LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	3.540	243	247	260	rBV	65028	105507	3.18%	0.433%
2	4.428	393	398	414	rBV	1404192	1684057	50.75%	6.906%
3	5.051	501	504	514	rBV	93966	118323	3.57%	0.485%
4	5.457	570	573	593	rBV	1459835	1359127	40.96%	5.574%
5	6.475	742	746	762	rBV	762058	812235	24.48%	3.331%
6	6.604	764	768	779	rVB	2532630	2402756	72.42%	9.854%
7	6.828	802	806	814	rBB	702872	626180	18.87%	2.568%
8	6.981	828	832	836	rBV	2315805	2348402	70.78%	9.631%
9	7.398	897	903	906	rBV	1651710	1830473	55.17%	7.507%
10	8.104	1020	1023	1027	rBV	920180	845947	25.50%	3.469%
11	8.628	1107	1112	1116	rBV3	21501	39587	1.19%	0.162%
12	9.181	1201	1206	1209	rBV	3098746	3318024	100.00%	13.607%
13	9.863	1317	1322	1326	rVB	935198	862562	26.00%	3.537%
14	10.651	1452	1456	1460	rBV	1429135	1439762	43.39%	5.905%
15	11.345	1571	1574	1578	rBV	814412	730010	22.00%	2.994%
16	12.386	1742	1751	1762	rBV2	80694	169776	5.12%	0.696%
17	12.745	1808	1812	1816	rBV	170458	154565	4.66%	0.634%
18	12.933	1839	1844	1847	rBV	2193921	2097427	63.21%	8.602%
19	13.404	1916	1924	1925	rBV	362234	405368	12.22%	1.662%
20	13.422	1925	1927	1934	rVV2	333713	543664	16.39%	2.230%
21	13.474	1934	1936	1941	rVB	160651	151637	4.57%	0.622%
22	13.827	1991	1996	2003	rBV	252492	261827	7.89%	1.074%
23	13.986	2020	2023	2029	rVB	571267	523227	15.77%	2.146%
24	14.086	2034	2040	2042	rBV	78686	97536	2.94%	0.400%
25	14.727	2144	2149	2166	rBV	859254	998852	30.10%	4.096%
26	15.451	2266	2272	2280	rVB	353503	457091	13.78%	1.875%

