LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111166.D
Acq On : 7 Dec 2018 4:06
Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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	5.004	488	496	502	rBV	351721	437754	6.62%	0.606%
2	5.422	562	567	570	rBV	6242027	6115814	92.49%	8.460%
3	6.434	734	739	748	rBV	7100423	6612398	100.00%	9.147%
4	6.575	759	763	766	rBV	7287671	6163417	93.21%	8.526%
5	6.810	799	803	806	rBV	3872030	3251922	49.18%	4.499%
6	6.963	825	829	833	rBV	5334517	4425602	66.93%	6.122%
7	7.363	890	897	900	rBV	4538105	3765718	56.95%	5.209%
8	8.086	1017	1020	1024	rBV	4572491	4004883	60.57%	5.540%
9	8.392	1065	1072	1075	rBV5	49278	73552	1.11%	0.102%
10	8.522	1091	1094	1097	rBV	98104	94147	1.42%	0.130%
11	8.692	1119	1123	1126	rBV	156936	141573	2.14%	0.196%
12	9.122	1194	1196	1199	rVB2	82431	69829	1.06%	0.097%
13	9.163	1200	1203	1207	rVV	6097665	5039365	76.21%	6.971%
14	9.257	1216	1219	1223	rBV2	212207	187947	2.84%	0.260%
15	9.422	1243	1247	1252	rBV7	51379	84523	1.28%	0.117%
16	9.504	1256	1261	1263	rBV5	69501	94452	1.43%	0.131%
17	9.557	1267	1270	1273	rBV	442320	374812	5.67%	0.518%
18	9.786	1306	1309	1313	rVB	223632	166334	2.52%	0.230%
19	9.845	1313	1319	1322	rBV	4189173	3582906	54.18%	4.956%
20	10.286	1391	1394	1396	rVB	218166	175856	2.66%	0.243%
21	10.504	1428	1431	1434	rBV	102063	99449	1.50%	0.138%
22	10.627	1448	1452	1455	rBV	2983574	2657318	40.19%	3.676%
23	10.757	1471	1474	1476	rBV	261608	246207	3.72%	0.341%
24	11.204	1547	1550	1553	rBV	204833	174264	2.64%	0.241%
25	11.239	1554	1556	1561	rVB	138041	114348	1.73%	0.158%
26	11.327	1567	1571	1573	rBV	3253519	3005977	45.46%	4.158%
27	11.345	1573	1574	1577	rVV	298968	224082	3.39%	0.310%
28	11.398	1581	1583	1586	rVB	100761	83192	1.26%	0.115%
29	11.633	1620	1623	1625	rBV	176351	150184	2.27%	0.208%
30	11.727	1636	1639	1643	rBV	1640490	1347164	20.37%	1.864%
31	11.857	1658	1661	1666	rBV	918746	761257	11.51%	1.053%
32	11.939	1671	1675	1677	rBV2	135336	155229	2.35%	0.215%
33	12.039	1690	1692	1694	rBV	161373	120012	1.81%	0.166%
34	12.380	1747	1750	1752	rBV	124141	110472	1.67%	0.153%

LSC Area Percent Report

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Acq On : 7 Dec 2018 4:06
Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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	12.416	1752	1756	1758	rBV	6207407	5311087	80.32%	7.347%
36	12.439	1758	1760	1762	rVB	3394373	2683920	40.59%	3.713%
37	12.521	1771	1774	1780	rBV2	622674	957302	14.48%	1.324%
38	12.645	1792	1795	1800	rVB	431395	405069	6.13%	0.560%
39	12.763	1811	1815	1818	rBV	491748	452144	6.84%	0.625%
40	12.910	1837	1840	1843	rBV	4198647	3388923	51.25%	4.688%
41	13.157	1879	1882	1887	rVB3	287552	278903	4.22%	0.386%
42	13.498	1938	1940	1943	rBV	323765	269311	4.07%	0.373%
43	13.827	1993	1996	2002	rVB2	431460	519581	7.86%	0.719%
44	13.963	2015	2019	2022	rBV	2600166	2471958	37.38%	3.420%
45	15.404	2261	2264	2268	rVB	1261294	1438660	21.76%	1.990%

Sum of corrected areas: 72288817

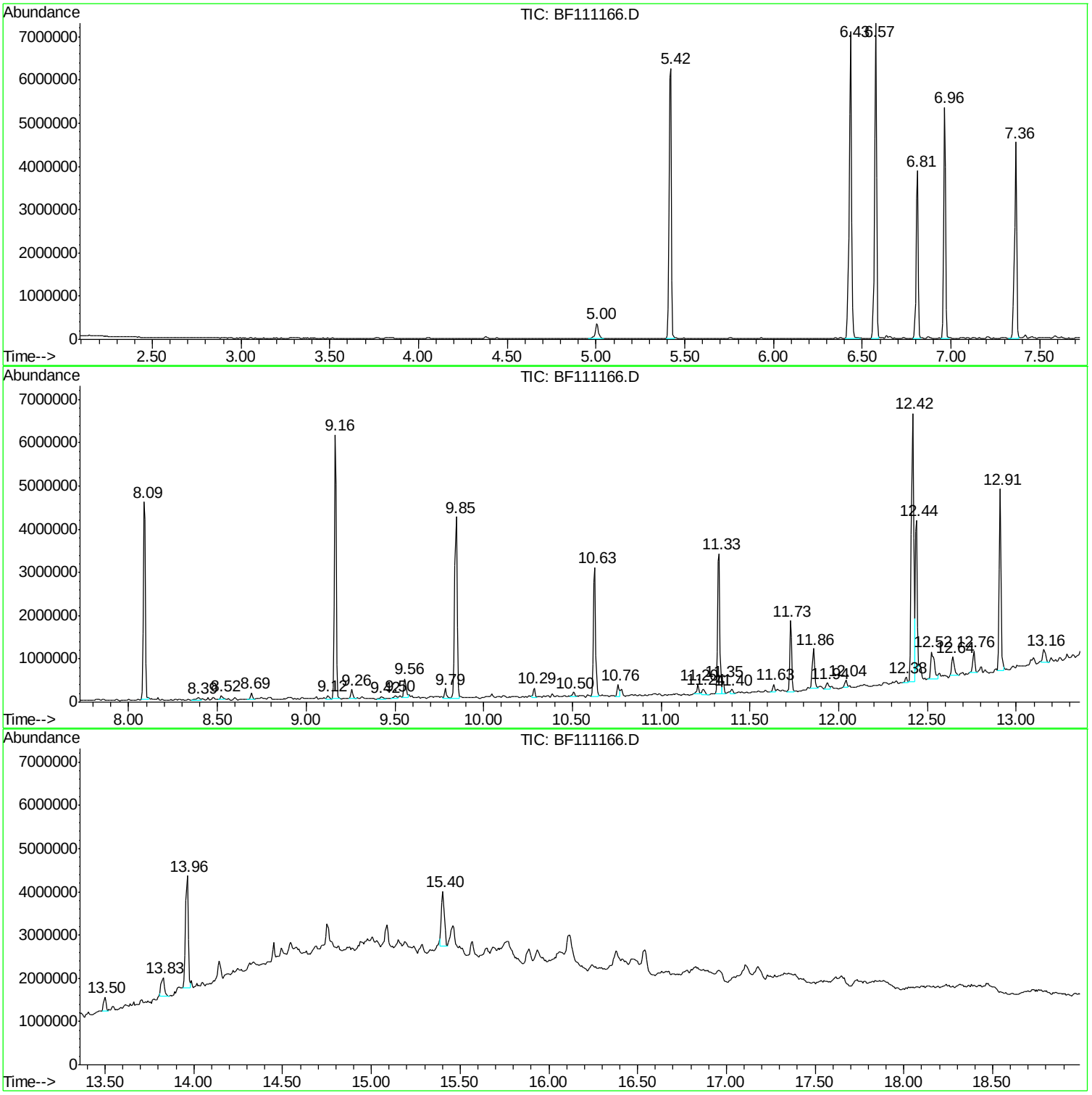
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111166.D
Acq On : 7 Dec 2018 4:06
Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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 : BF111166.D
Acq On : 7 Dec 2018 4:06
Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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

