LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

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-BF120818.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	4.993	485	494	501	rVB2	113645	133662	4.07%	0.374%
2	5.410	561	565	579	rVB	2381253	2131971	64.95%	5.969%
3	6.422	734	737	751	rBV	2302015	2263210	68.94%	6.336%
4	6.569	758	762	770	rBV	2493442	2156054	65.68%	6.036%
5	6.804	798	802	805	rBV	2984966	2532014	77.13%	7.089%
6	6.957	824	828	832	rBV	2004096	1613590	49.15%	4.518%
7	7.204	865	870	873	rBV4	40939	40653	1.24%	0.114%
8	7.357	889	896	899	rBV	1409327	1220602	37.18%	3.417%
9	7.410	903	905	909	rVV	67389	58815	1.79%	0.165%
10	7.457	909	913	916	rVB6	32339	50048	1.52%	0.140%
11	7.828	970	976	978	rBV5	35787	62903	1.92%	0.176%
12	7.922	988	992	995	rVB4	26864	42837	1.30%	0.120%
13	8.087	1015	1020	1023	rBV	3367847	3068166	93.47%	8.590%
14	8.387	1066	1071	1074	rBV6	43245	56218	1.71%	0.157%
15	8.516	1090	1093	1095	rBV	57457	52053	1.59%	0.146%
16	8.592	1103	1106	1109	rBV2	57860	55575	1.69%	0.156%
17	8.687	1118	1122	1124	rBV2	127186	105466	3.21%	0.295%
18	8.786	1136	1139	1145	rVB4	38955	62359	1.90%	0.175%
19	9.116	1193	1195	1199	rVB2	70924	61635	1.88%	0.173%
20	9.157	1199	1202	1208	rBV	2032152	1689985	51.48%	4.732%
21	9.251	1215	1218	1222	rVB	121724	103735	3.16%	0.290%
22	9.551	1267	1269	1271	rBV	117627	101384	3.09%	0.284%
23	9.781	1306	1308	1311	rBV	102889	71240	2.17%	0.199%
24	9.839	1314	1318	1322	rVV	2789648	2334503	71.12%	6.536%
25	10.281	1390	1393	1395	rVB	109203	89243	2.72%	0.250%
26	10.504	1426	1431	1433	rBV2	46880	54717	1.67%	0.153%
27	10.622	1447	1451	1455	rBV	908694	778292	23.71%	2.179%
28	10.751	1470	1473	1480	rVB	128617	170974	5.21%	0.479%
29	11.069	1524	1527	1533	rVB2	195559	238807	7.27%	0.669%
30	11.198	1547	1549	1551	rBV	85109	68196	2.08%	0.191%
31	11.233	1553	1555	1560	rVB2	57756	52921	1.61%	0.148%
32	11.322	1566	1570	1573	rBV	2120308	1781918	54.28%	4.989%
33	11.345	1573	1574	1577	rVB	107839	56167	1.71%	0.157%
34	11.627	1619	1622	1624	rBV	84939	61926	1.89%	0.173%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

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-BF120818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.722	1635	1638	1642	rBV	920164	808957	24.64%	2.265%
36	11.851	1657	1660	1665	rBV2	217214	182226	5.55%	0.510%
37	11.922	1669	1672	1676	rVV5	66152	102205	3.11%	0.286%
38	12.033	1689	1691	1694	rBV2	59497	49941	1.52%	0.140%
39	12.251	1726	1728	1729	rBV2	75942	49642	1.51%	0.139%
40	12.410	1752	1755	1757	rBV	3860550	3282659	100.00%	9.191%
41	12.433	1757	1759	1762	rVB	3489742	2643948	80.54%	7.402%
42	12.516	1770	1773	1779	rBV2	460952	479243	14.60%	1.342%
43	12.563	1779	1781	1783	rVV3	112589	77359	2.36%	0.217%
44	12.639	1792	1794	1799	rBV3	163760	175499	5.35%	0.491%
45	12.757	1812	1814	1817	rBV	138025	116494	3.55%	0.326%
46	12.904	1836	1839	1844	rBV	1350380	1232306	37.54%	3.450%
47	13.957	2015	2018	2021	rVB	1686352	1504128	45.82%	4.211%
48	15.398	2260	2263	2267	rBV	763194	879835	26.80%	2.463%
49	15.486	2276	2278	2280	rBV3	269763	318151	9.69%	0.891%
50	17.862	2680	2682	2687	rBV6	219294	392786	11.97%	1.100%

Sum of corrected areas: 35717218

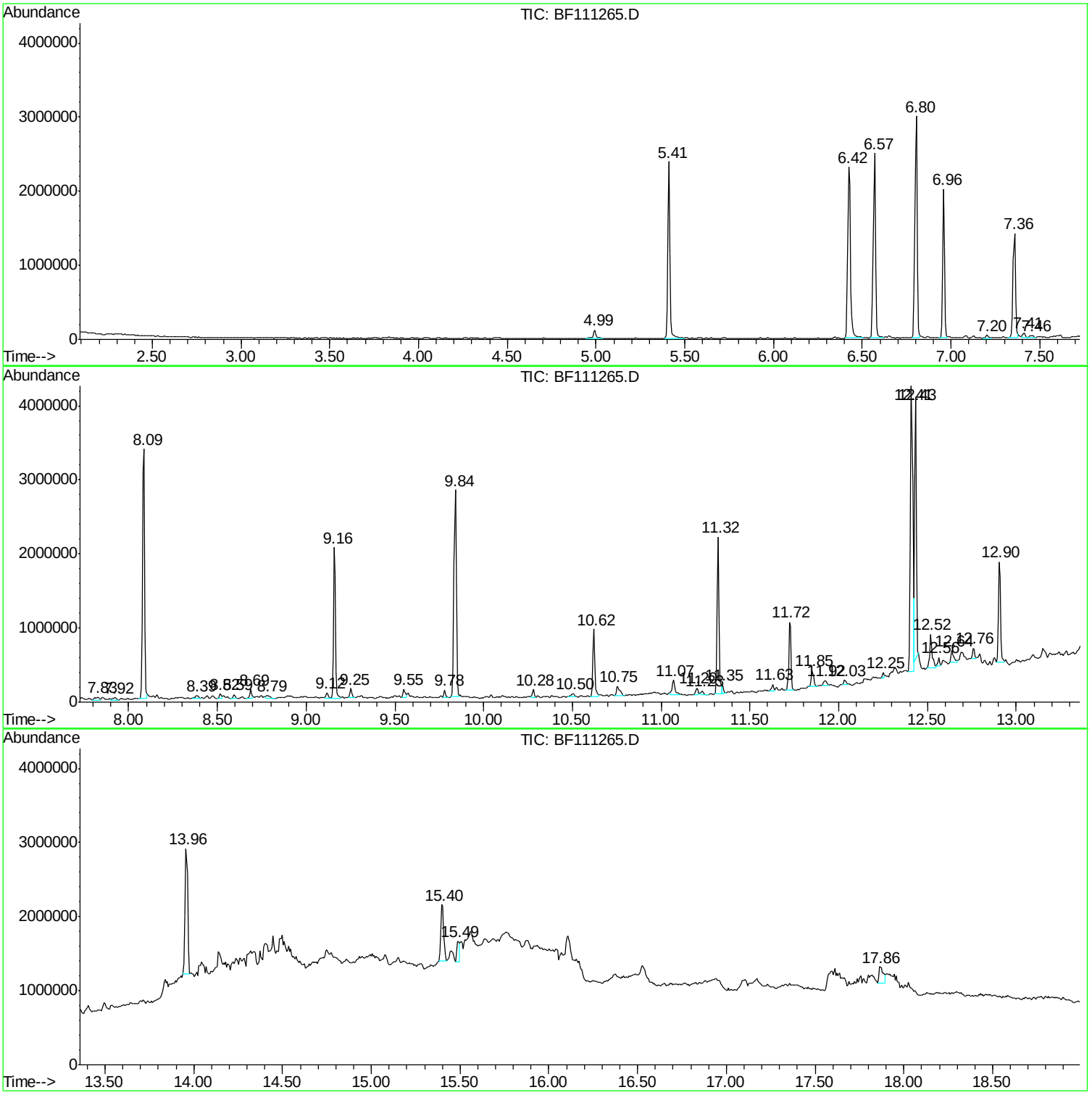
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