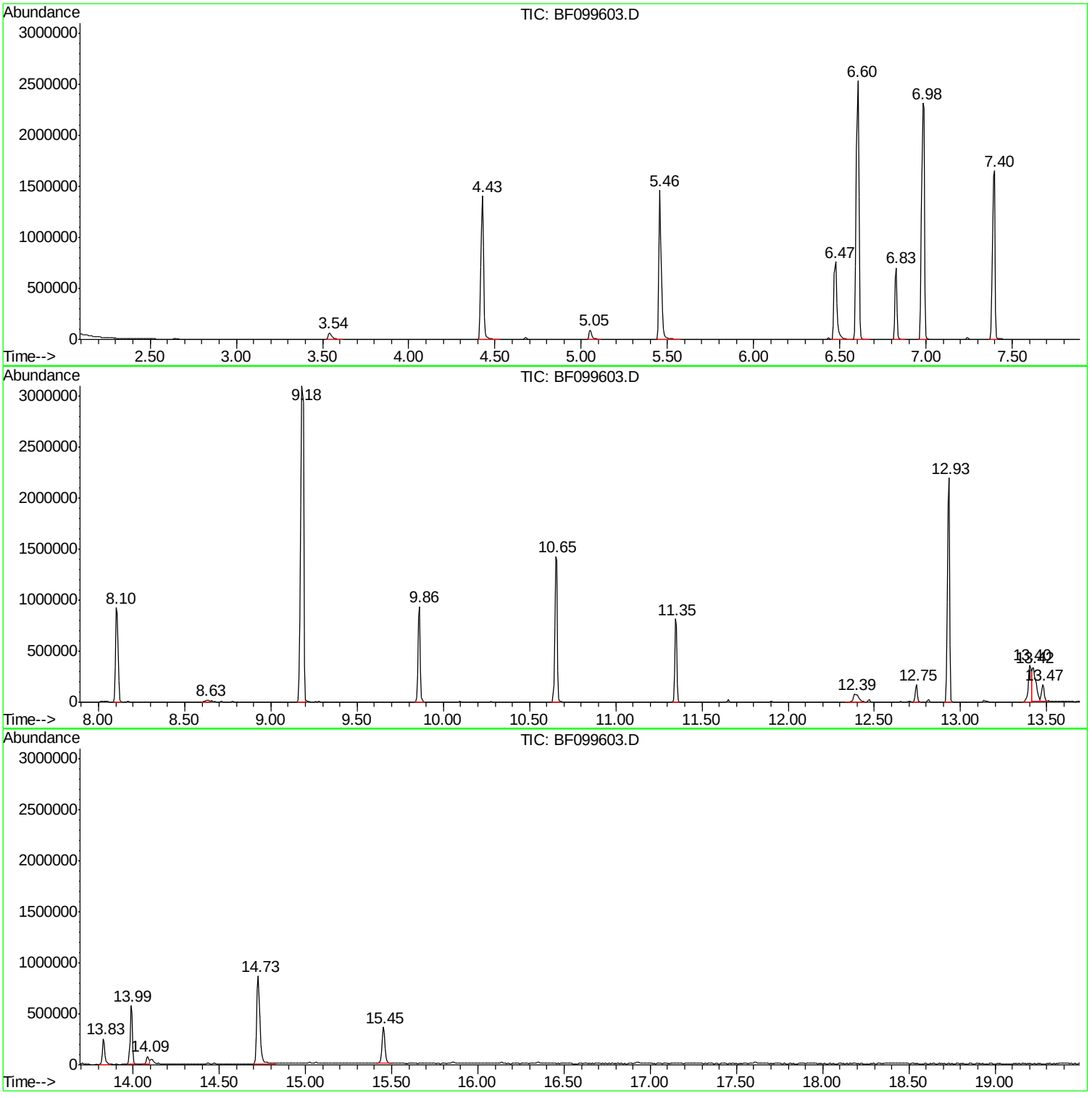
Sum of corrected areas: 24383922

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

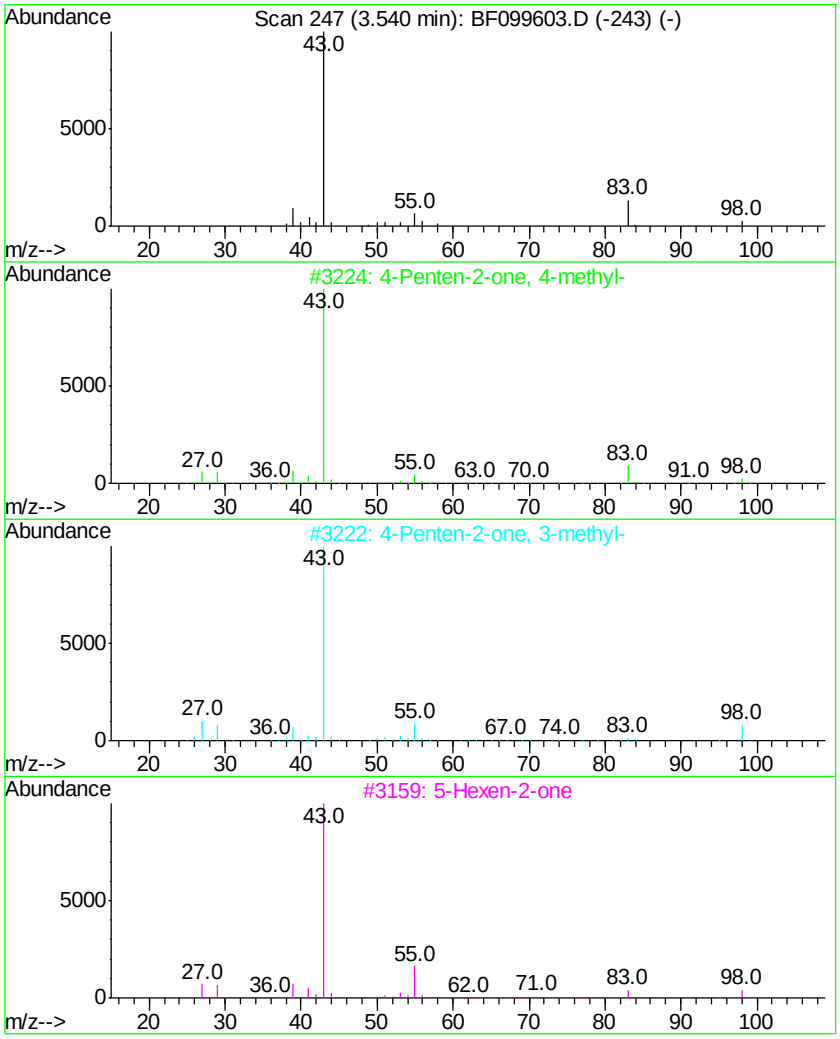
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