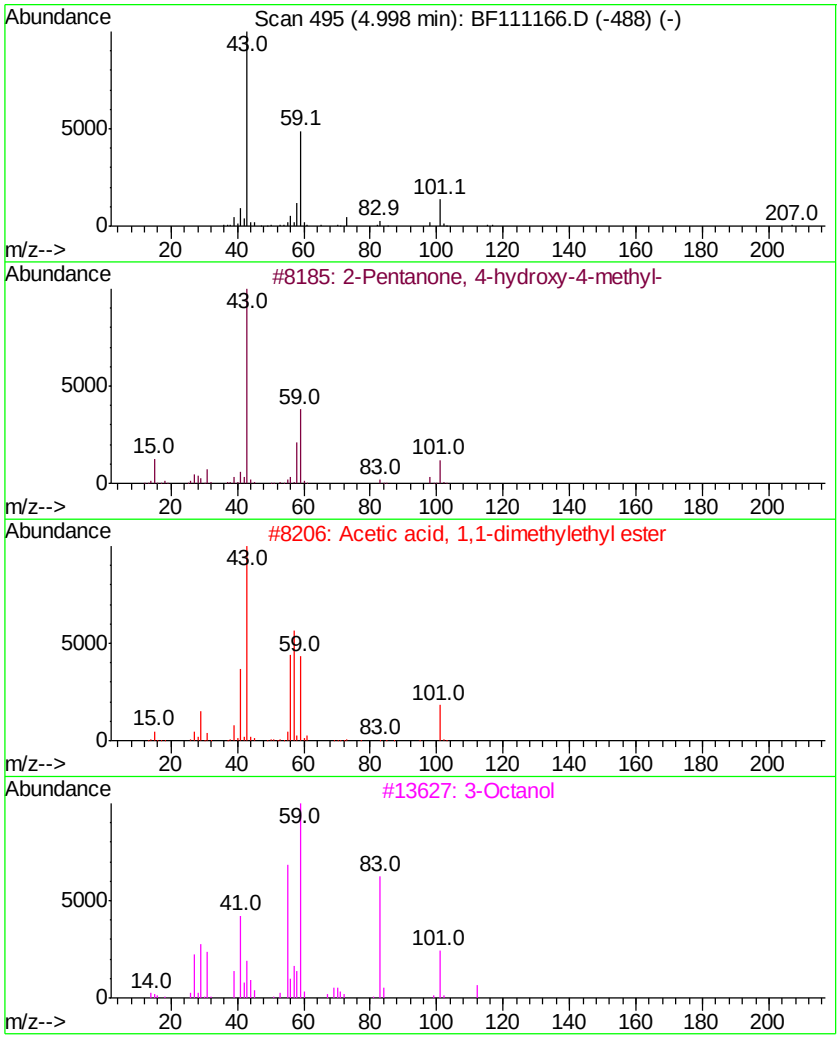
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

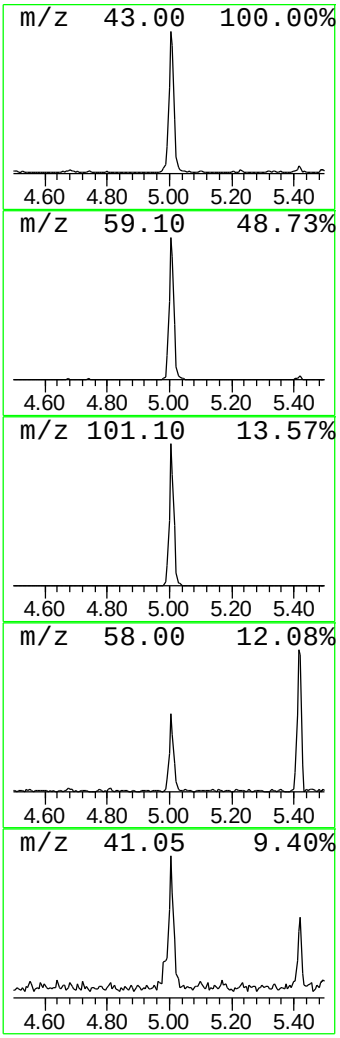
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.69 ng	437754	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Octanol	130	C8H18O	000589-98-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	dl-Erythro-O-methylthreonine	133	C5H11NO3	1000214-70-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111166.D
Acq On : 7 Dec 2018 4:06
Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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