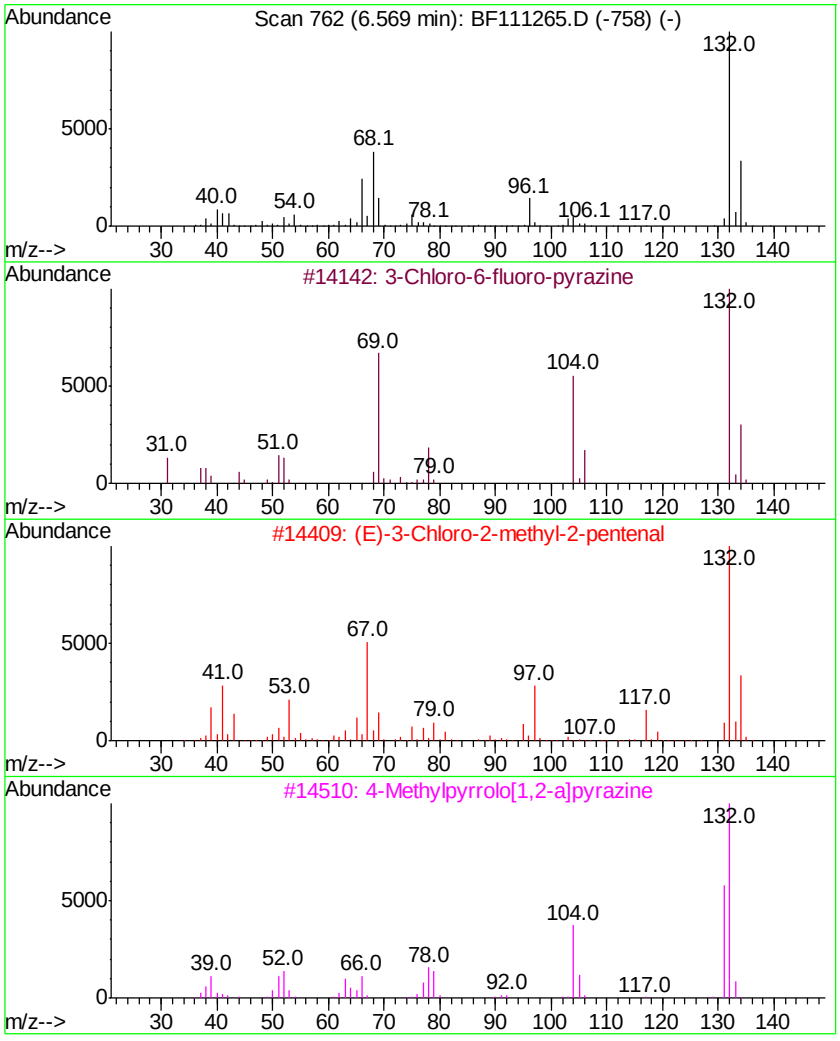
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

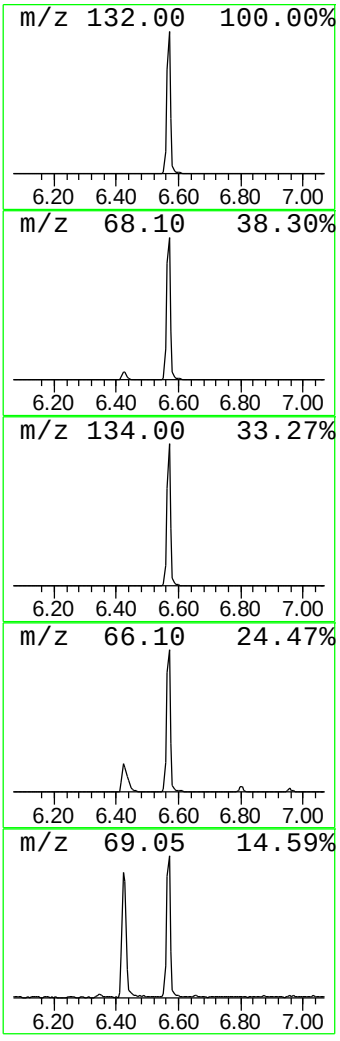
****

Peak Number 1 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	17.03 ng	2156050	1,4-Dichlorobenzene-d4	6.80

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	12
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