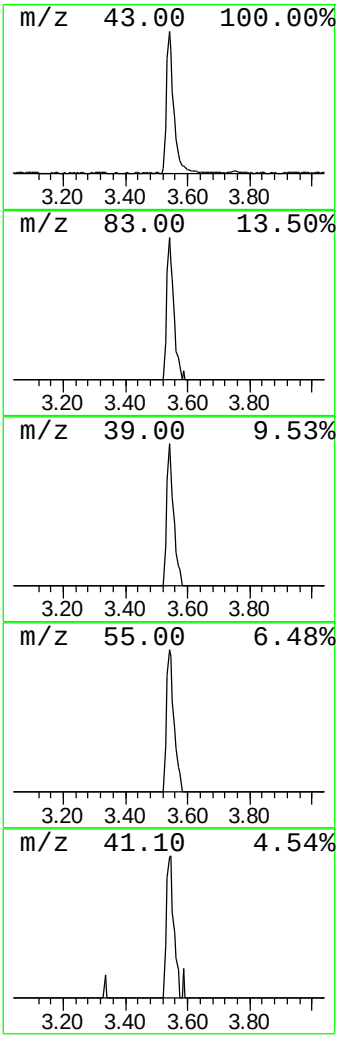
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	3.37 ng	105507	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	37
3	5-Hexen-2-one	98	C6H10O	000109-49-9	32
4	4-Hexen-2-one	98	C6H10O	025659-22-7	9
5	2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

