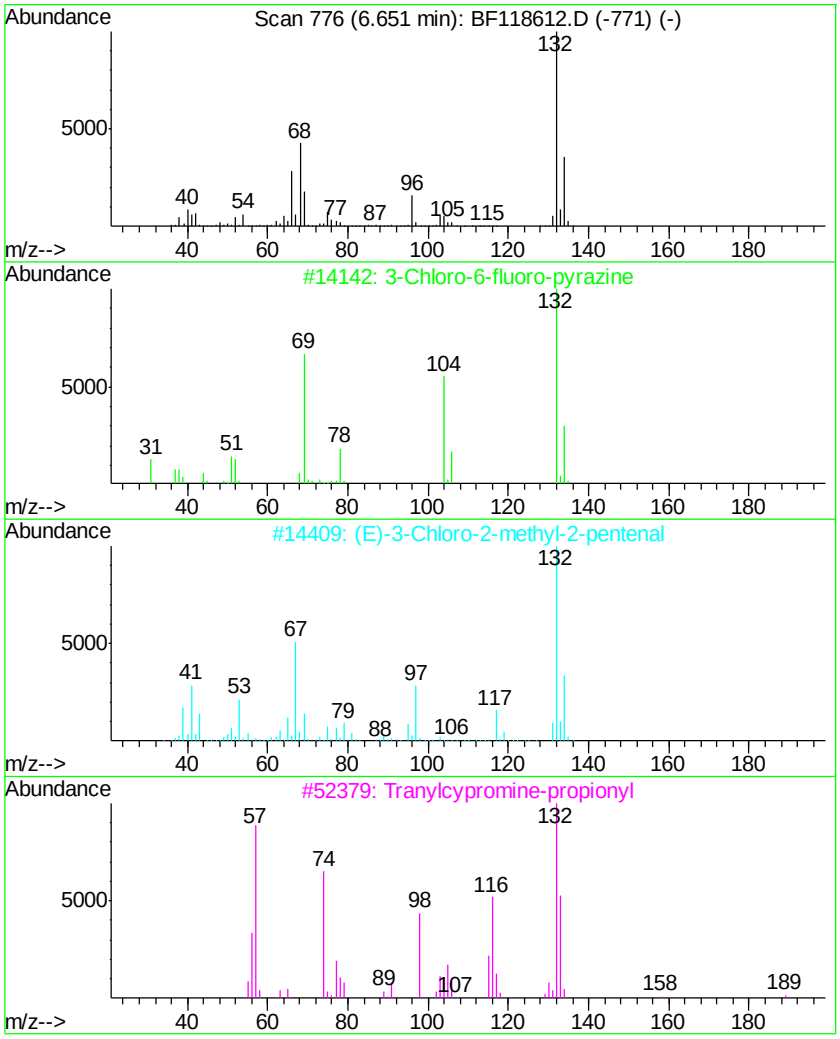
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

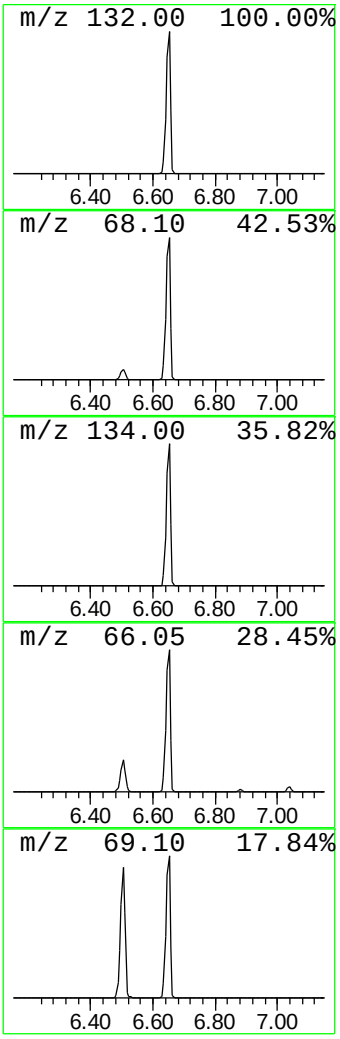
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	66.92 ng	9012630	1,4-Dichlorobenzene-d4	6.88

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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