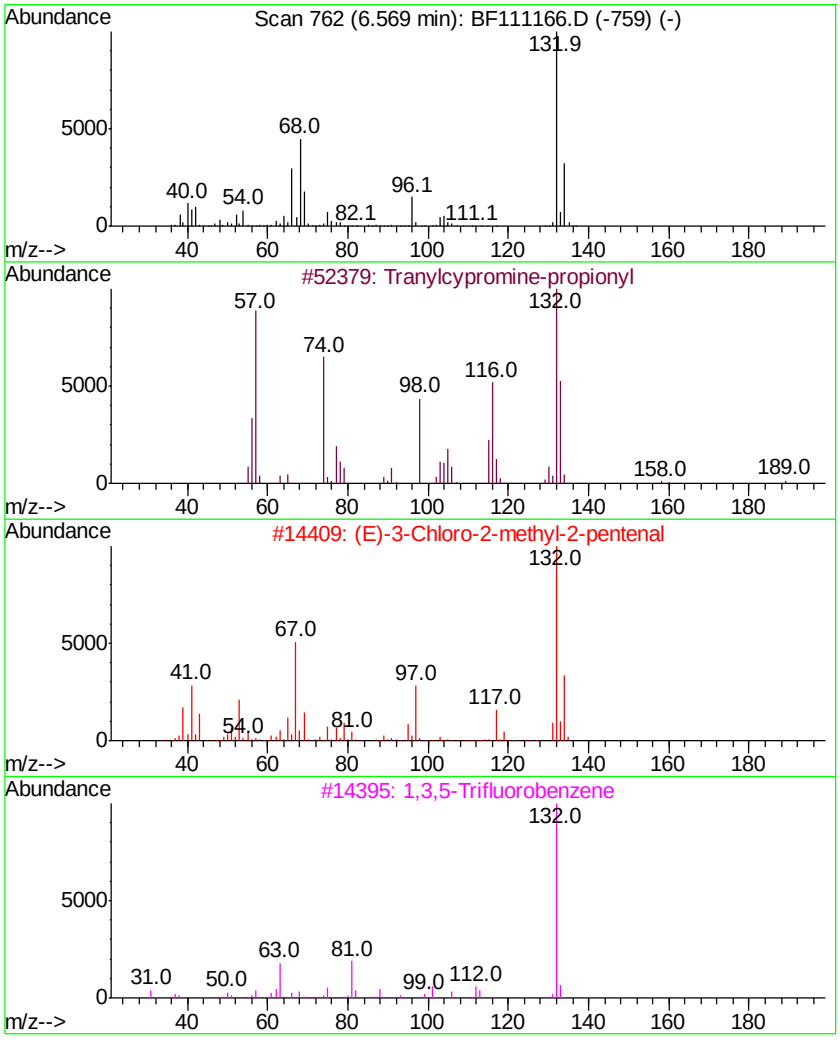
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

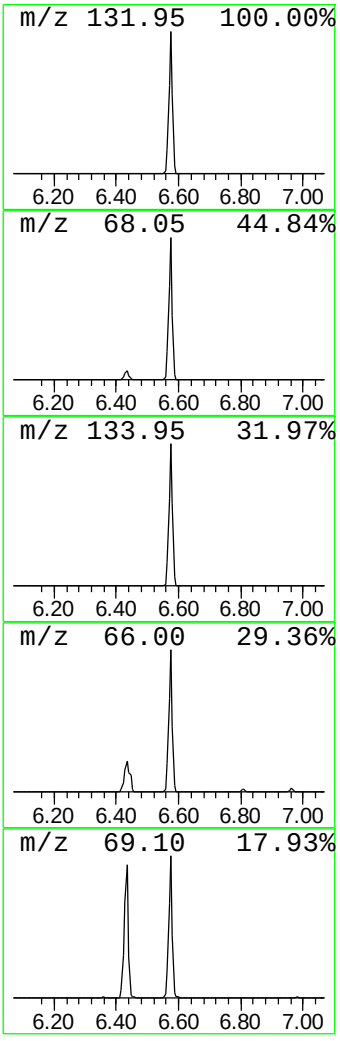
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	37.91 ng	6163420	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111166.D
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Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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

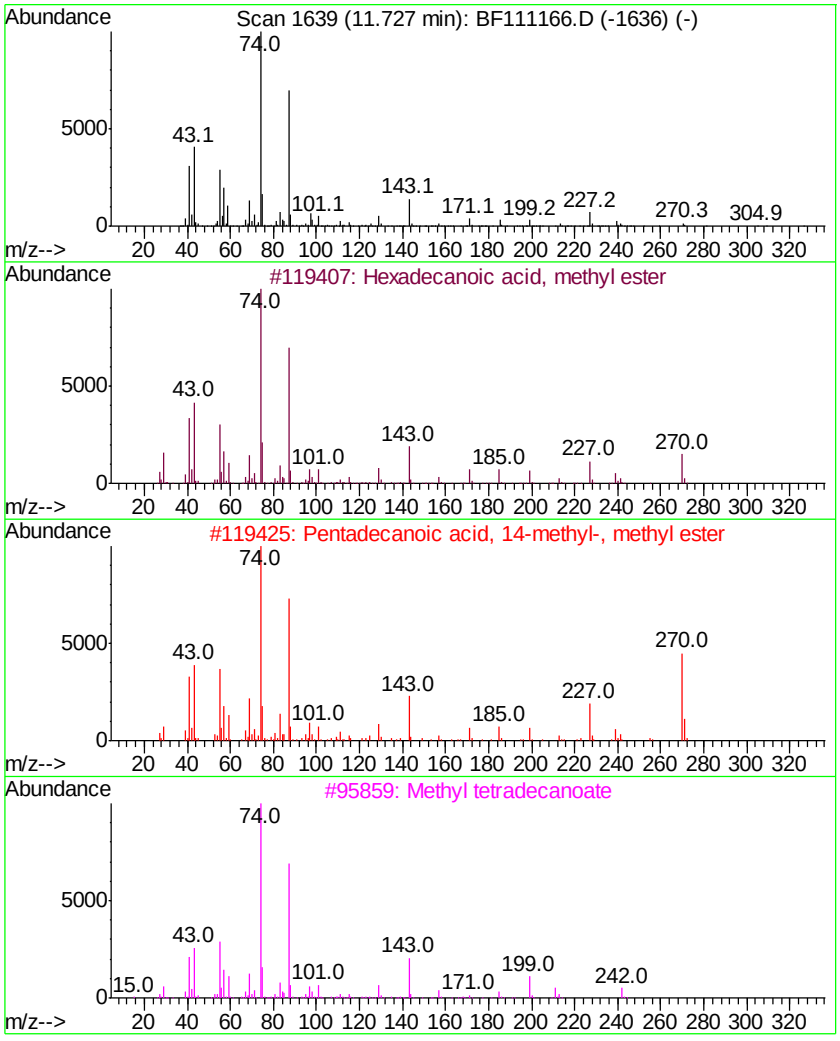
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

