LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111159.D
Acq On : 7 Dec 2018 00:55
Operator : JU/SJ
Sample : J6188-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-120418-A

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-BF120518.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	3.234	193	195	206	rBV	120663	266925	2.16%	0.236%
2	5.016	489	498	504	rVB	644166	823939	6.66%	0.727%
3	5.422	561	567	570	rBV	10860086	10839904	87.58%	9.571%
4	6.434	733	739	744	rBV2	10693298	12376489	100.00%	10.927%
5	6.575	758	763	766	rBV	11859136	11222268	90.67%	9.908%
6	6.804	798	802	806	rBV	4138138	3212648	25.96%	2.836%
7	6.963	825	829	832	rVB	9662702	8124886	65.65%	7.174%
8	7.363	892	897	900	rBV	8017503	7429764	60.03%	6.560%
9	8.086	1016	1020	1022	rBV	5304211	4256842	34.39%	3.758%
10	8.104	1022	1023	1028	rVB	273311	205931	1.66%	0.182%
11	9.163	1198	1203	1206	rBV	11992128	10619357	85.80%	9.376%
12	9.257	1213	1219	1223	rVB3	153204	165514	1.34%	0.146%
13	9.551	1266	1269	1272	rBV	1687249	1445242	11.68%	1.276%
14	9.781	1306	1308	1312	rVB	169082	137607	1.11%	0.121%
15	9.839	1312	1318	1322	rBV2	5339634	4494653	36.32%	3.968%
16	10.280	1391	1393	1396	rVB	179986	141985	1.15%	0.125%
17	10.622	1447	1451	1455	rBV	6507392	6181897	49.95%	5.458%
18	10.757	1471	1474	1475	rBV	165266	152647	1.23%	0.135%
19	11.204	1547	1550	1553	rBV3	129919	124367	1.00%	0.110%
20	11.322	1566	1570	1572	rBV	4352037	3577788	28.91%	3.159%
21	11.345	1572	1574	1577	rVV	597401	448827	3.63%	0.396%
22	11.392	1577	1582	1585	rVB2	204344	221916	1.79%	0.196%
23	11.727	1636	1639	1642	rVB	954574	714135	5.77%	0.631%
24	11.780	1645	1648	1652	rBV3	102208	160005	1.29%	0.141%
25	11.857	1657	1661	1666	rBV2	2255747	2101836	16.98%	1.856%
26	11.933	1671	1674	1677	rBV	145514	138471	1.12%	0.122%
27	12.410	1752	1755	1757	rBV	1968644	1686456	13.63%	1.489%
28	12.433	1757	1759	1762	rVB	2148640	1601914	12.94%	1.414%
29	12.527	1770	1775	1779	rBV2	927271	1146487	9.26%	1.012%
30	12.563	1779	1781	1789	rVB5	187398	318334	2.57%	0.281%
31	12.639	1791	1794	1800	rBV	999873	998391	8.07%	0.881%
32	12.757	1809	1814	1818	rBV	822602	849961	6.87%	0.750%
33	12.910	1836	1840	1843	rBV	7438656	6380690	51.55%	5.634%
34	13.810	1990	1993	2001	rVB	1468989	1509821	12.20%	1.333%

LSC Area Percent Report

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Sample : J6188-01
Misc :
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Instrument : BNA_F
ClientSampleId : BU-03-120418-A

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-BF120518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.957	2013	2018	2020	rBV2	3230849	3245458	26.22%	2.865%
36	13.980	2020	2022	2025	rVB	390847	303086	2.45%	0.268%
37	14.139	2046	2049	2052	rBV	168009	165044	1.33%	0.146%
38	14.445	2098	2101	2106	rBV2	319680	378366	3.06%	0.334%
39	14.745	2150	2152	2156	rBV2	139429	169165	1.37%	0.149%
40	14.821	2162	2165	2168	rVB	668479	574621	4.64%	0.507%
41	14.974	2188	2191	2199	rBV	348151	690625	5.58%	0.610%
42	15.080	2206	2209	2211	rBV2	252071	253499	2.05%	0.224%
43	15.268	2239	2241	2246	rVB	223240	270415	2.18%	0.239%
44	15.327	2249	2251	2254	rVB	268110	245970	1.99%	0.217%
45	15.392	2258	2262	2266	rVV	1765360	2131350	17.22%	1.882%
46	15.921	2349	2352	2363	rVB4	435206	756891	6.12%	0.668%