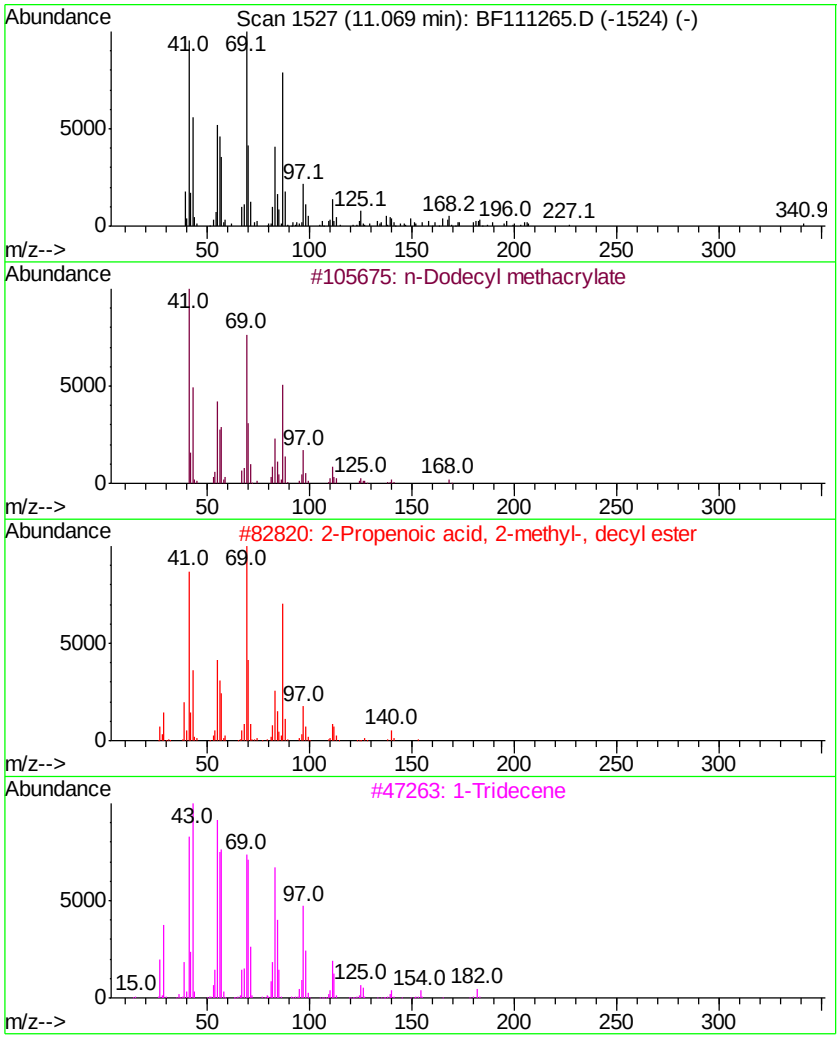
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

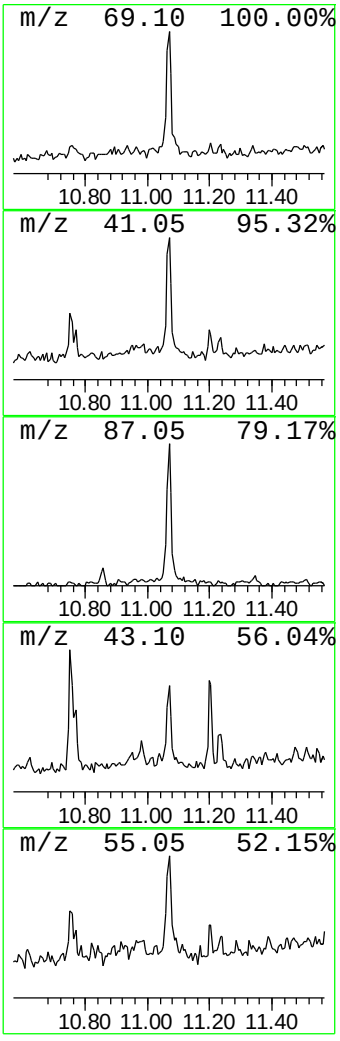
****

Peak Number 3 n-Dodecyl methacrylate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.07	2.68 ng	238807	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	91
2	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	91
3	1-Tridecene	182	C13H26	002437-56-1	86
4	6-Dodecene, (E)-	168	C12H24	007206-17-9	62
5	Cyclotetradecane	196	C14H28	000295-17-0	56





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

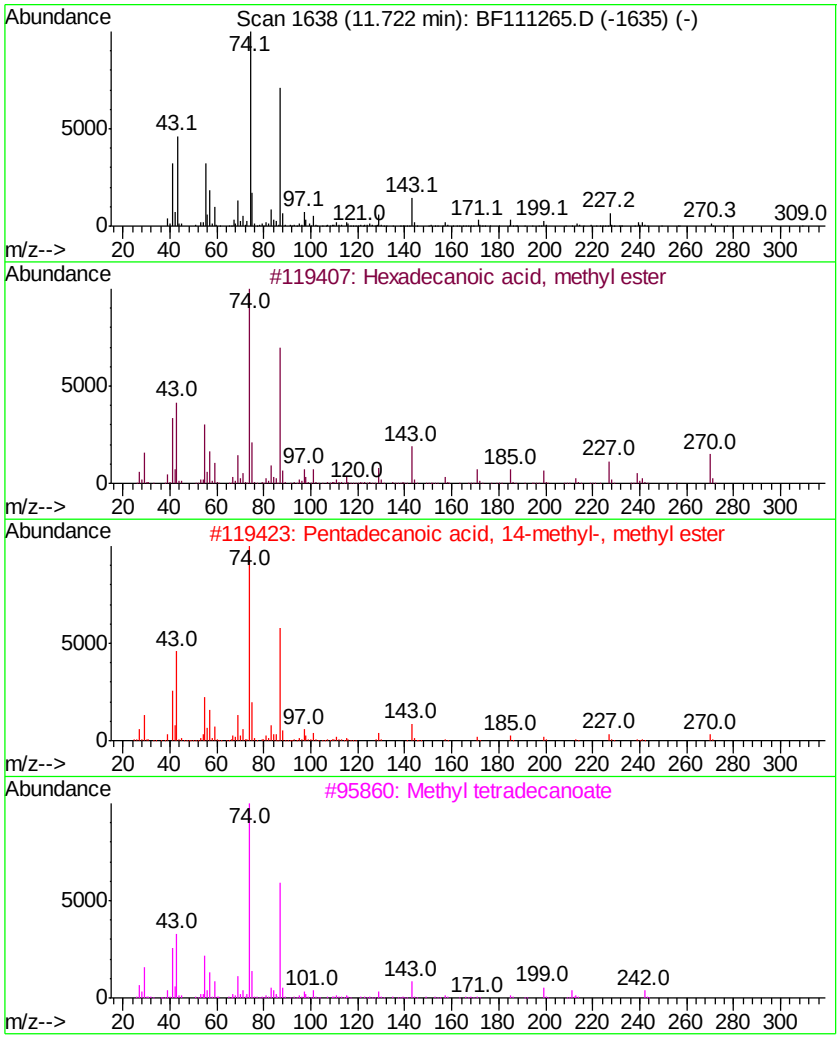
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