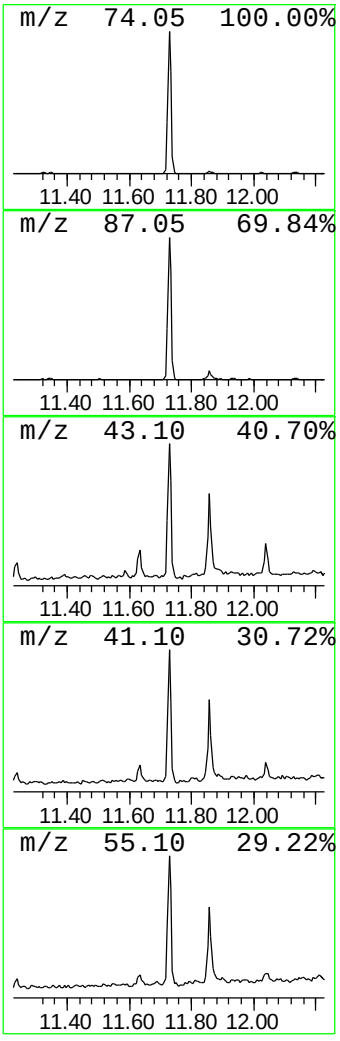
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	8.96 ng	1347160	Phenanthrene-d10	11.33

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	96
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90





Library Search Compound Report

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

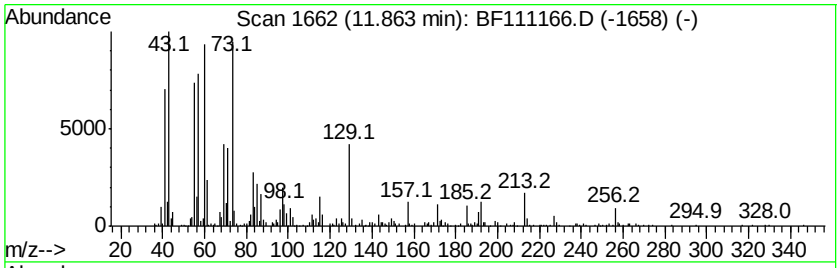
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

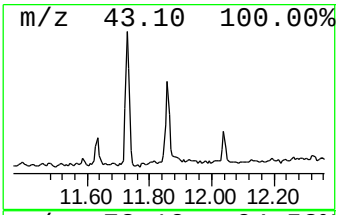
****

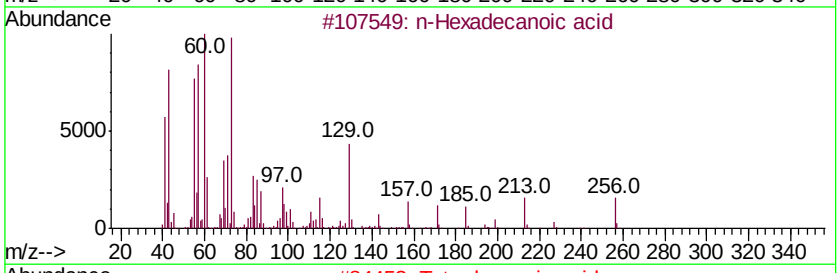
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

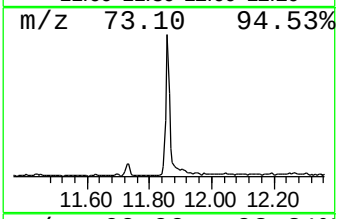
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	5.06 ng	761257	Phenanthrene-d10	11.33

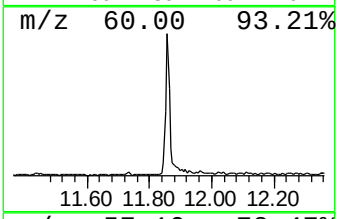
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	95
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58

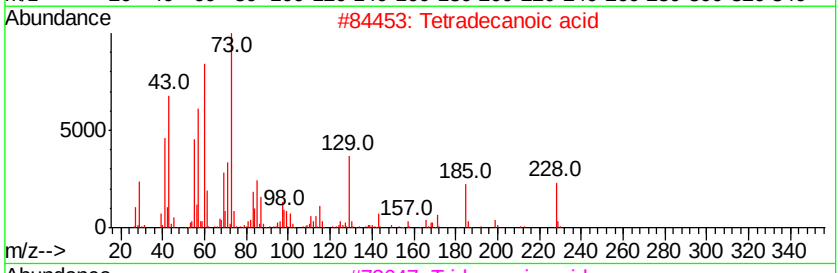


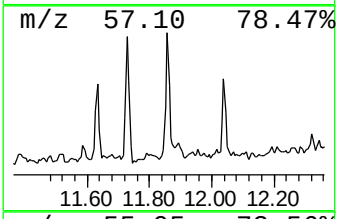


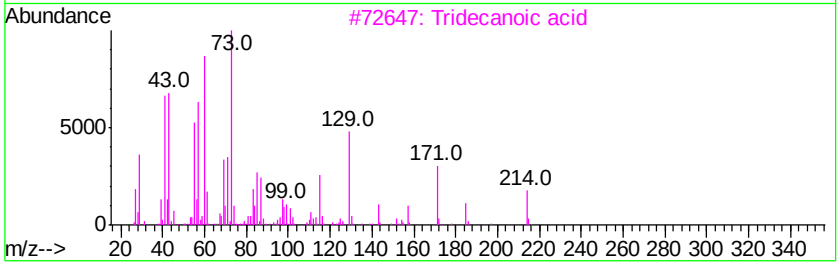


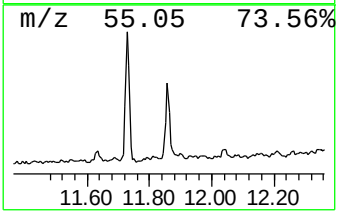












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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