Sum of corrected areas: 113262387

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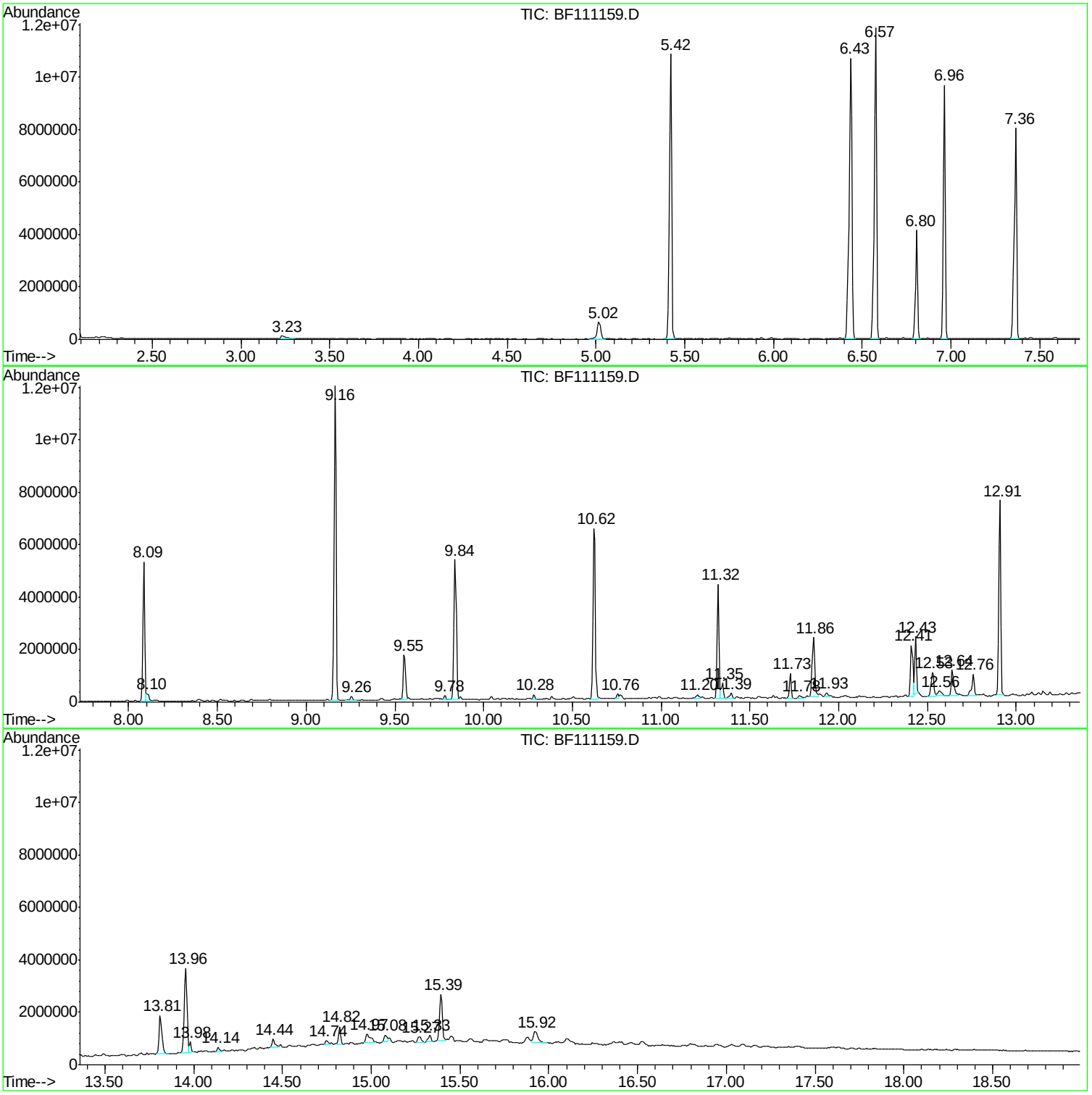
Instrument : BNA_F
ClientSampleId : BU-03-120418-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111159.D
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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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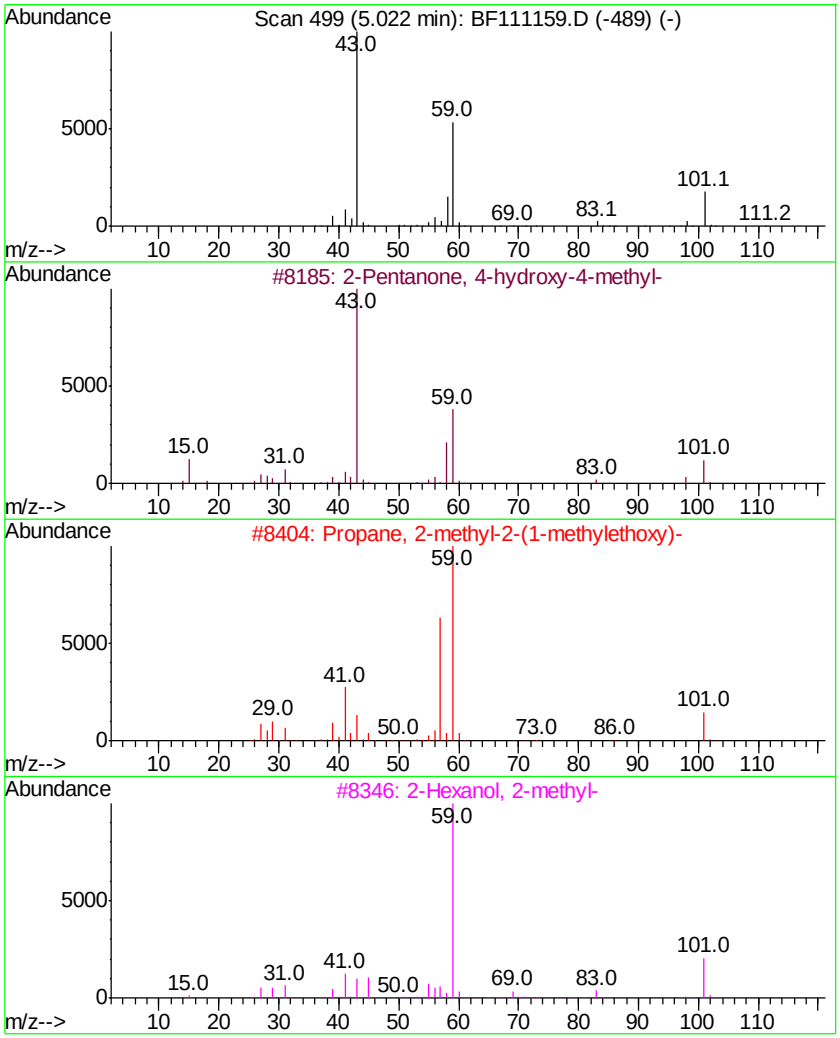
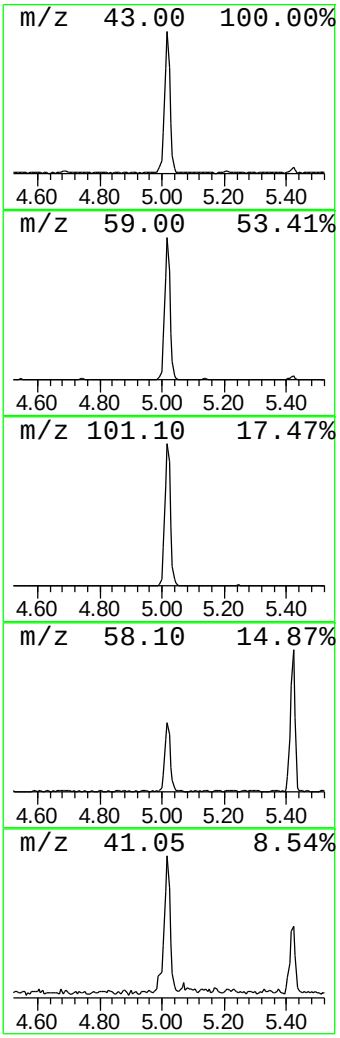
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	5.13 ng	823939	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111159.D
Acq On : 7 Dec 2018 00:55
Operator : JU/SJ
Sample : J6188-01
Misc :
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Instrument : BNA_F
ClientSampleId : BU-03-120418-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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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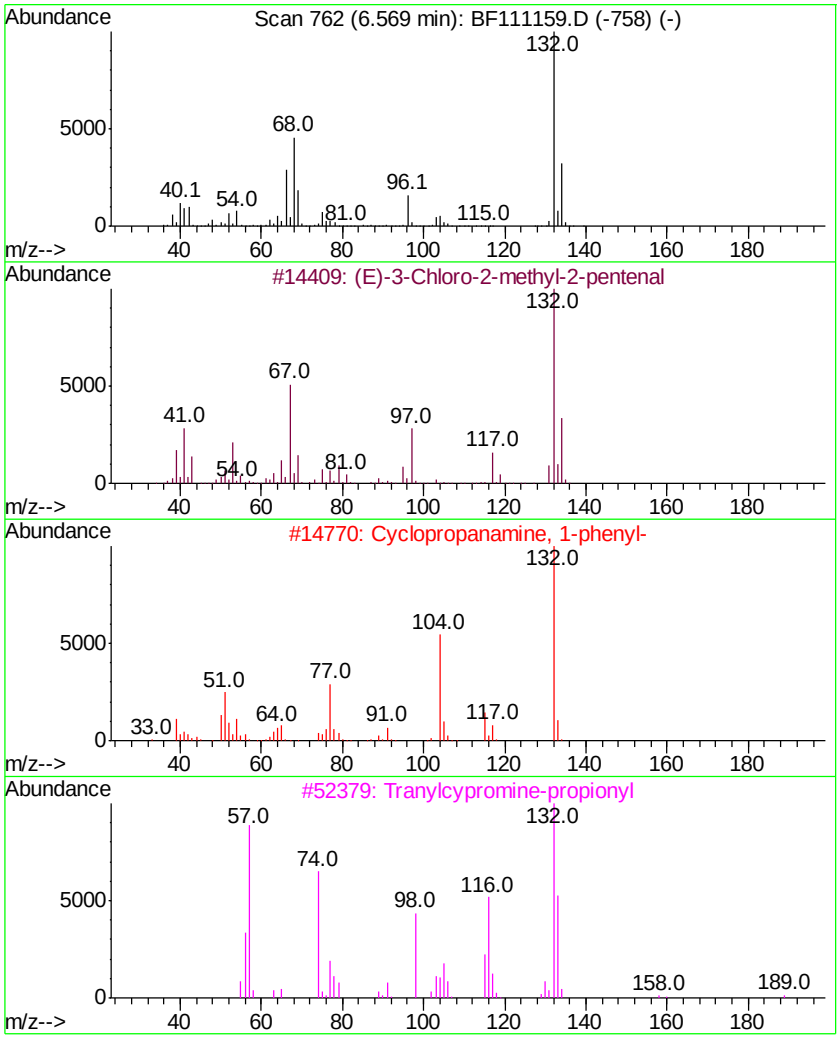
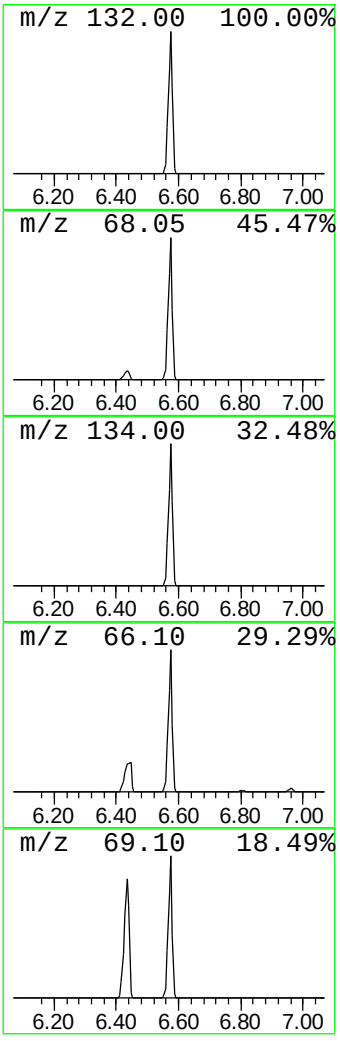
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	69.86 ng	11222300	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9