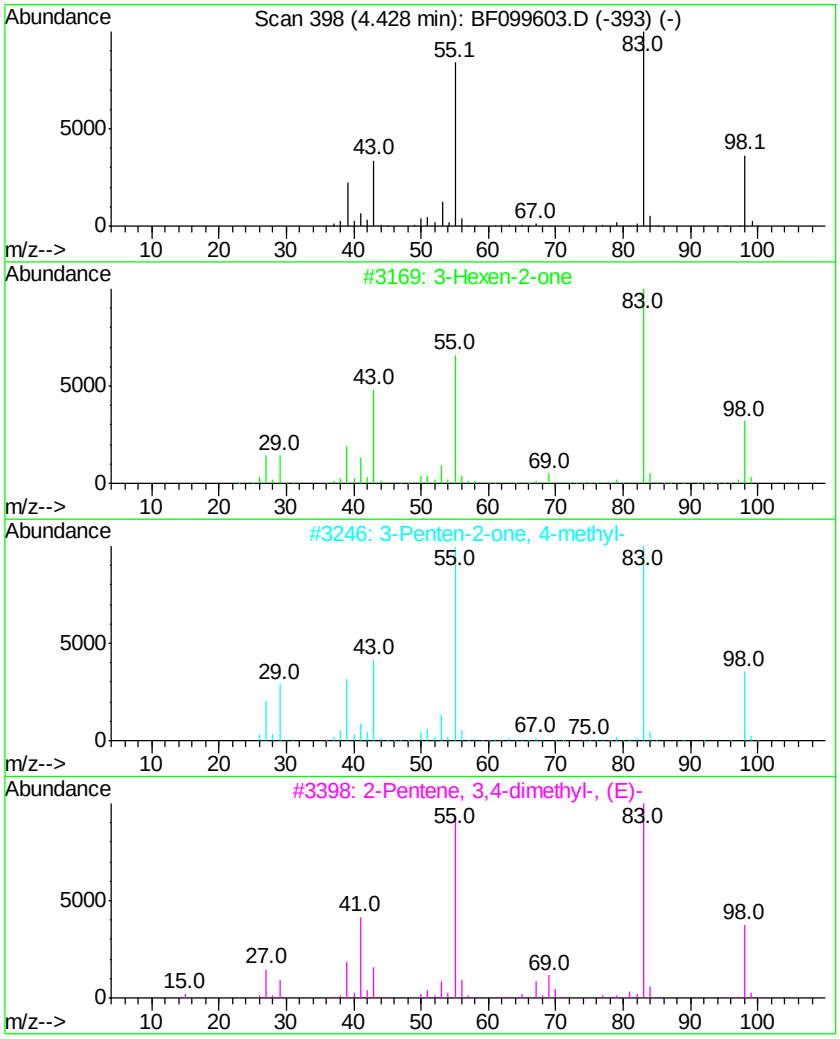
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

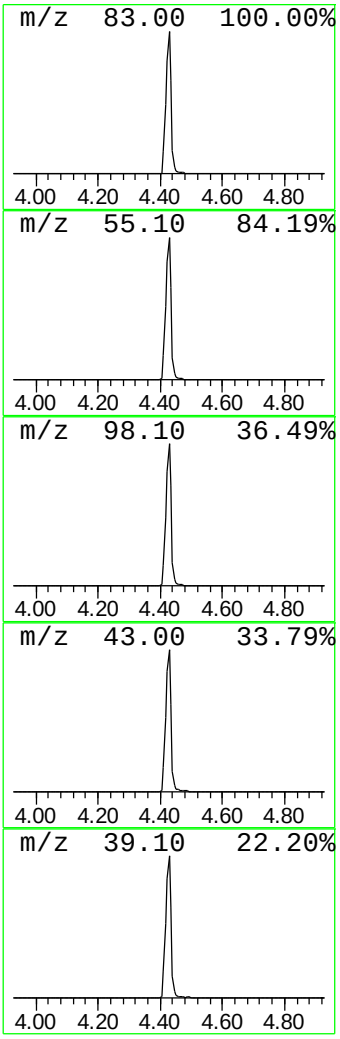
****

Peak Number 2 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.43	53.79 ng	1684060	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