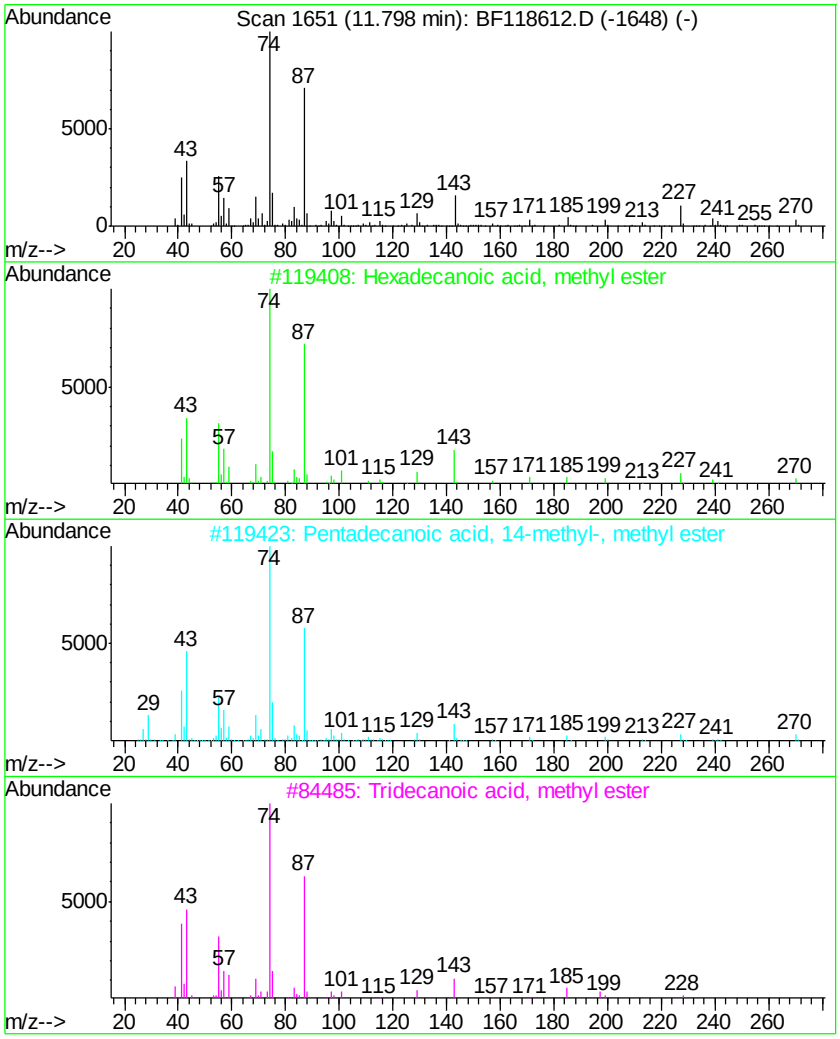
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

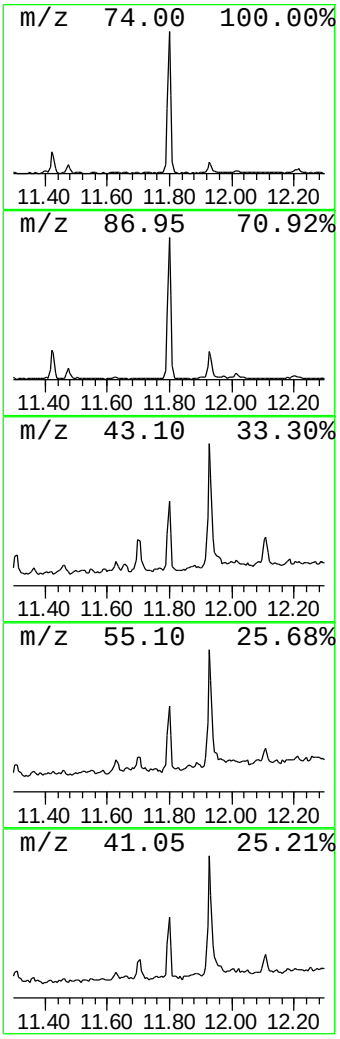
****

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.68 ng	392376	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	98
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83





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Operator : CG/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