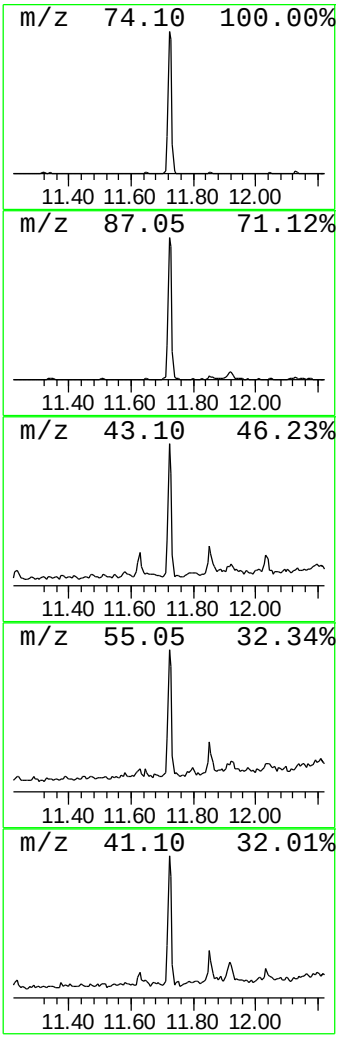
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	9.08 ng	808957	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

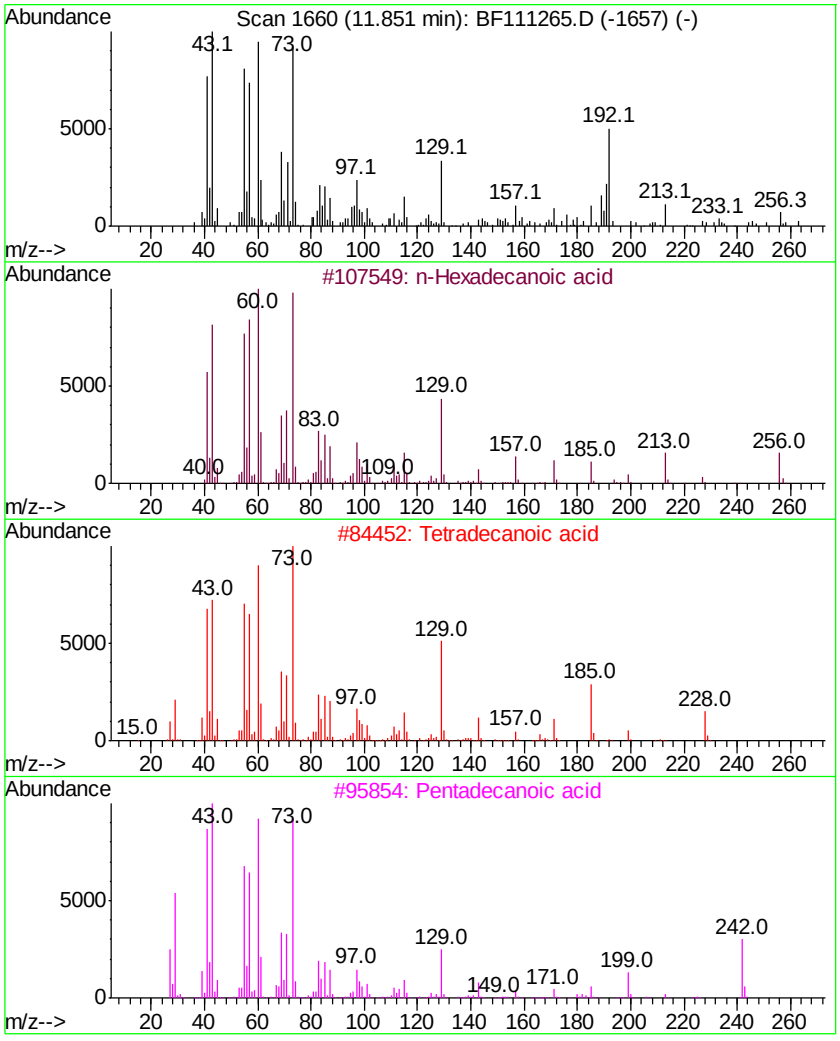
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

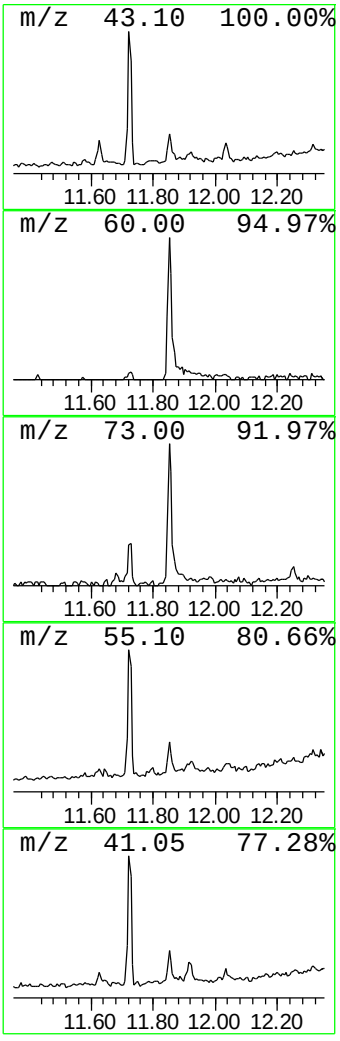
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.05 ng	182226	Phenanthrene-d10	11.32

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	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	49