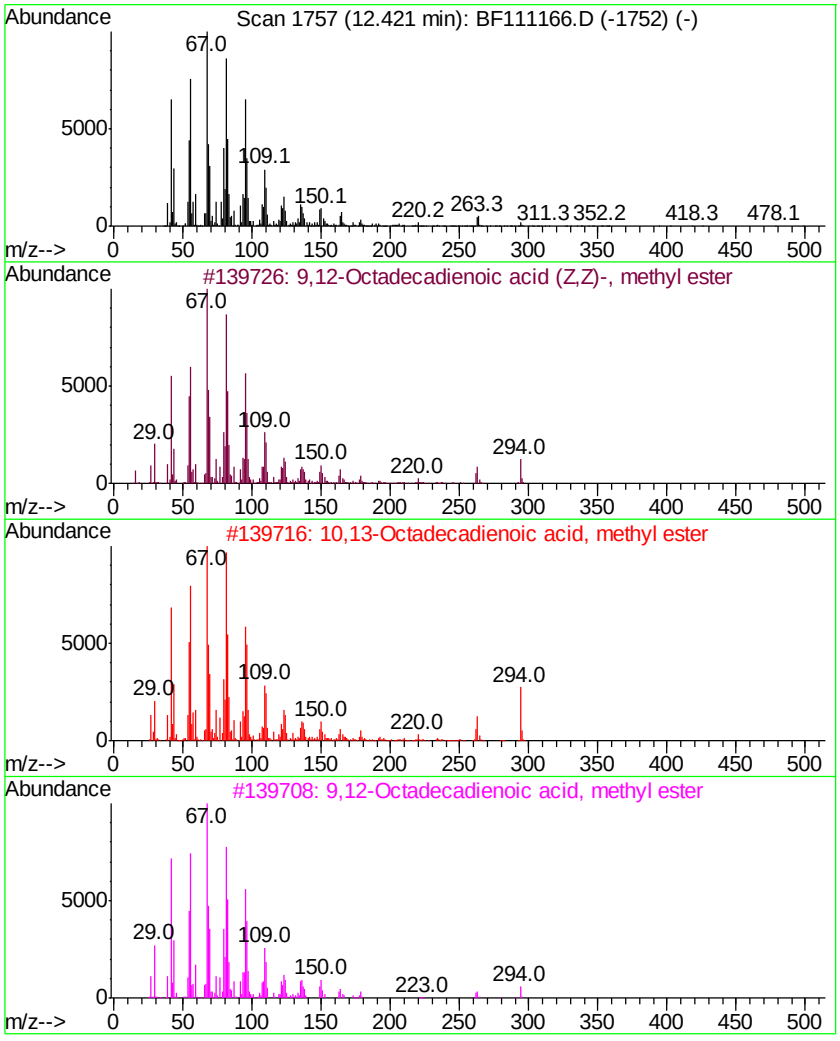
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

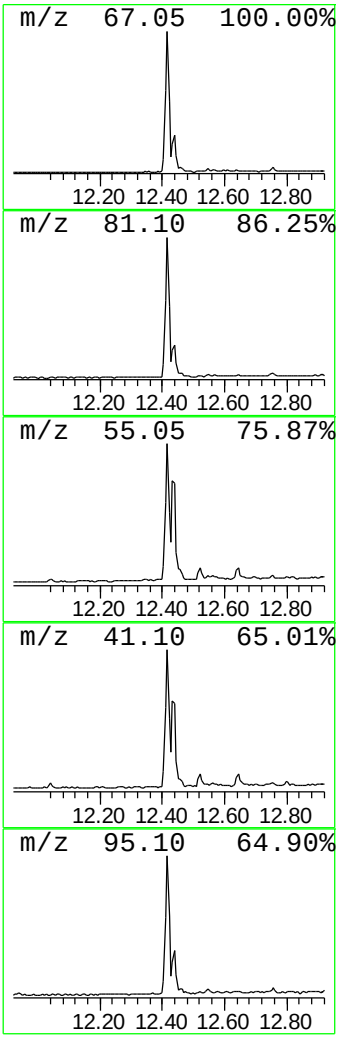
****

Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	35.34 ng	5311090	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	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 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99





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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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

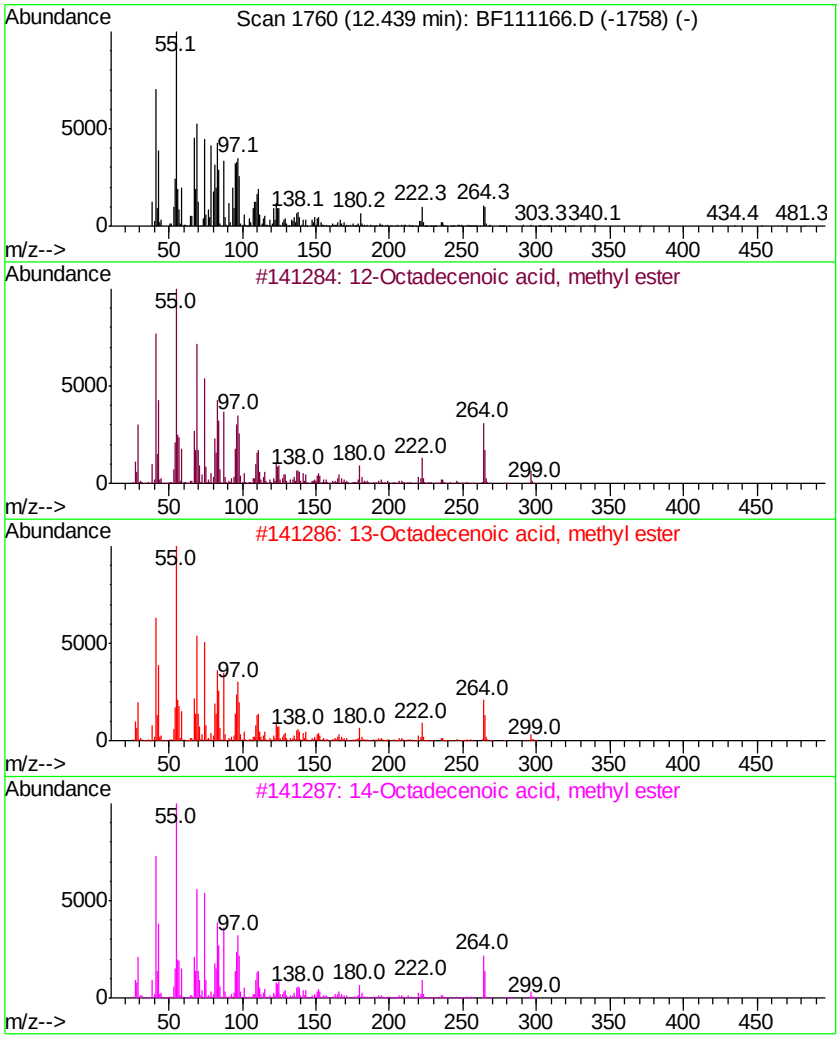
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