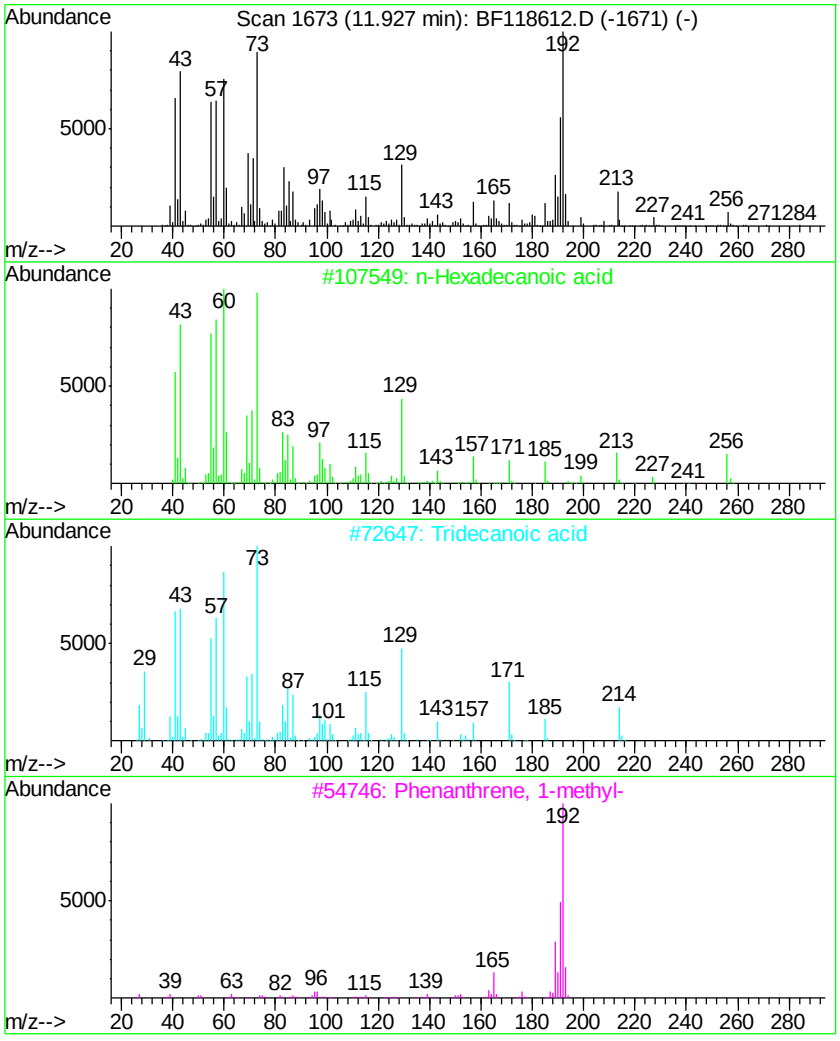
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

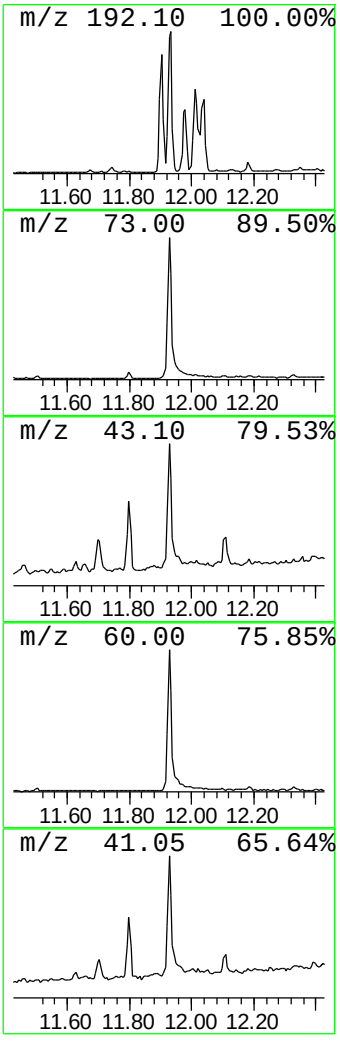
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	5.89 ng	861736	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91