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Acq On : 7 Dec 2018 00:55
Operator : JU/SJ
Sample : J6188-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-120418-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

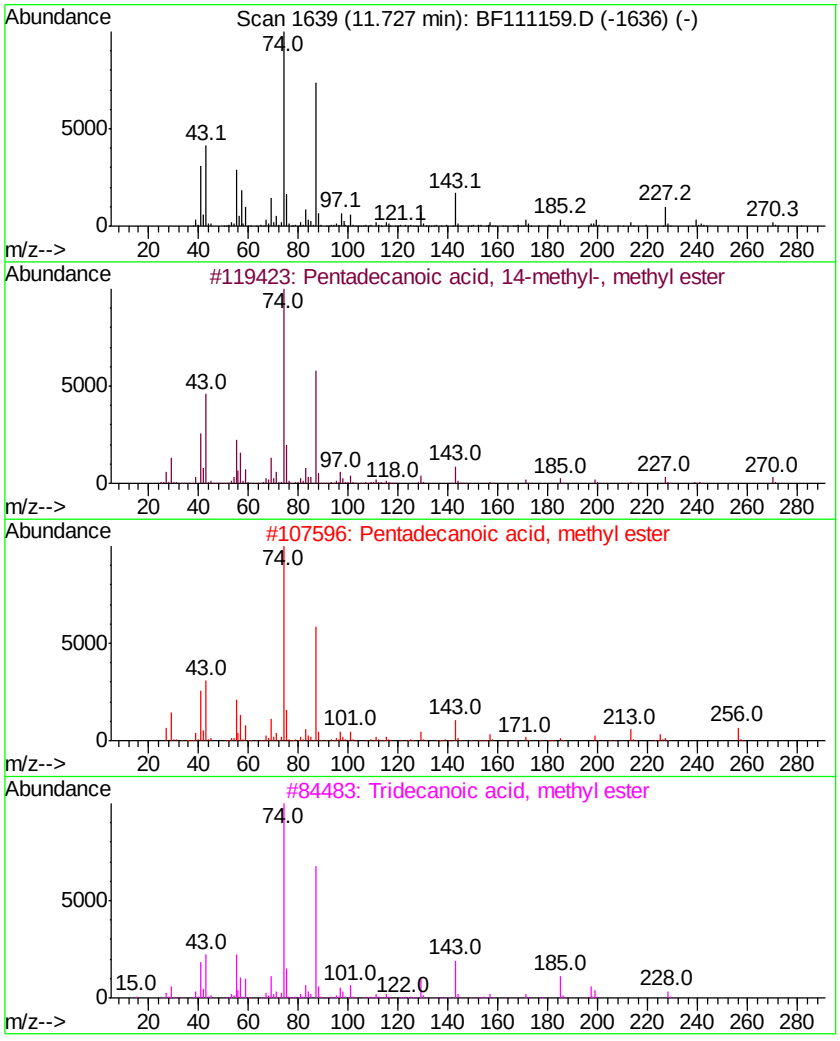
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

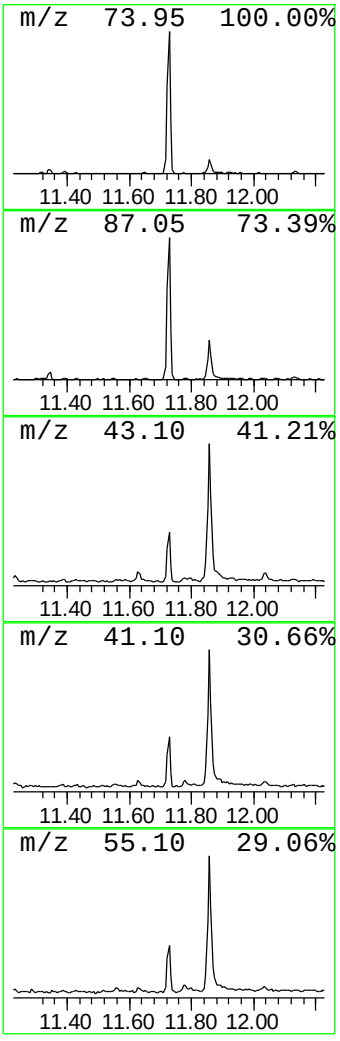
****

Peak Number 4 Pentadecanoic acid, 14-meth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	3.99 ng	714135	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





Library Search Compound Report

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Sample : J6188-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-120418-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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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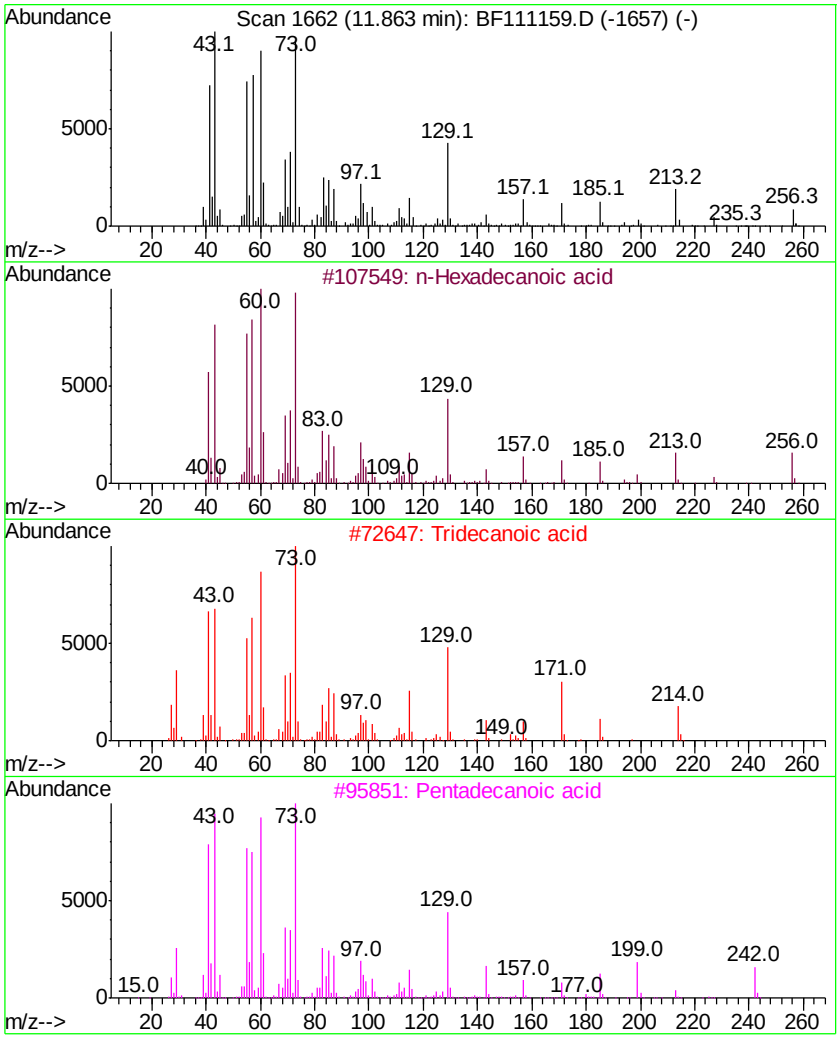
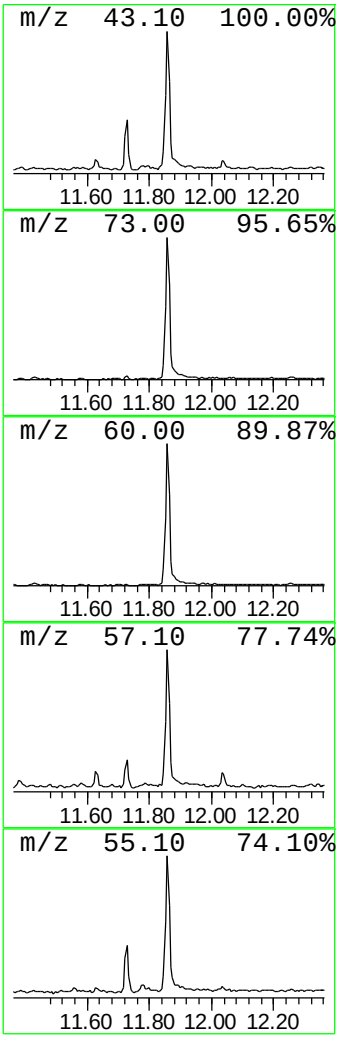
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	11.75 ng	2101840	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	87