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

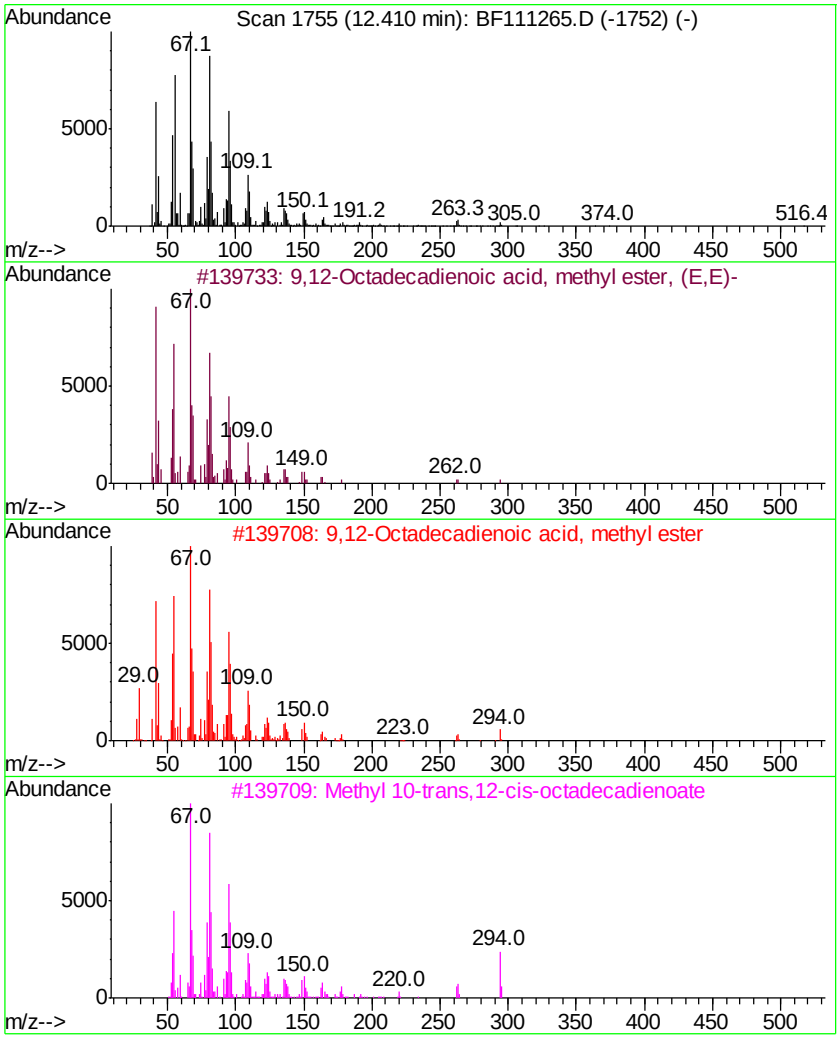
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

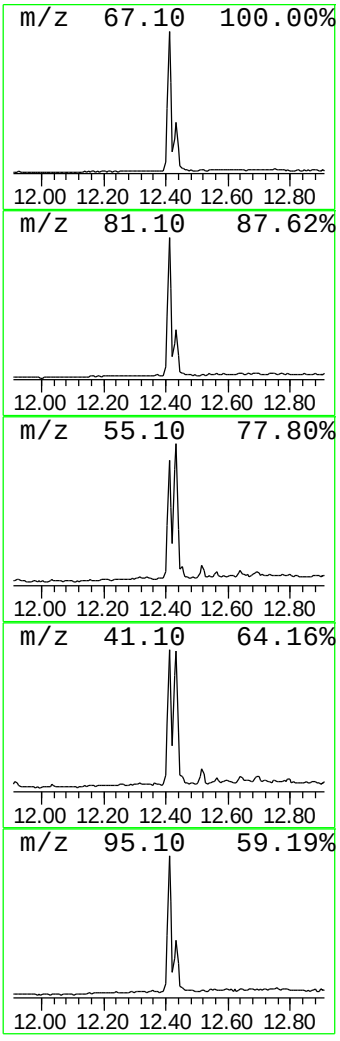
****

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	36.84 ng	3282660	Phenanthrene-d10	11.32

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	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

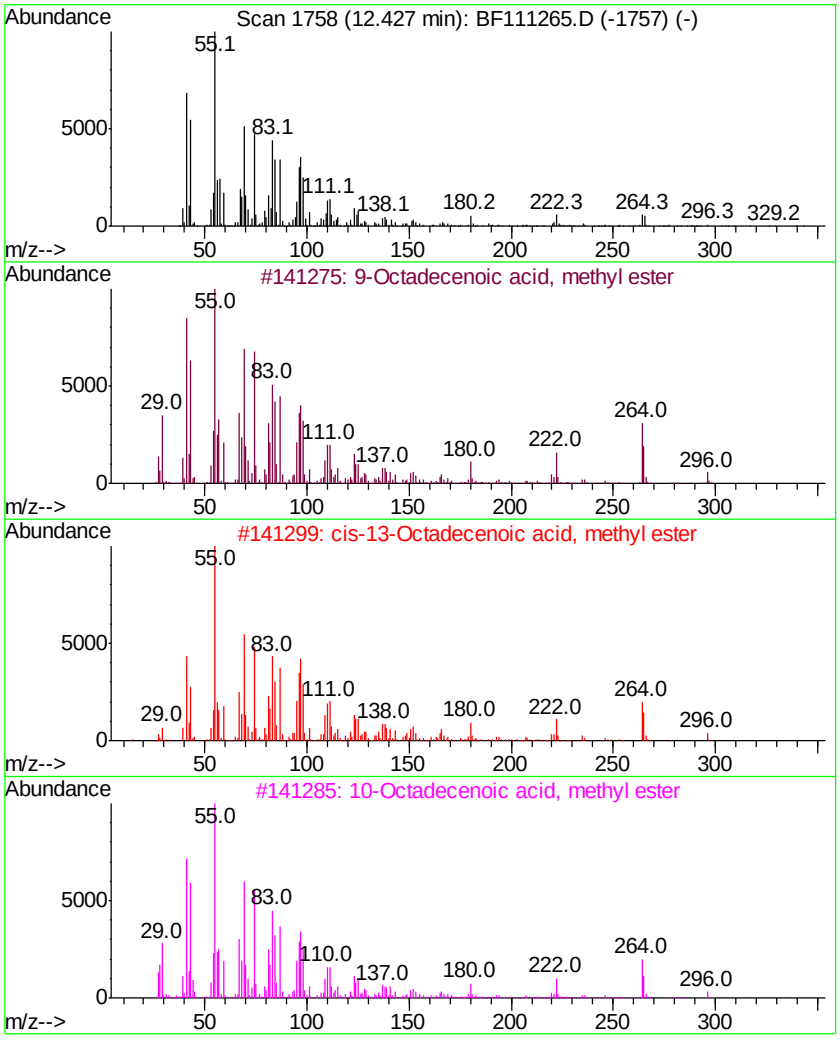
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