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Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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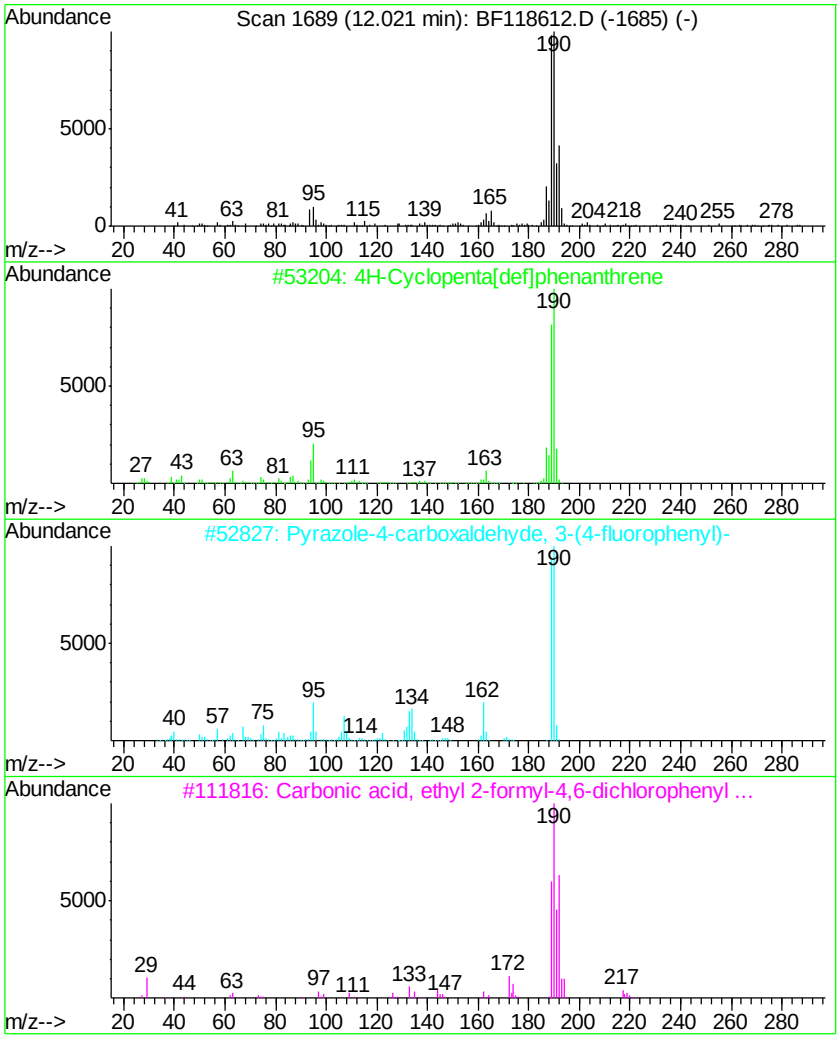
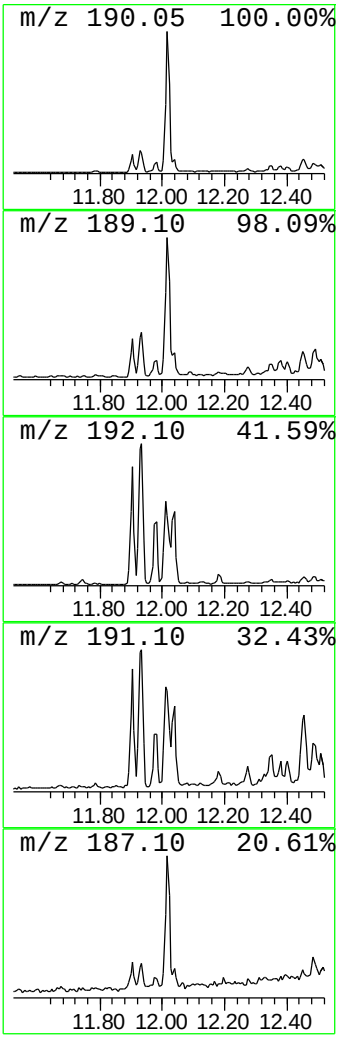
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.27 ng	331750	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	52
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	2,6-Dichlorobenzaldoxime	189	C7H5Cl2NO	025185-95-9	25