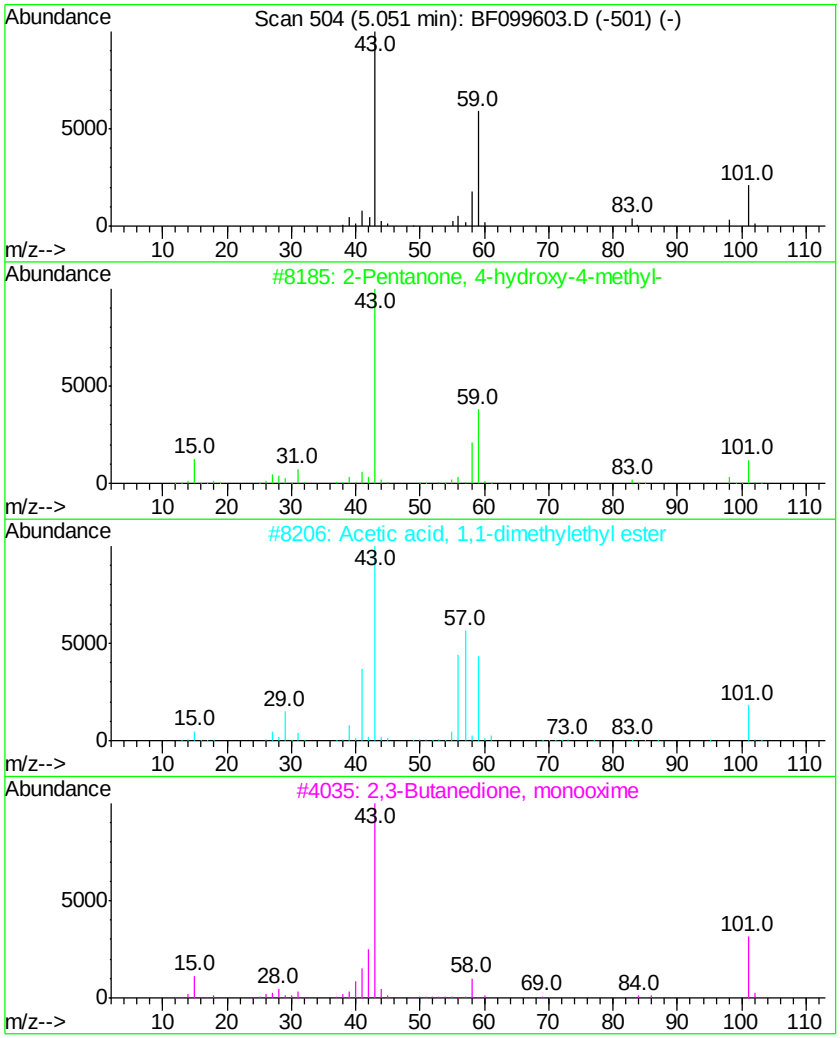
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

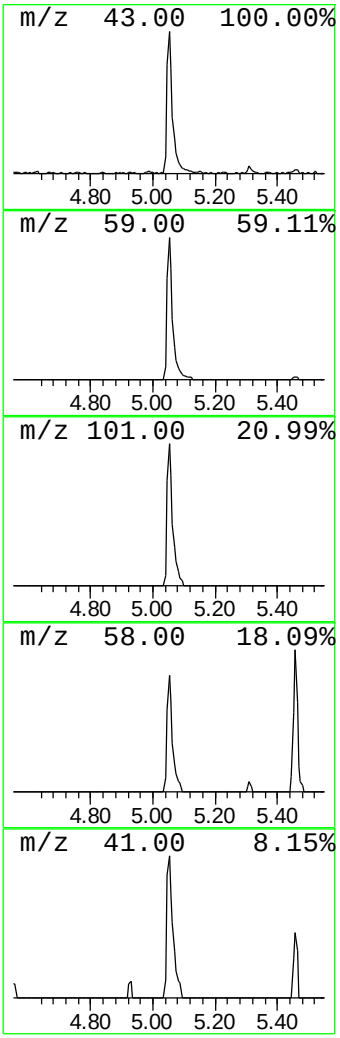
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	3.78 ng	118323	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