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Operator : JU/SJ
Sample : J6188-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-120418-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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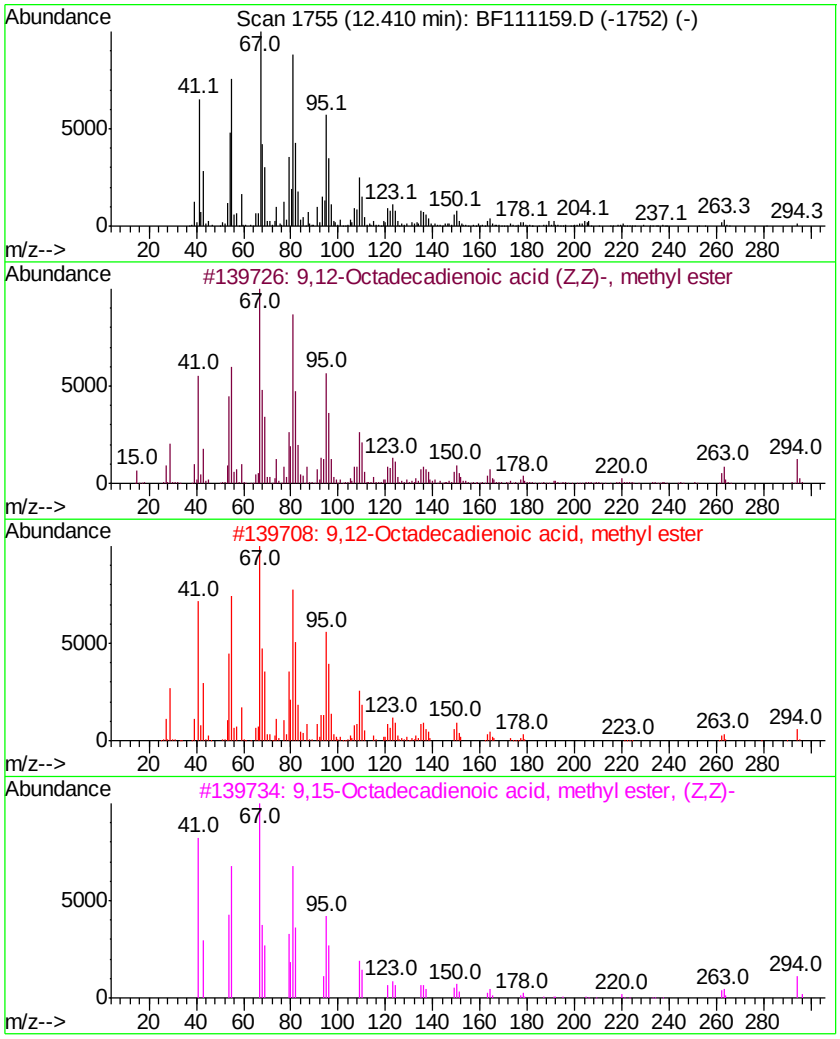
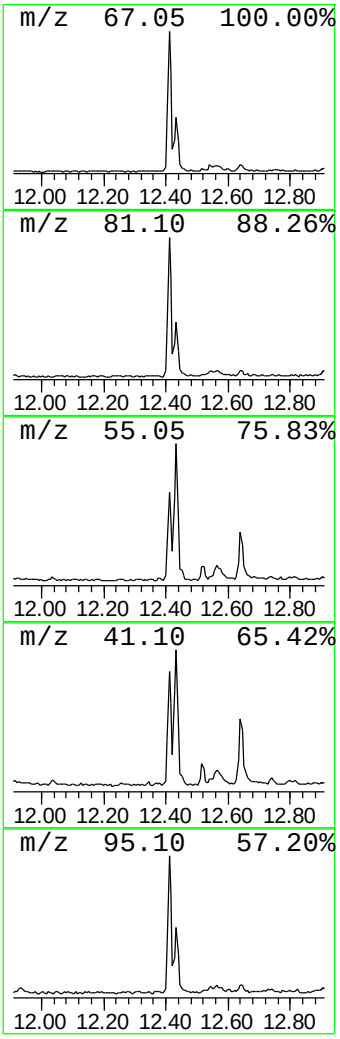
Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	9.43 ng	1686460	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
4	9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	93
5	7-Hexadecyne	222	C16H30	074685-28-2	93





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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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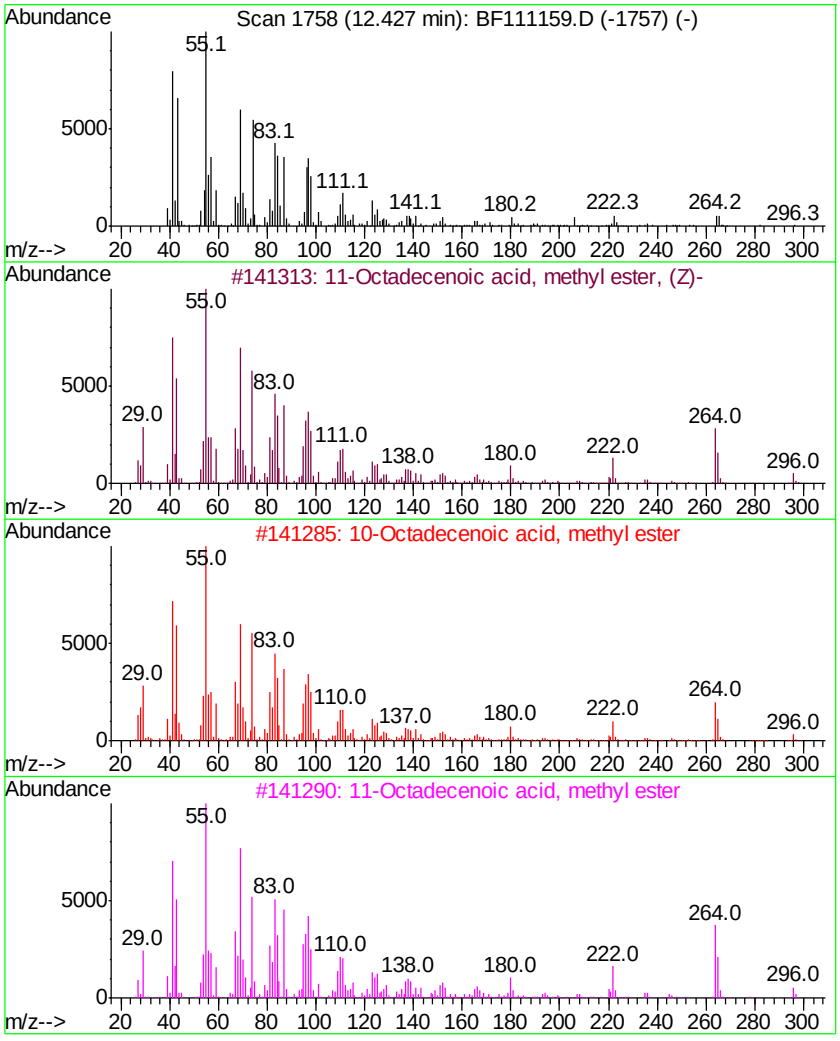
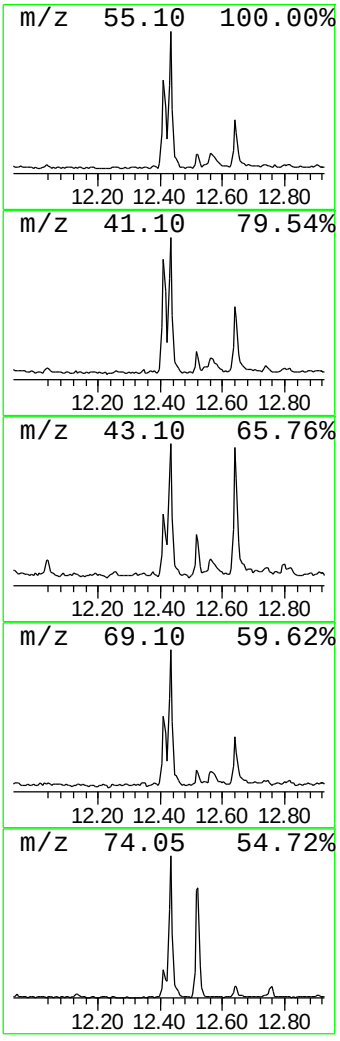
Peak Number 7 11-Octadecenoic acid, methy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	8.95 ng	1601910	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	98
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	96
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	96