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Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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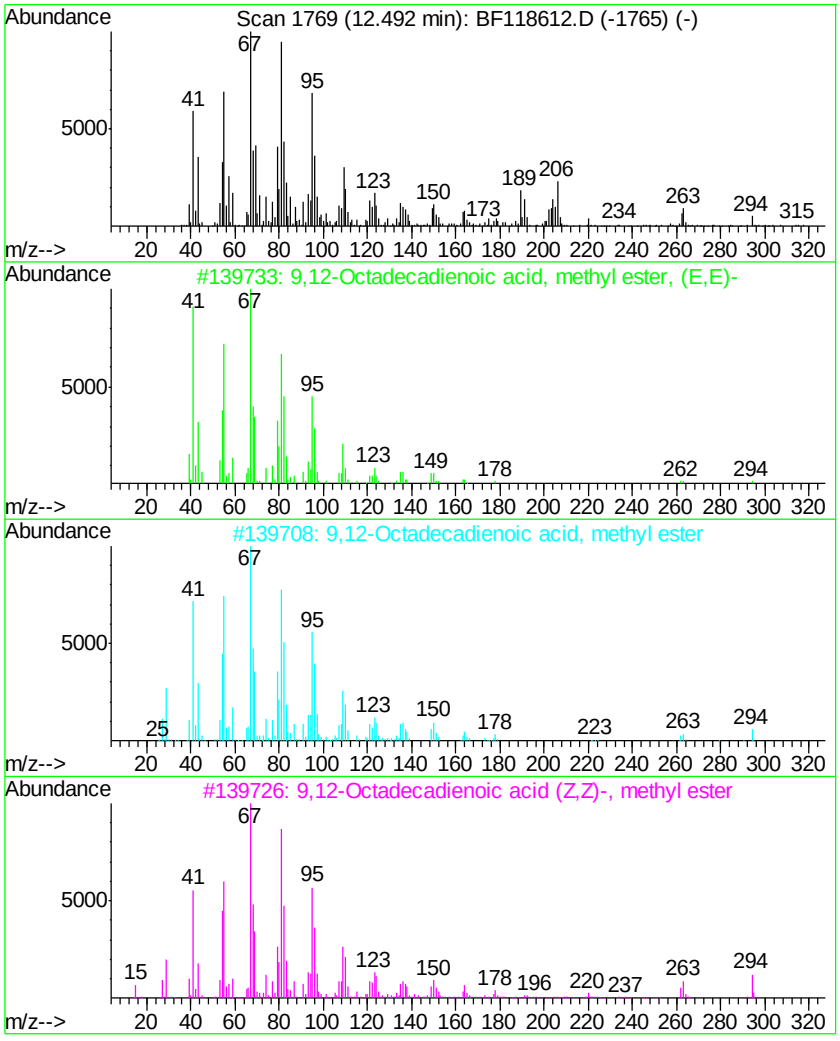
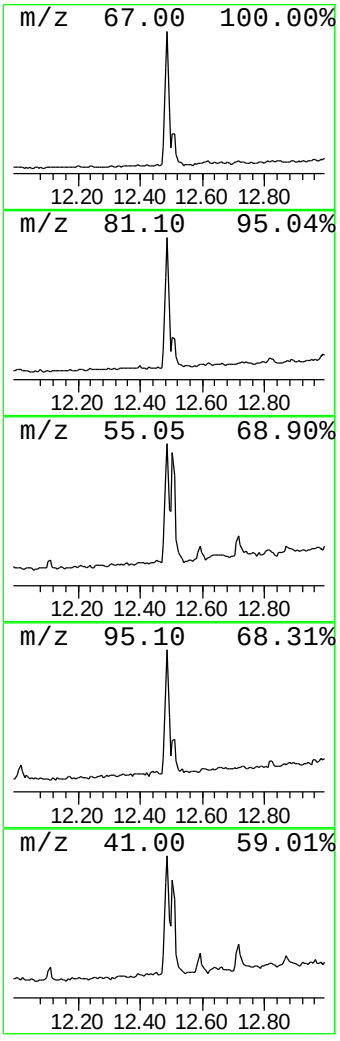
Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	10.23 ng	1497300	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	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99