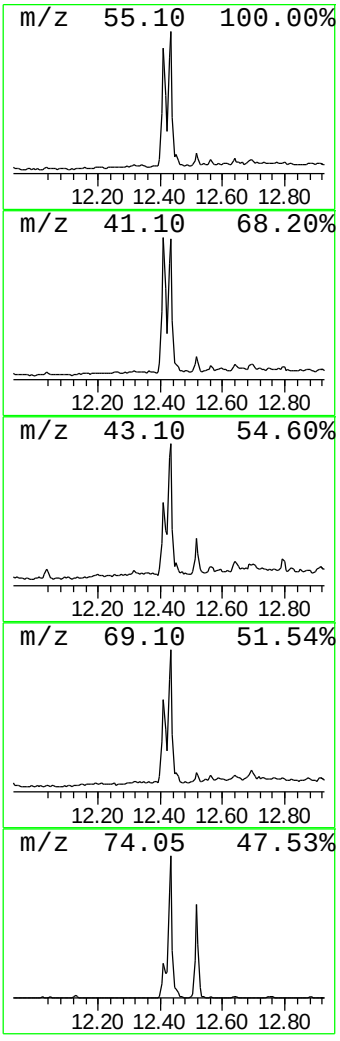
****

Peak Number 7 9-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	29.68 ng	2643950	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
2	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	99
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

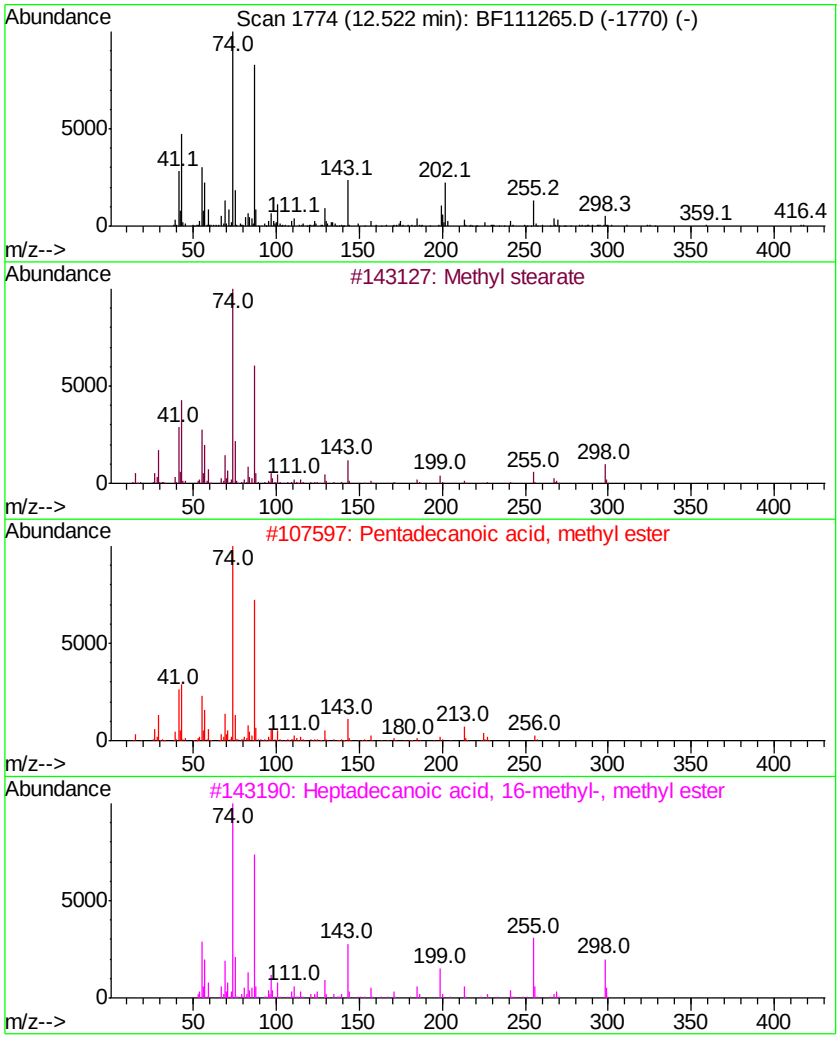
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

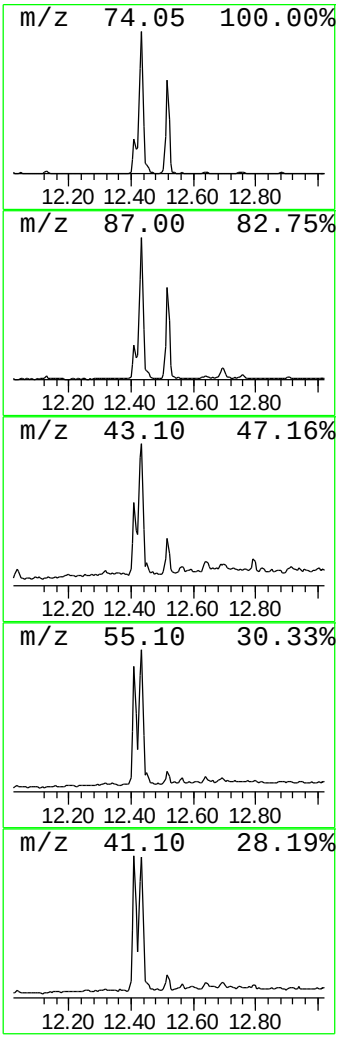
****

Peak Number 8 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	5.38 ng	479243	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	93
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90
5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

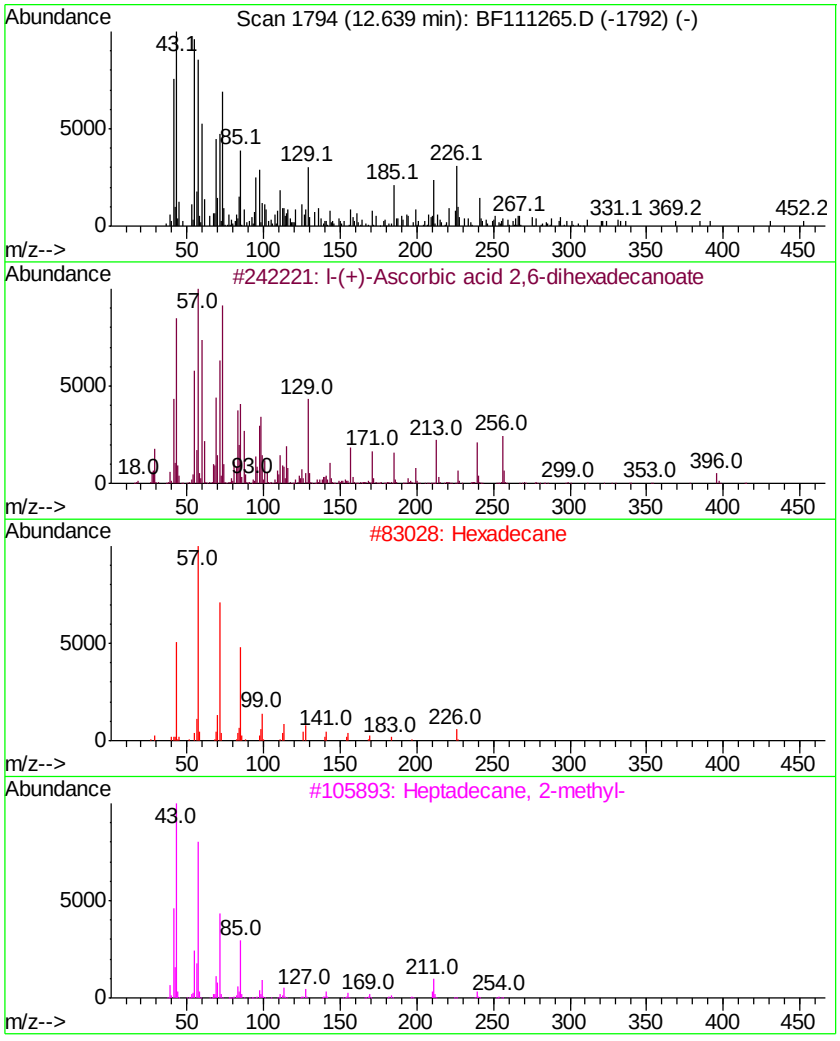
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