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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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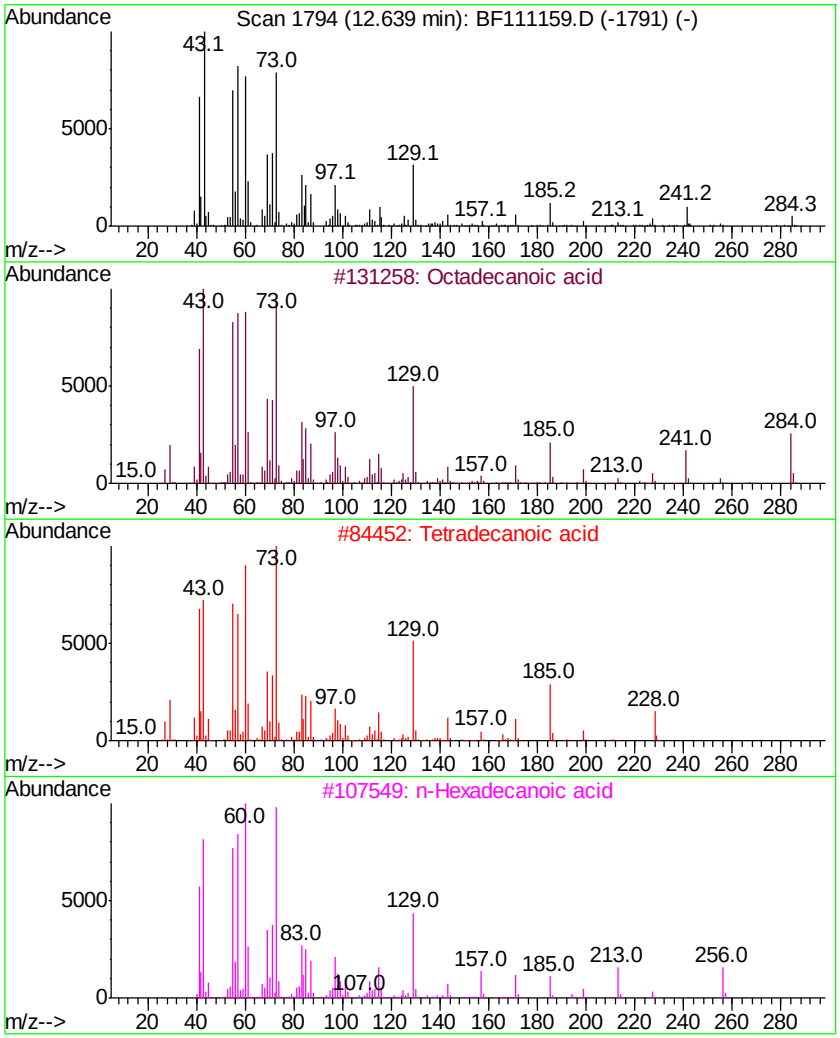
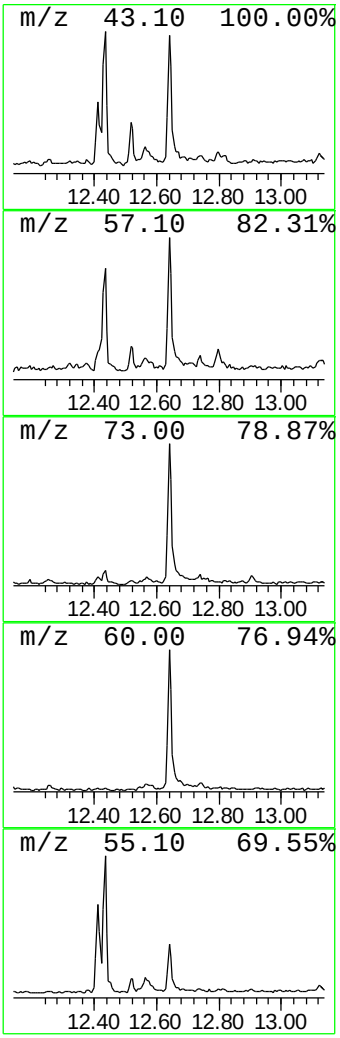
Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	6.15 ng	998391	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Data File : BF111159.D
Acq On : 7 Dec 2018 00:55
Operator : JU/SJ
Sample : J6188-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-120418-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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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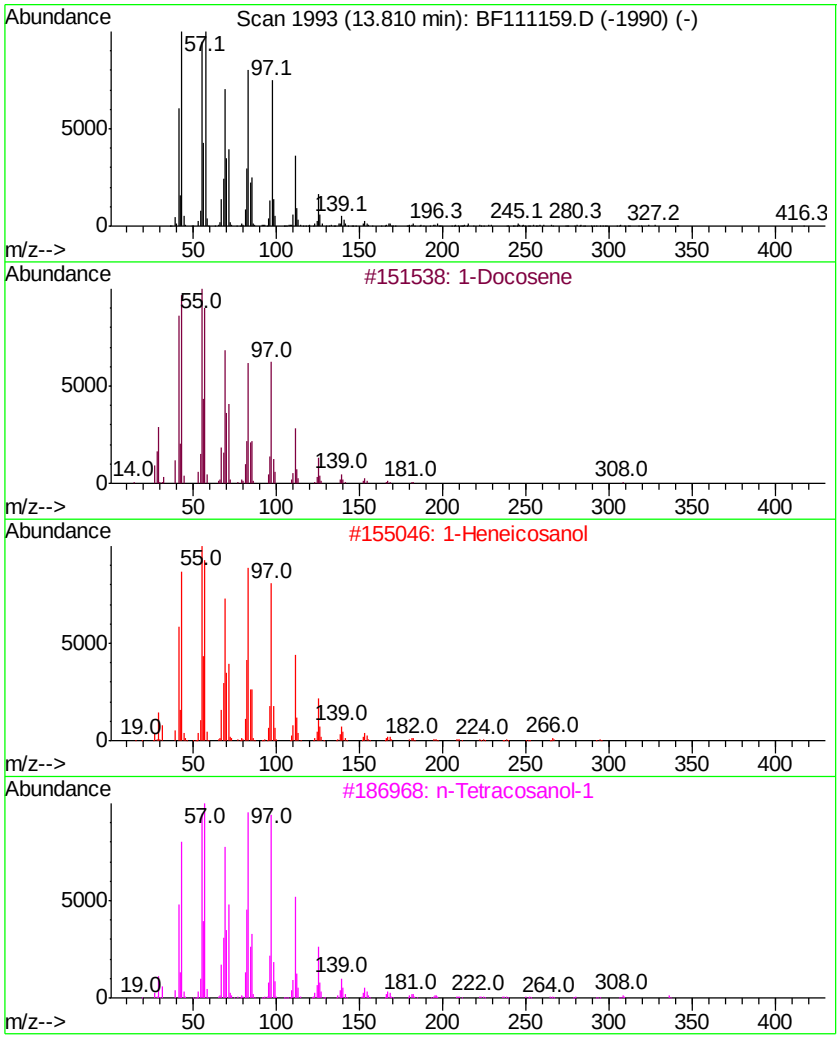
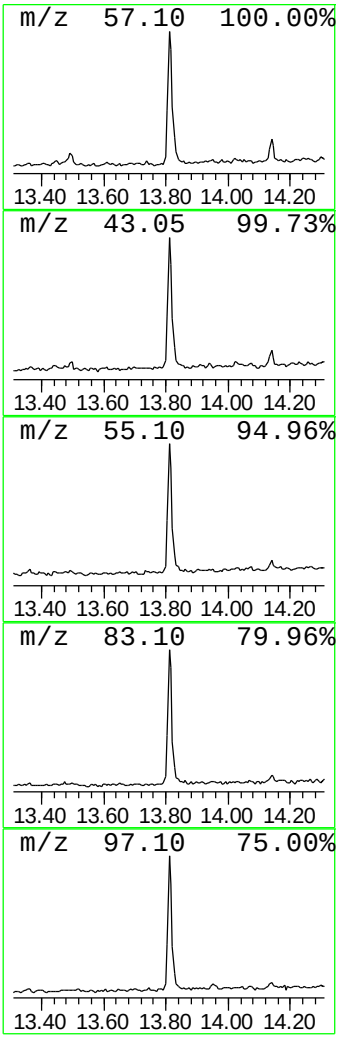
Peak Number 9 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	9.30 ng	1509820	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5	Cyclotetracosane	336	C24H48	000297-03-0	91