Library Search Compound Report

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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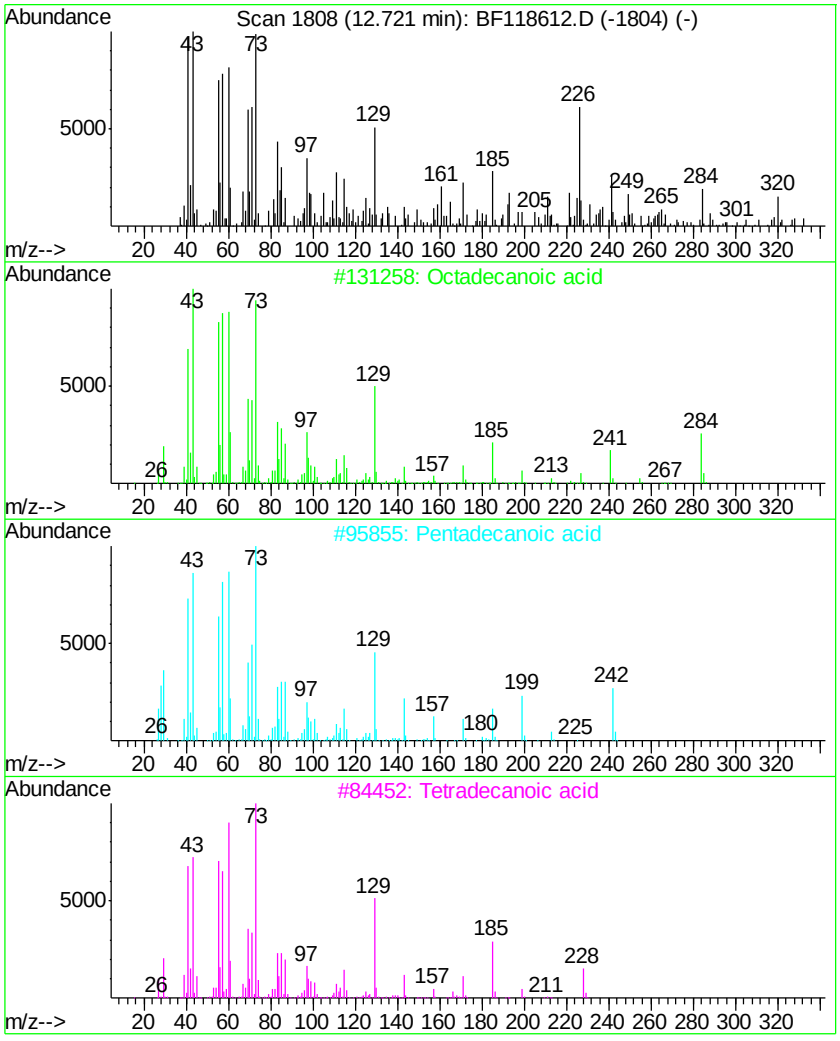
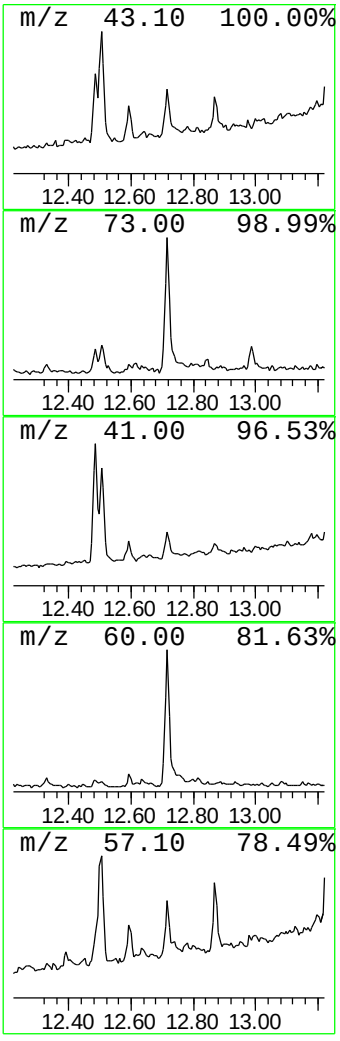
Peak Number 10 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.34 ng	342532	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	Dodecanoic acid	200	C12H24O2	000143-07-7	46
5	Isopropyl stearate	326	C21H42O2	000112-10-7	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118612.D
Acq On : 21 Jan 2020 1:03
Operator : CG/JU
Sample : L1164-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