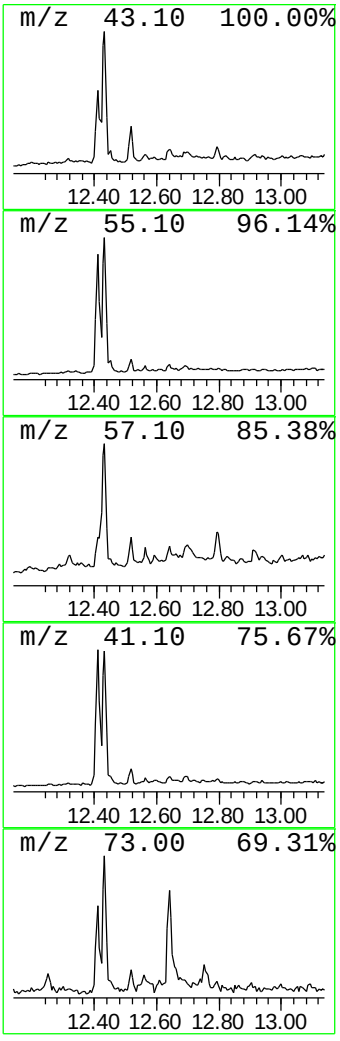
****

Peak Number 9 unknown12.64 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.33 ng	175499	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	49
2	Hexadecane	226	C16H34	000544-76-3	42
3	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	42
4	Eicosane, 9-cyclohexyl-	364	C26H52	004443-61-2	38
5	Nonadecanoic acid	298	C19H38O2	000646-30-0	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

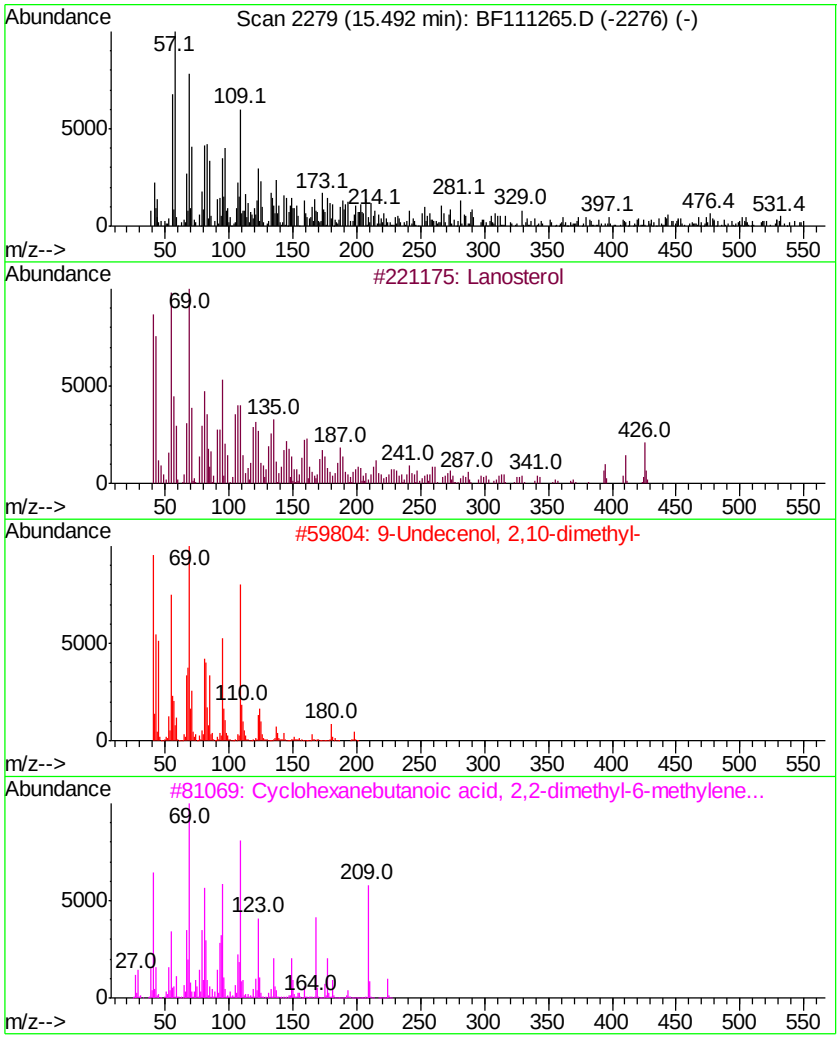
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

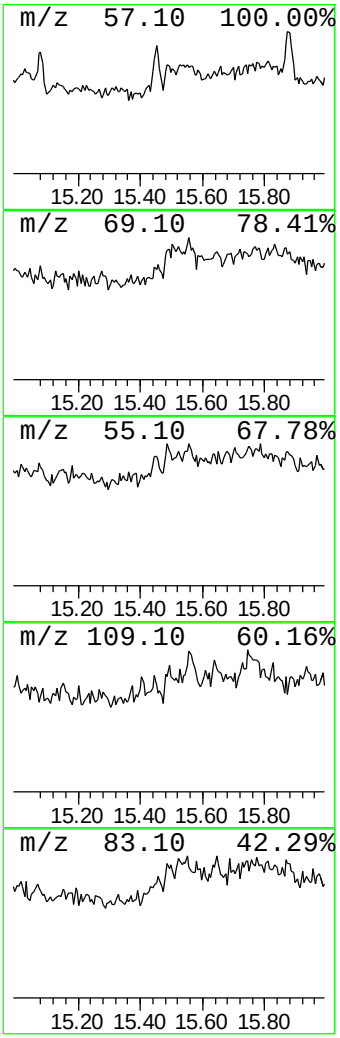
****

Peak Number 10 unknown15..49 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	7.23 ng	318151	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lanosterol	426	C30H50O	000079-63-0	43
2	9-Undecenol, 2,10-dimethyl-	198	C13H26O	1000131-86-0	38
3	Cyclohexanebutanoic acid, 2,2-di...	224	C14H24O2	095452-15-6	32
4	Bicyclo[3.3.1]nonan-9-one, 2,4-d...	211	C11H17NO3	129967-64-2	25
5	Silane, chlorodiethylnonyloxy-	264	C13H29ClOSi	1000363-09-4	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