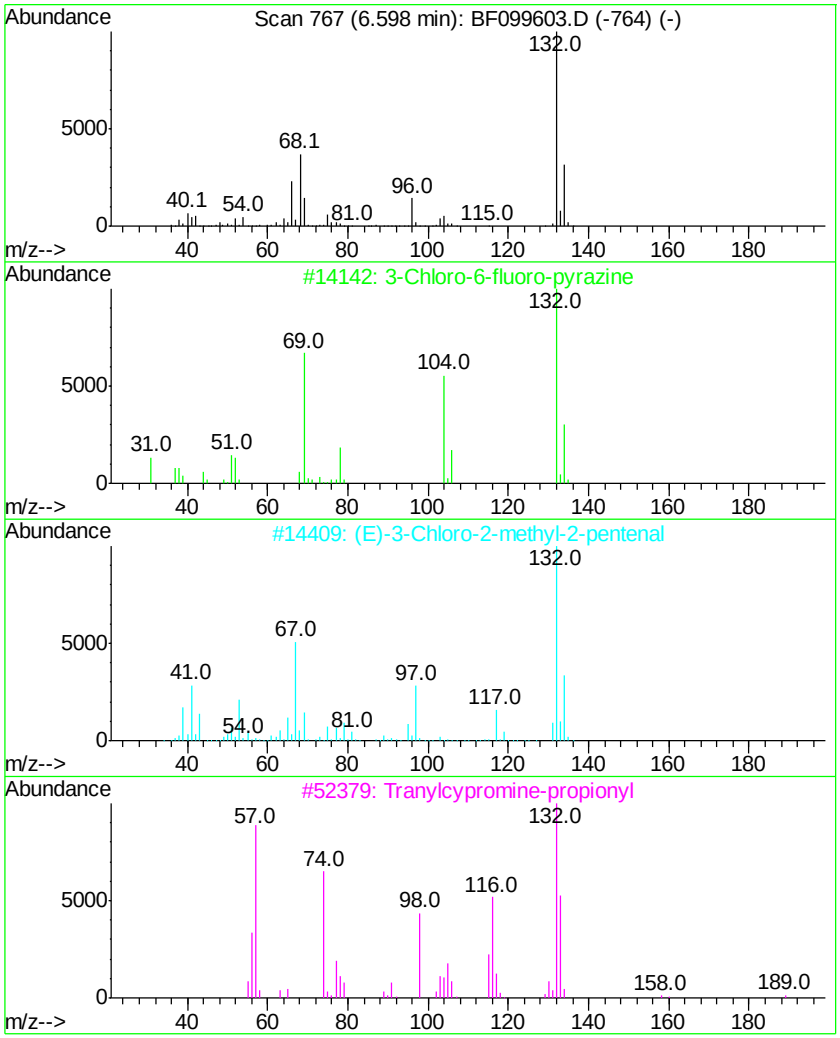
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

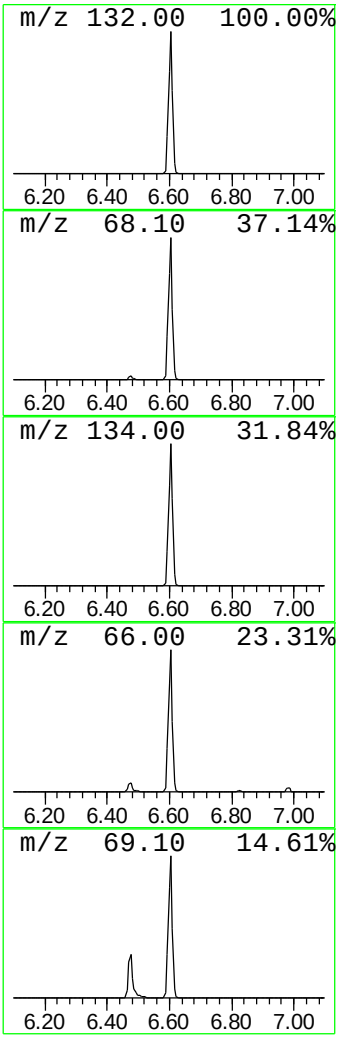
****

Peak Number 4 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	76.74 ng	2402760	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