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Acq On : 7 Dec 2018 00:55
Operator : JU/SJ
Sample : J6188-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-120418-A

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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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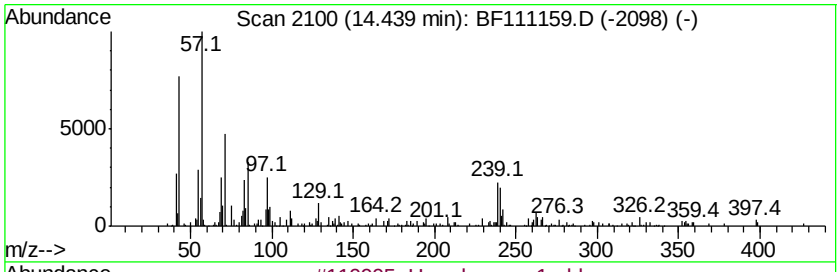
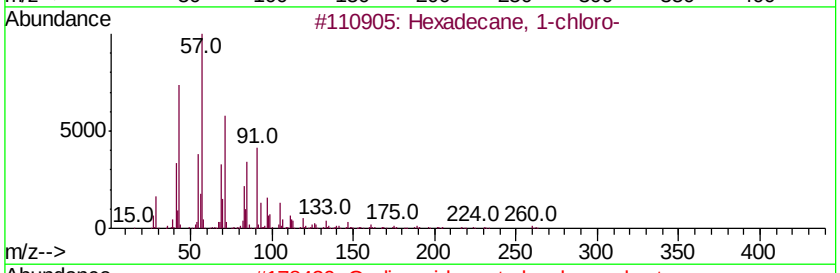
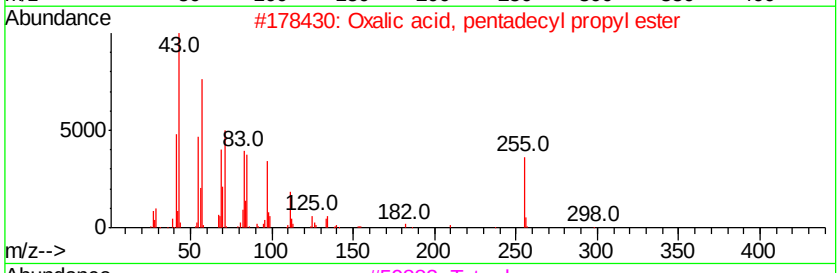
Peak Number 10 Hexadecane, 1-chloro- Concentration Rank 14

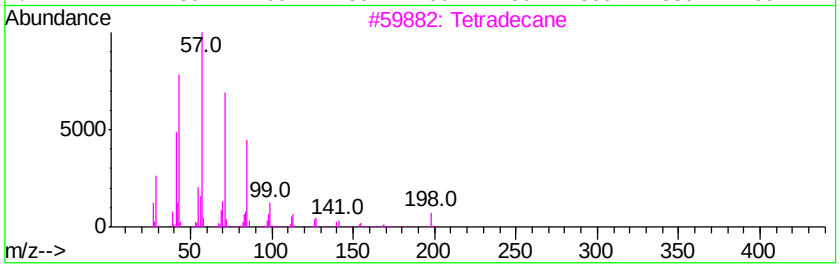
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.33 ng	378366	Chrysene-d12	13.96

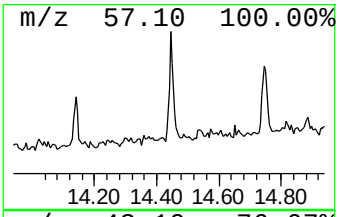
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	81
2	Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	64
3	Tetradecane	198	C14H30	000629-59-4	64
4	Eicosane	282	C20H42	000112-95-8	60
5	Nonadecane	268	C19H40	000629-92-5	60

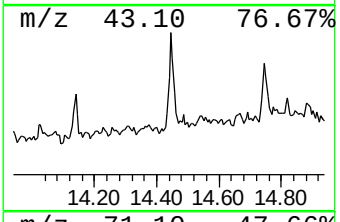


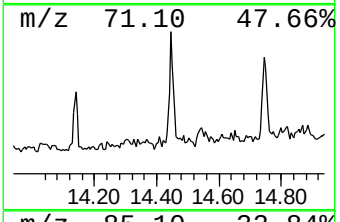


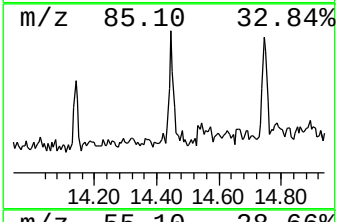


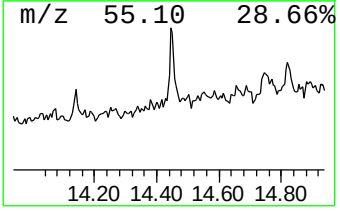












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Data File : BF111159.D
Acq On : 7 Dec 2018 00:55
Operator : JU/SJ
Sample : J6188-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-120418-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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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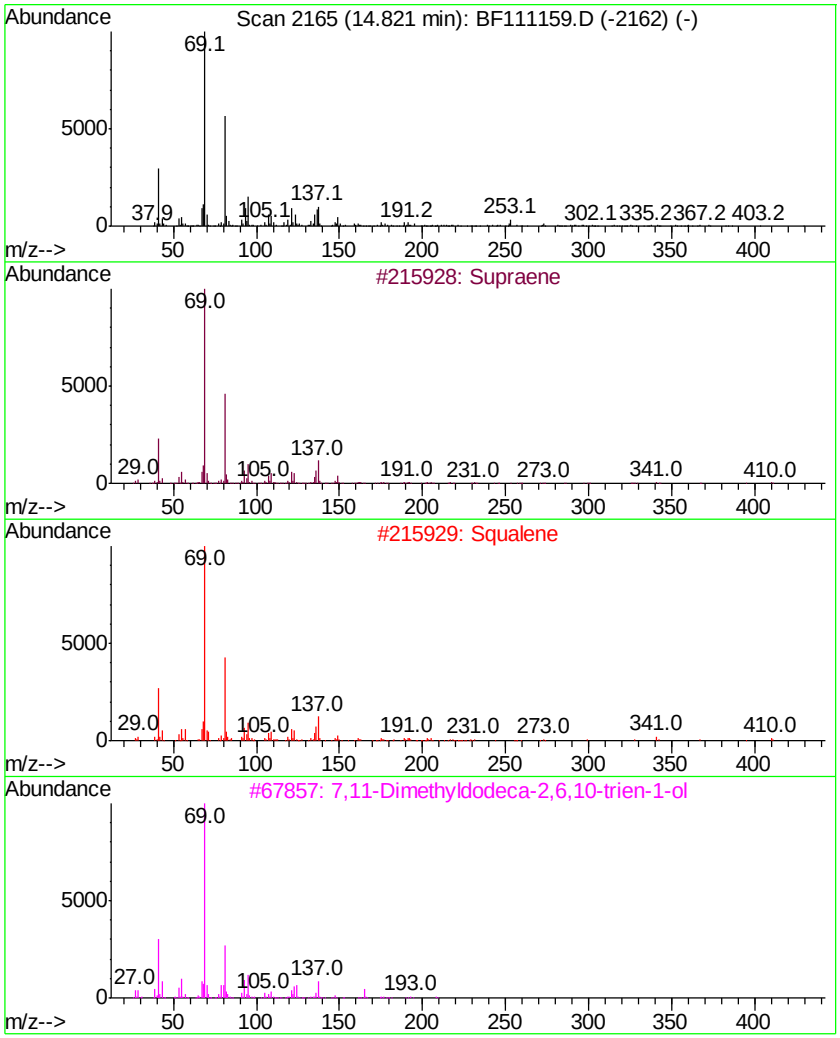
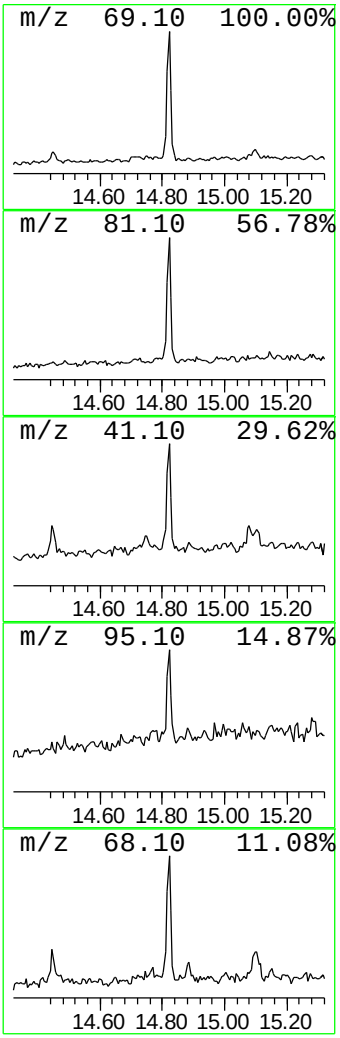
Peak Number 11 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	5.39 ng	574621	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	74
2	Squalene	410	C30H50	000111-02-4	72
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	58
5	trans-Geranylgeraniol	290	C20H34O	024034-73-9	53