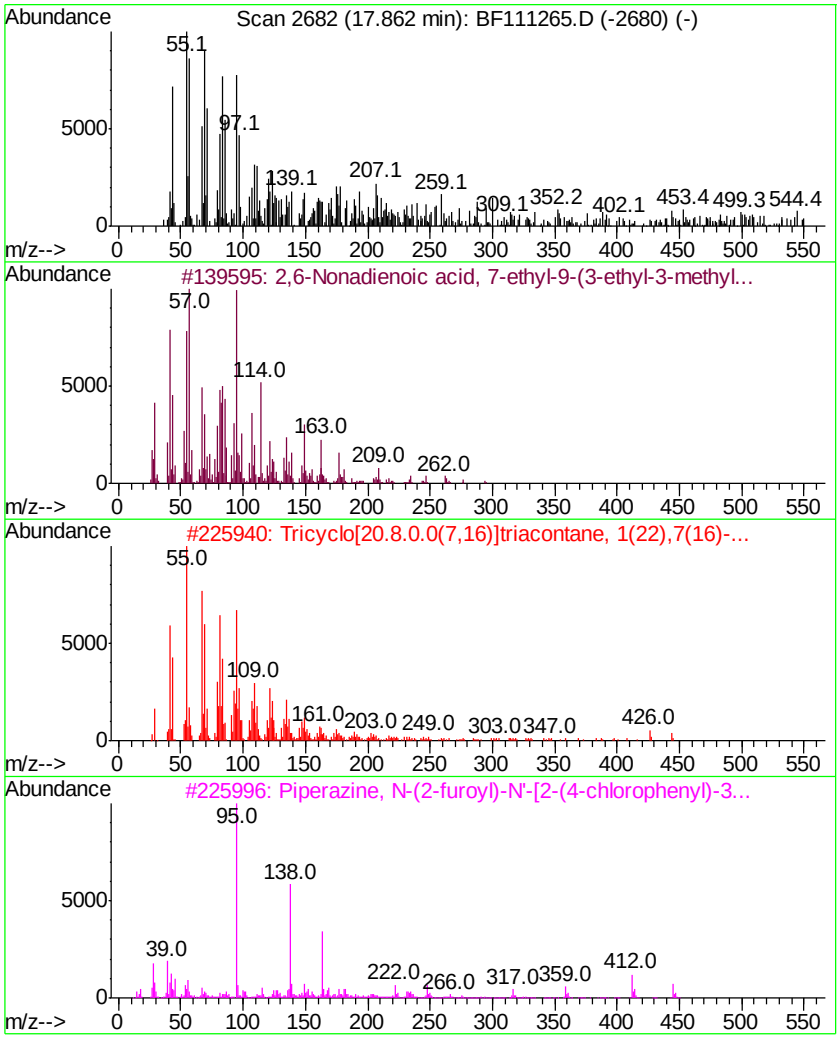
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

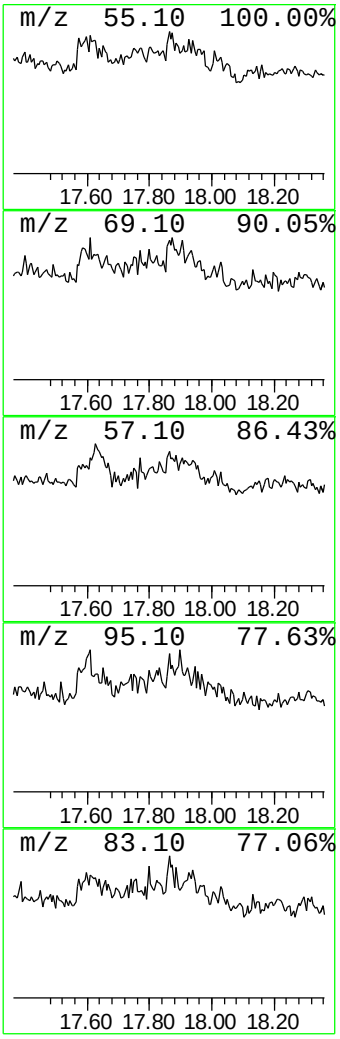
****

Peak Number 11 2,6-Nonadienoic acid, 7-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.86	8.93 ng	392786	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Nonadienoic acid, 7-ethyl-9-...	294	C18H30O3	013804-51-8	60
2	Tricyclo[20.8.0.0(7,16)]triacont...	444	C30H52O2	1000155-90-7	60
3	Piperazine, N-(2-furoyl)-N'-[2-(...	445	C22H24ClN3O3S	156483-16-8	49
4	11,13-Dimethyl-12-tetradecen-1-o...	282	C18H34O2	1000130-81-0	49
5	7,9-Dimethyl-8-nitrobicyclo[4.3....	225	C12H19NO3	129967-66-4	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121018\
Data File : BF111265.D
Acq On : 11 Dec 2018 1:48
Operator : JU/SJ
Sample : J6196-05 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-120718-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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
unknown6.57	6.57	17.0	ng	2156050	1	6.80	2532010	20.0
n-Dodecyl methacr...	11.07	2.7	ng	238807	4	11.32	1781920	20.0
Hexadecanoic acid...	11.72	9.1	ng	808957	4	11.32	1781920	20.0
n-Hexadecanoic acid	11.85	2.0	ng	182226	4	11.32	1781920	20.0
9,12-Octadecadien...	12.41	36.8	ng	3282660	4	11.32	1781920	20.0
9-Octadecenoic ac...	12.43	29.7	ng	2643950	4	11.32	1781920	20.0
Methyl stearate	12.52	5.4	ng	479243	4	11.32	1781920	20.0
unknown12.64	12.64	2.3	ng	175499	5	13.96	1504130	20.0
unknown15..49	15.49	7.2	ng	318151	6	15.40	879835	20.0
2,6-Nonadienoic a...	17.86	8.9	ng	392786	6	15.40	879835	20.0