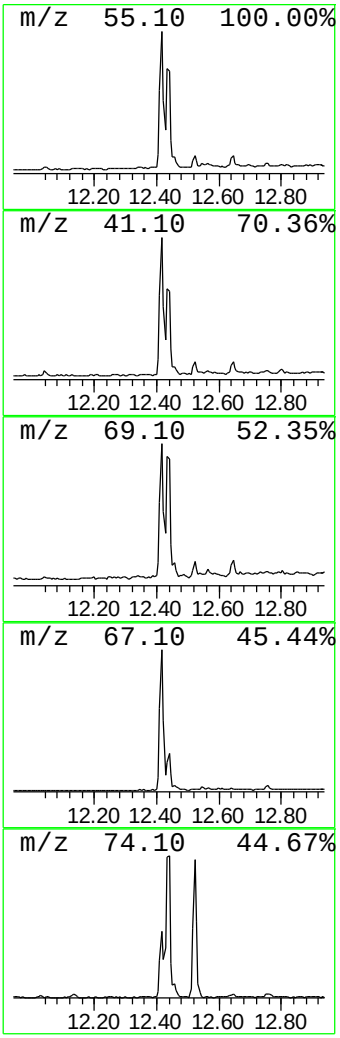
****

Peak Number 7 12-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	17.86 ng	2683920	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	97
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	97
5	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	95





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111166.D
Acq On : 7 Dec 2018 4:06
Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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

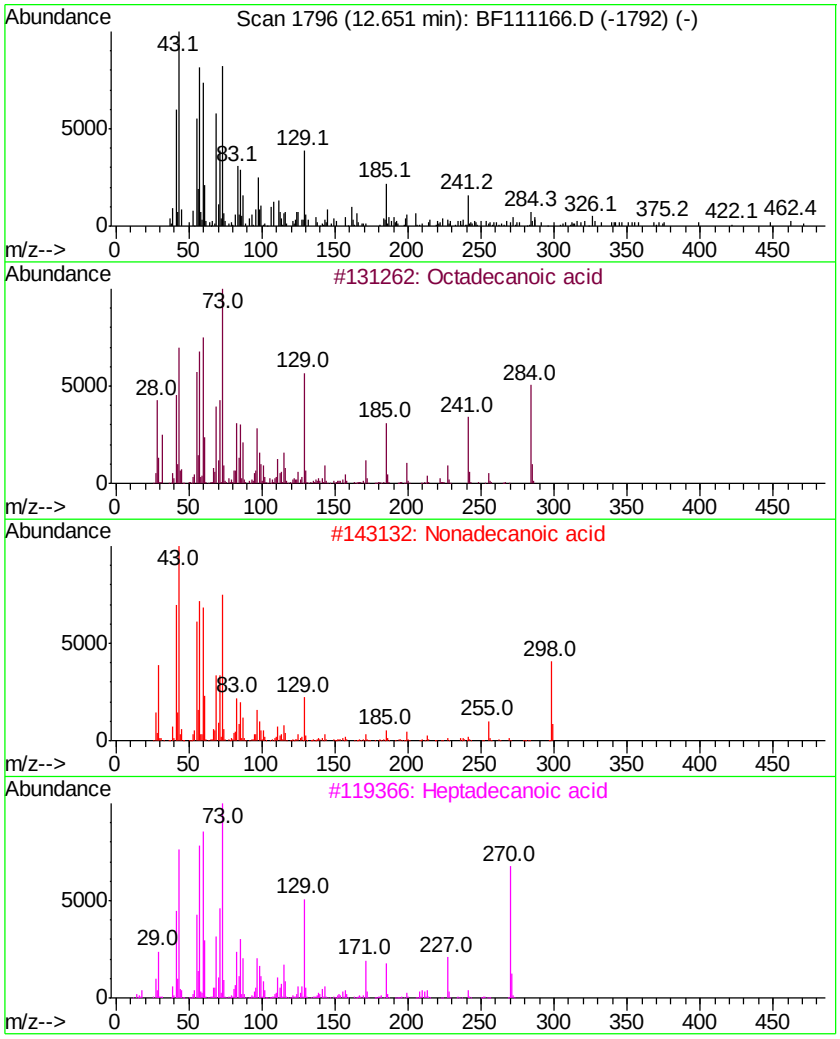
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

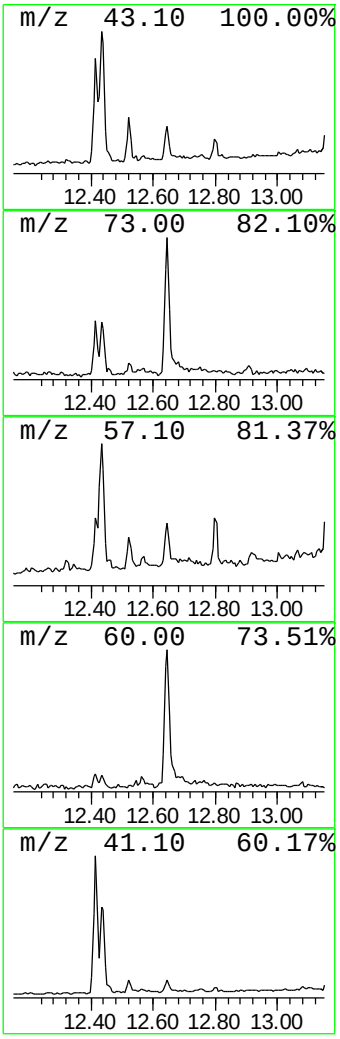
****

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.70 ng	405069	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Nonadecanoic acid	298	C19H38O2	000646-30-0	70
3	Heptadecanoic acid	270	C17H34O2	000506-12-7	68
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111166.D
Acq On : 7 Dec 2018 4:06
Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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