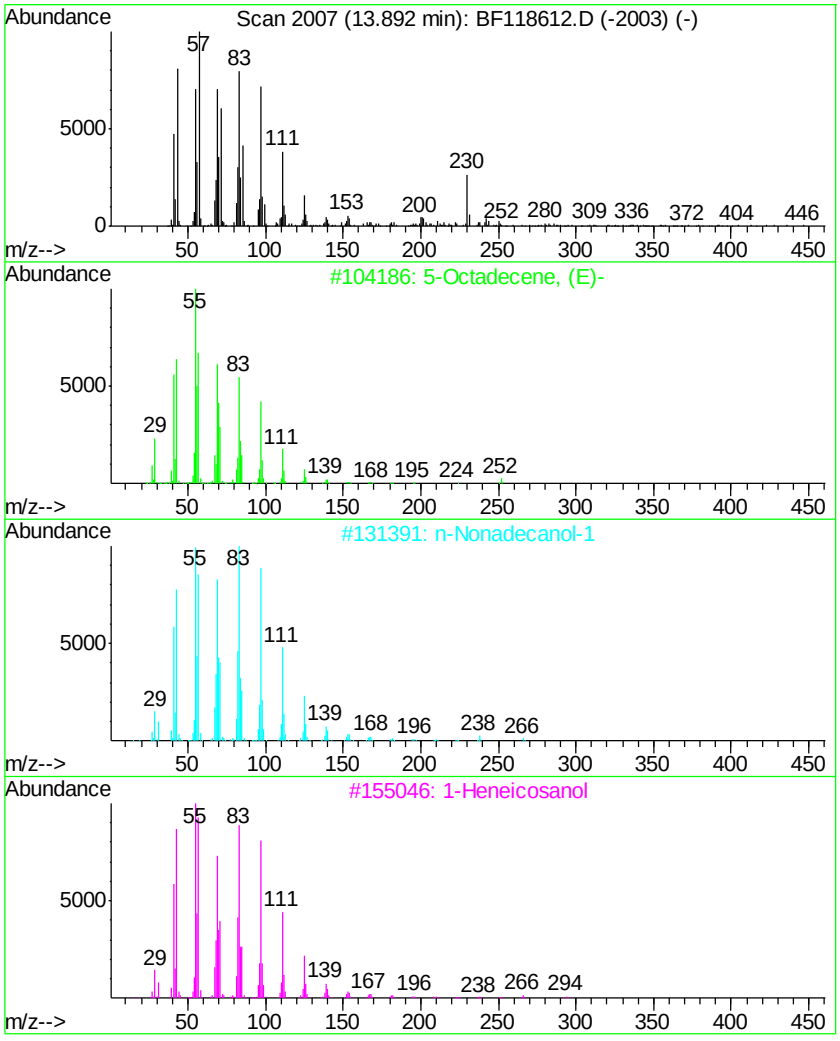
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

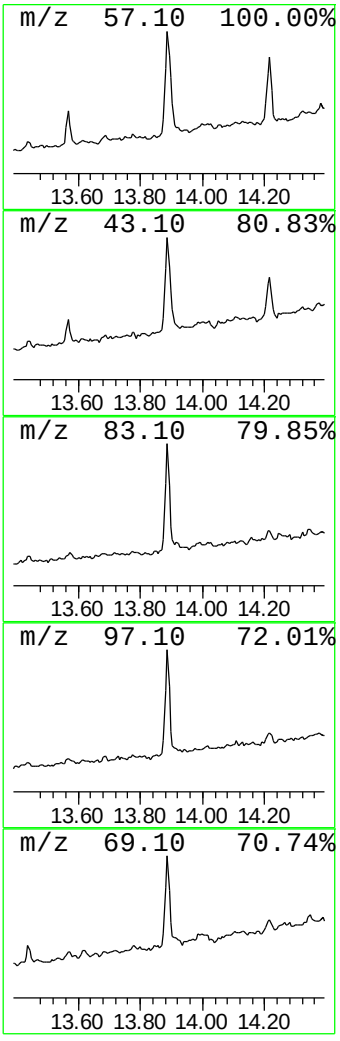
****

Peak Number 11 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	6.83 ng	1470280	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012020\
Data File : BF118612.D
Acq On : 21 Jan 2020 1:03
Operator : CG/JU
Sample : L1164-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QVD-SB-0203-0-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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...	2.15	15.3	ng	2054910	1	6.88	2693580	20.0
2-Pentanone, 4-hy...	5.09	13.3	ng	1787630	1	6.88	2693580	20.0
unknown6.65	6.65	66.9	ng	9012630	1	6.88	2693580	20.0
Hexadecanoic acid...	11.80	2.7	ng	392376	4	11.40	2928050	20.0
n-Hexadecanoic acid	11.93	5.9	ng	861736	4	11.40	2928050	20.0
4H-Cyclopenta[def...	12.02	2.3	ng	331750	4	11.40	2928050	20.0
9,12-Octadecadien...	12.49	10.2	ng	1497300	4	11.40	2928050	20.0
Octadecanoic acid	12.72	2.3	ng	342532	4	11.40	2928050	20.0
5-Octadecene, (E)-	13.89	6.8	ng	1470280	5	14.04	4308310	20.0