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Operator : JU/SJ
Sample : J6188-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-120418-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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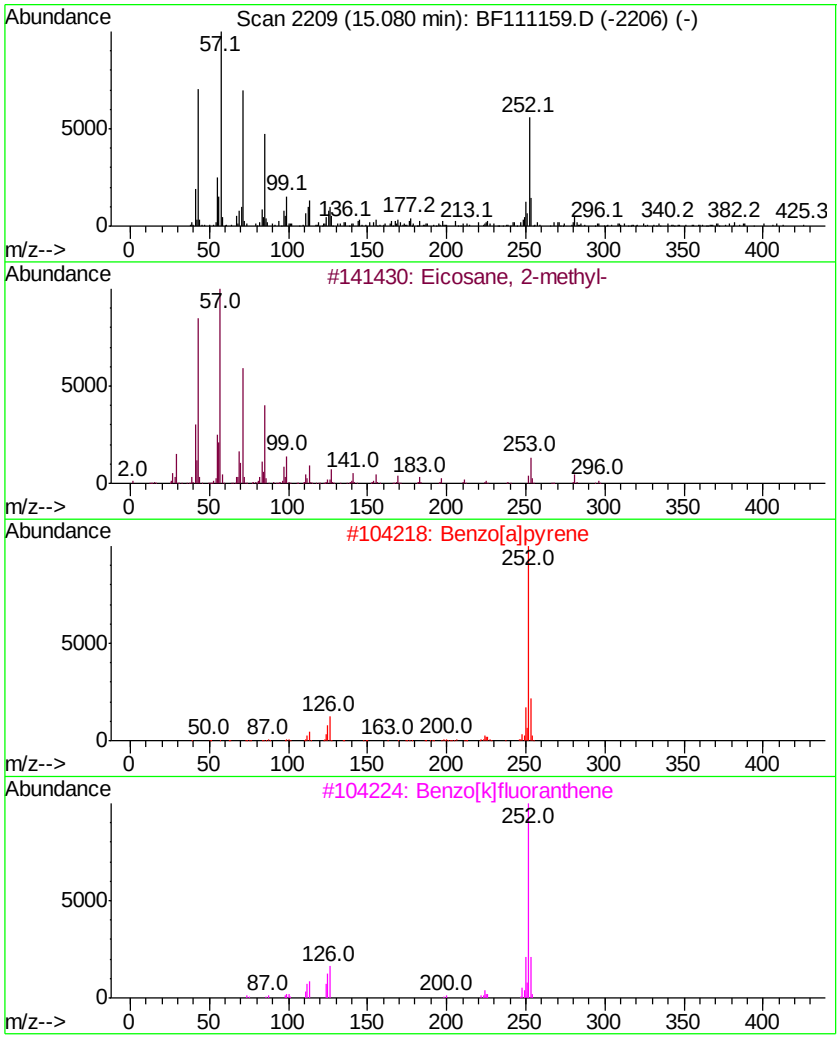
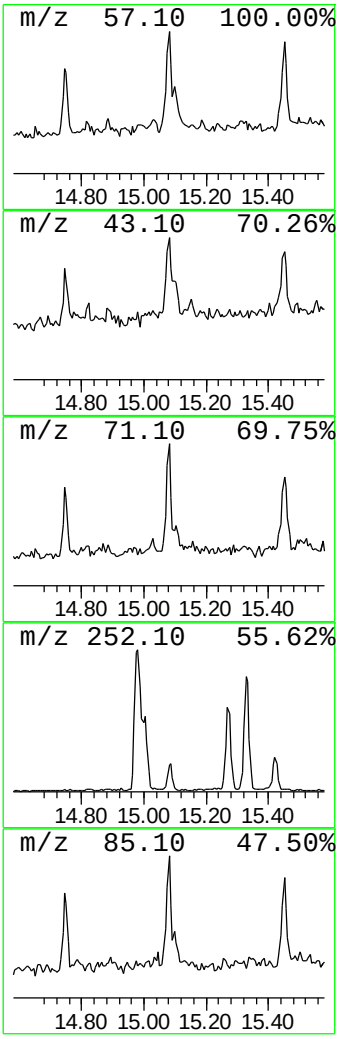
Peak Number 12 Eicosane, 2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	2.38 ng	253499	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 2-methyl-	296	C21H44	001560-84-5	62
2	Benzo[a]pyrene	252	C20H12	000050-32-8	58
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	50
4	Hexadecane	226	C16H34	000544-76-3	50
5	Nonadecane	268	C19H40	000629-92-5	45