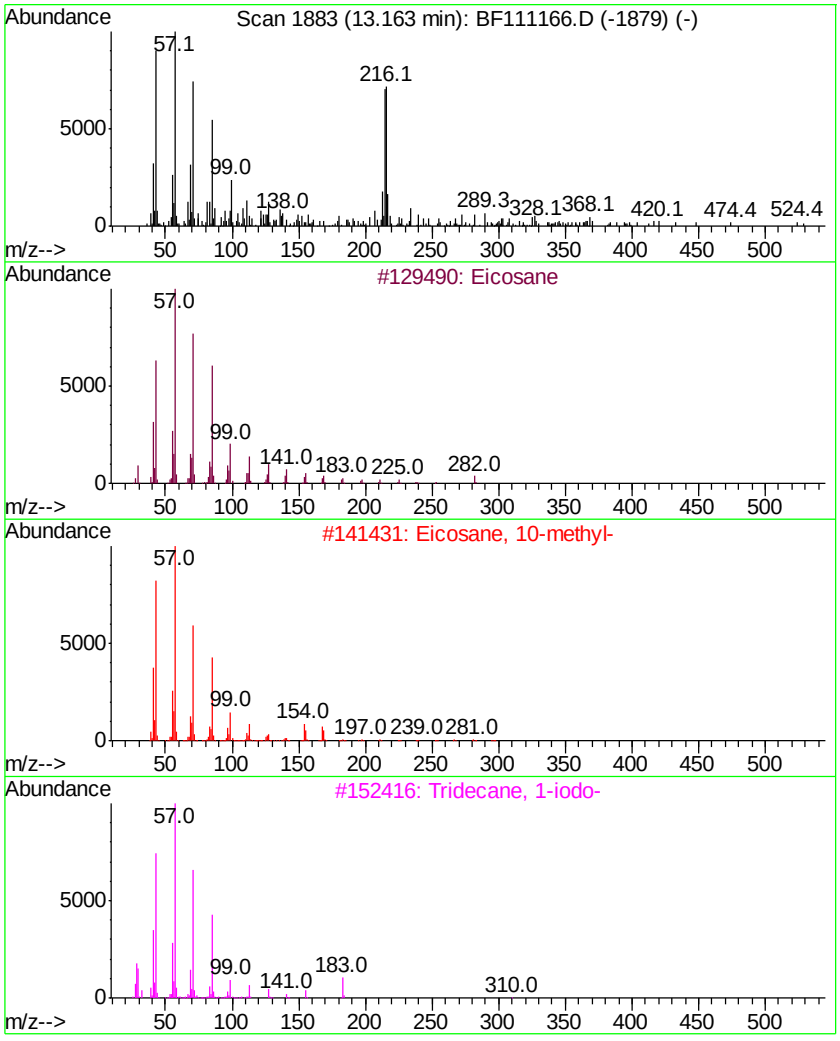
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

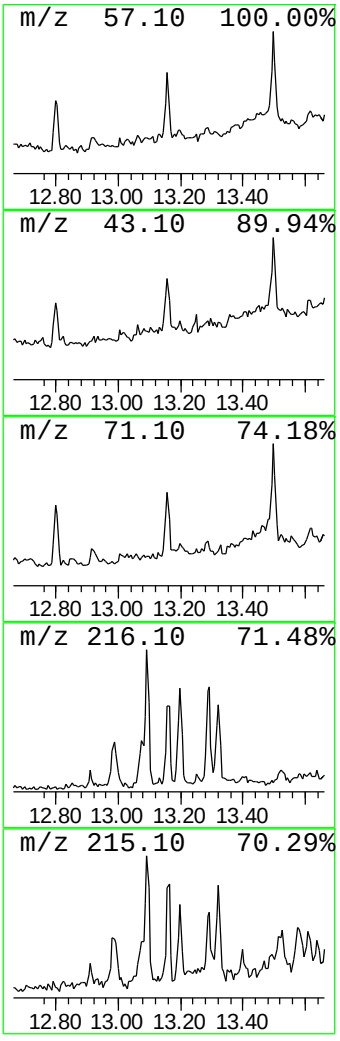
****

Peak Number 9 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.16	2.26 ng	278903	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	83
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	83
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	78
4	Heptadecane	240	C17H36	000629-78-7	78
5	Tetracosane	338	C24H50	000646-31-1	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111166.D
Acq On : 7 Dec 2018 4:06
Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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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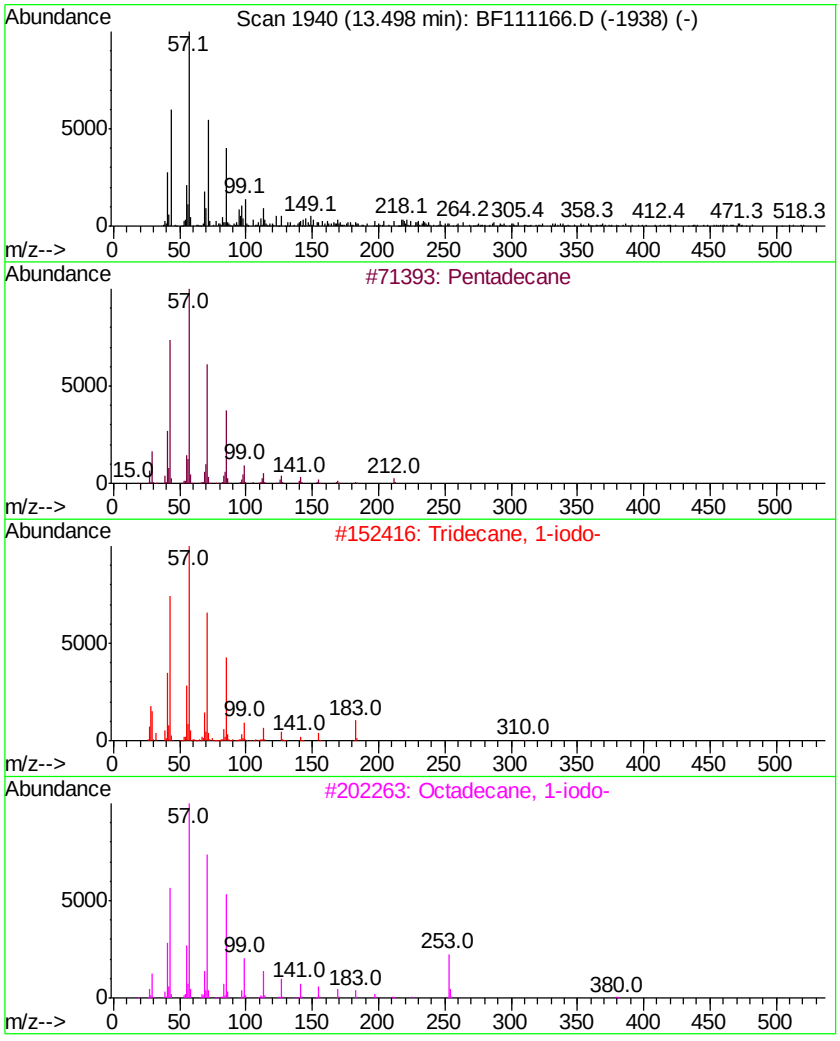
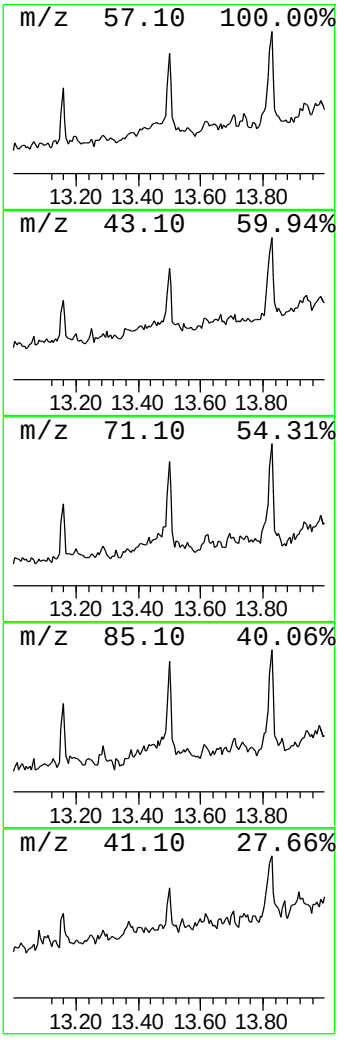
Peak Number 10 Pentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	2.18 ng	269311	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	93
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tricosane	324	C23H48	000638-67-5	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111166.D
Acq On : 7 Dec 2018 4:06
Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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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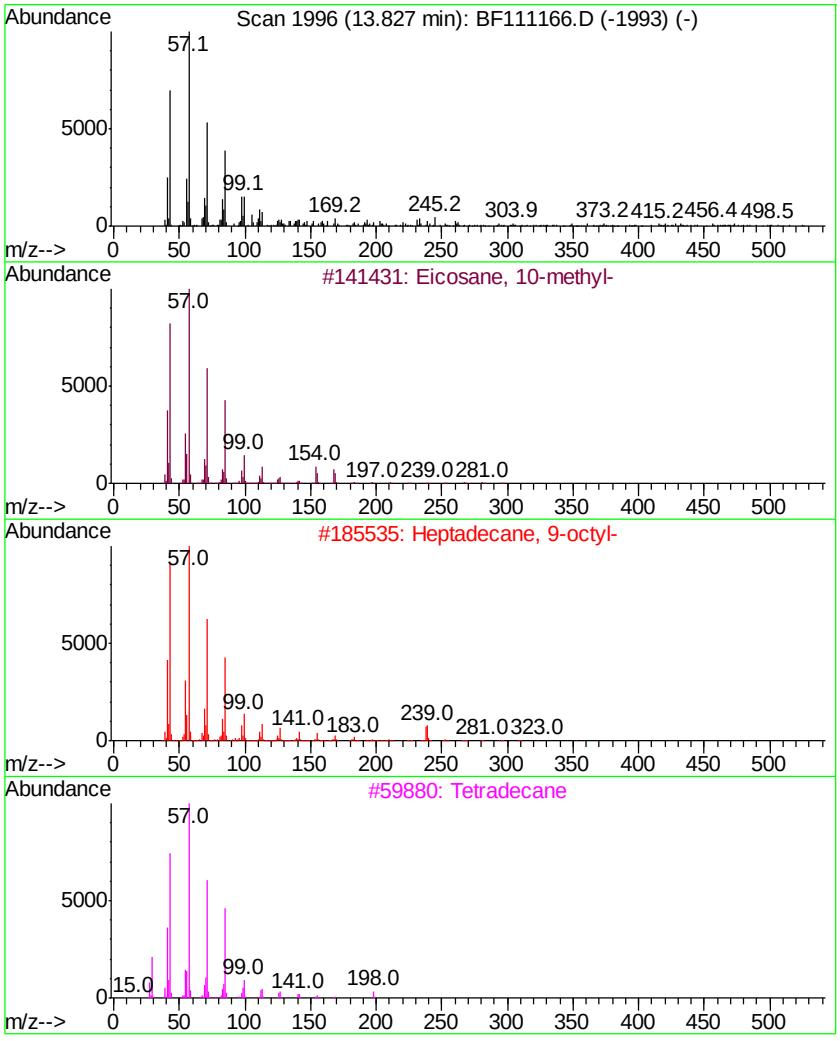
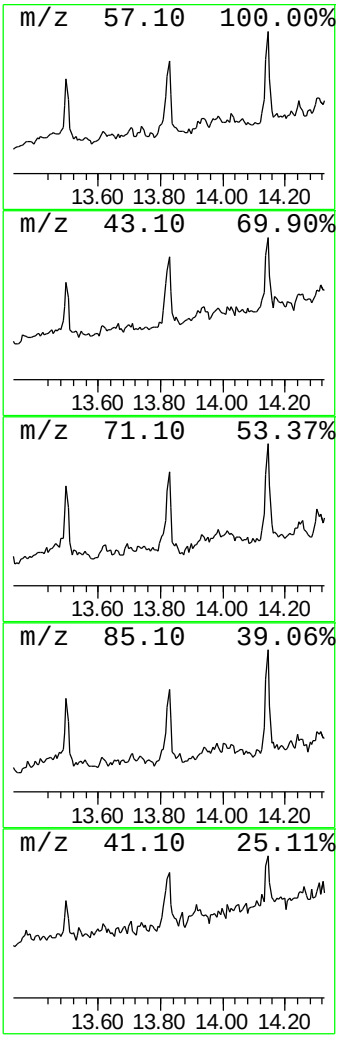
Peak Number 11 Eicosane, 10-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.20 ng	519581	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	81
3	Tetradecane	198	C14H30	000629-59-4	81
4	Hexacosane	366	C26H54	000630-01-3	81
5	1-Iodoundecane	282	C11H23I	004282-44-4	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120618\
Data File : BF111166.D
Acq On : 7 Dec 2018 4:06
Operator : JU/SJ
Sample : J6199-03 2X
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-120518-B

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	2.7	ng	437754	1	6.81	3251920	20.0
unknown6.57	6.57	37.9	ng	6163420	1	6.81	3251920	20.0
Hexadecanoic acid...	11.73	9.0	ng	1347160	4	11.33	3005980	20.0
n-Hexadecanoic acid	11.86	5.1	ng	761257	4	11.33	3005980	20.0
9,12-Octadecadien...	12.42	35.3	ng	5311090	4	11.33	3005980	20.0
12-Octadecenoic a...	12.44	17.9	ng	2683920	4	11.33	3005980	20.0
Octadecanoic acid	12.65	2.7	ng	405069	4	11.33	3005980	20.0
Eicosane	13.16	2.3	ng	278903	5	13.96	2471960	20.0
Pentadecane	13.50	2.2	ng	269311	5	13.96	2471960	20.0
Eicosane, 10-methyl-	13.83	4.2	ng	519581	5	13.96	2471960	20.0