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Operator : JU/SJ
Sample : J6188-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-120418-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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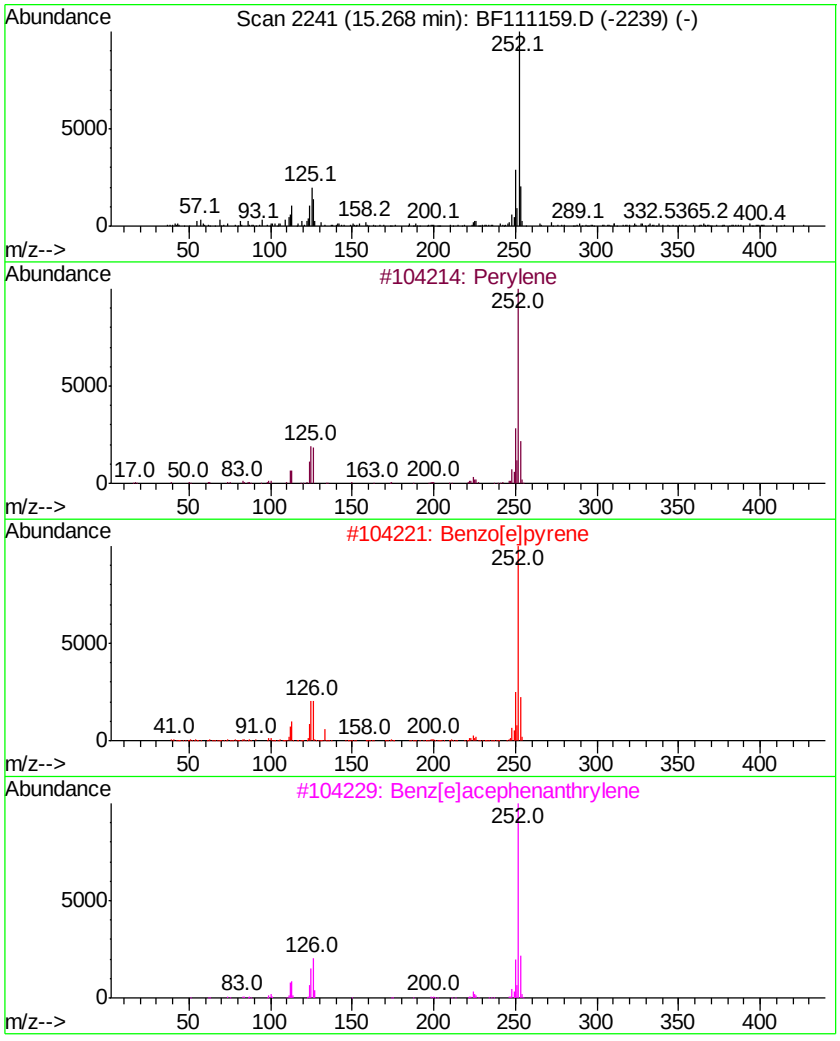
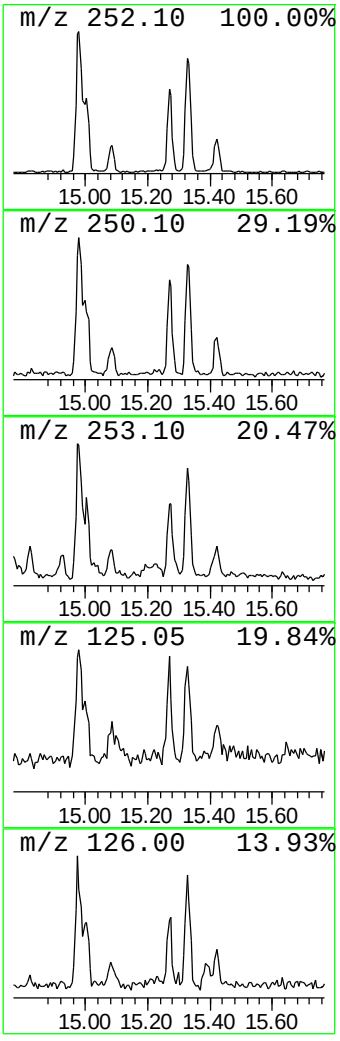
Peak Number 13 Perylene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	2.54 ng	270415	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	96
2	Benzo[e]pyrene	252	C20H12	000192-97-2	95
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111159.D
Acq On : 7 Dec 2018 00:55
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Sample : J6188-01
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ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-120418-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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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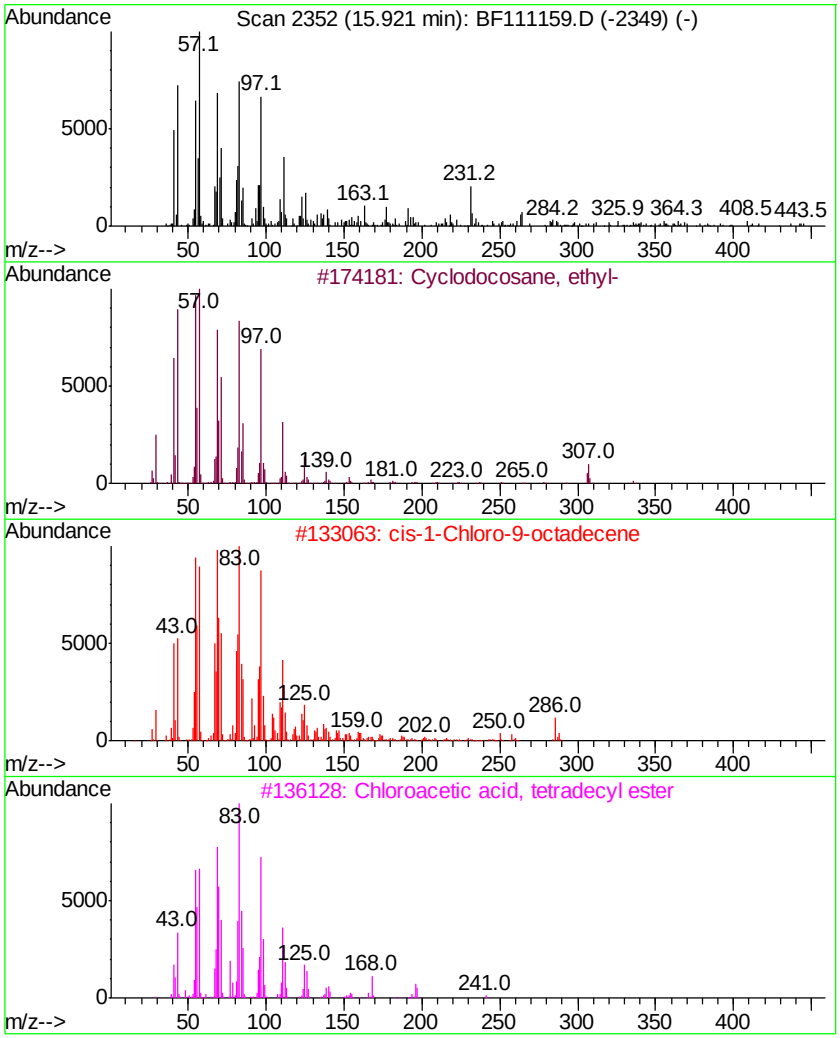
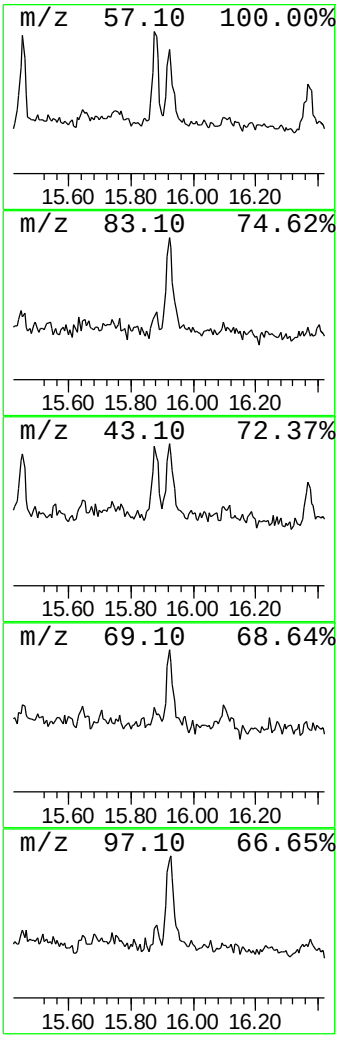
Peak Number 14 Cyclodocosane, ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	7.10 ng	756891	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	94
2	cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	87
3	Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	80
4	Fumaric acid, octadecyl 2,2,3,3,...	582	C27H42F8O4	1000348-79-4	72
5	Octacosanol	410	C28H58O	000557-61-9	64





Tentatively Identified Compound (LSC) summary

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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : BU-03-120418-A

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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...	5.02	5.1	ng	823939	1	6.80	3212650	20.0
unknown6.57	6.57	69.9	ng	11222300	1	6.80	3212650	20.0
Pentadecanoic aci...	11.73	4.0	ng	714135	4	11.32	3577790	20.0
n-Hexadecanoic acid	11.86	11.8	ng	2101840	4	11.32	3577790	20.0
9,12-Octadecadien...	12.41	9.4	ng	1686460	4	11.32	3577790	20.0
11-Octadecenoic a...	12.43	8.9	ng	1601910	4	11.32	3577790	20.0
Octadecanoic acid	12.64	6.2	ng	998391	5	13.96	3245460	20.0
1-Docosene	13.81	9.3	ng	1509820	5	13.96	3245460	20.0
Hexadecane, 1-chl...	14.44	2.3	ng	378366	5	13.96	3245460	20.0
Supraene	14.82	5.4	ng	574621	6	15.39	2131350	20.0
Eicosane, 2-methyl-	15.08	2.4	ng	253499	6	15.39	2131350	20.0
Perylene	15.27	2.5	ng	270415	6	15.39	2131350	20.0
Cyclodocosane, et...	15.92	7.1	ng	756891	6	15.39	2131350	20.0