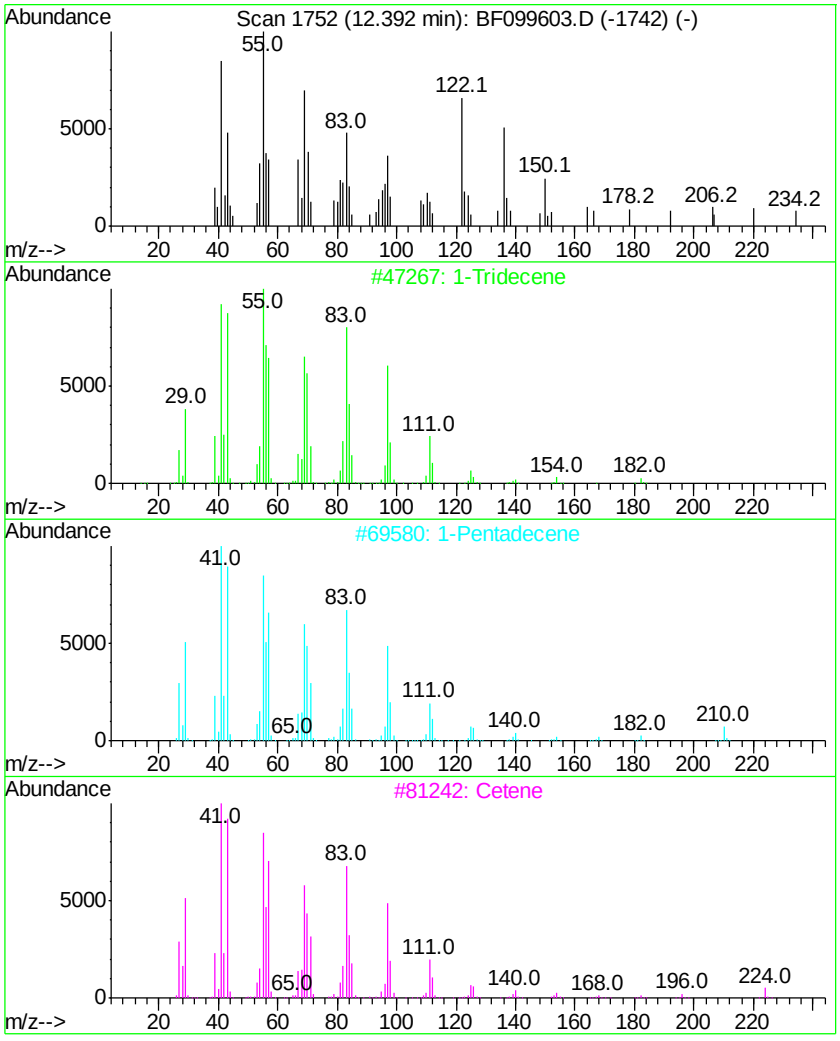
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

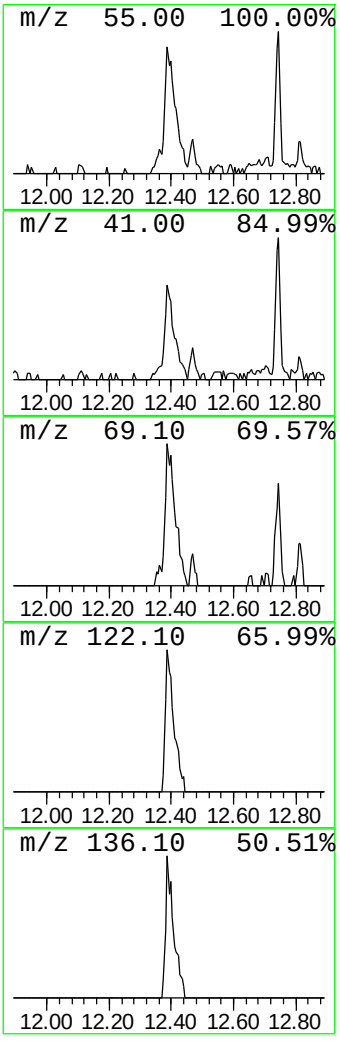
****

Peak Number 6 unknown12.39 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	4.65 ng	169776	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecene	182	C13H26	002437-56-1	38
2	1-Pentadecene	210	C15H30	013360-61-7	30
3	Cetene	224	C16H32	000629-73-2	27
4	1-Dodecanol	186	C12H26O	000112-53-8	18
5	2-Butenedioic acid (Z)-, monodod...	284	C16H28O4	002424-61-5	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

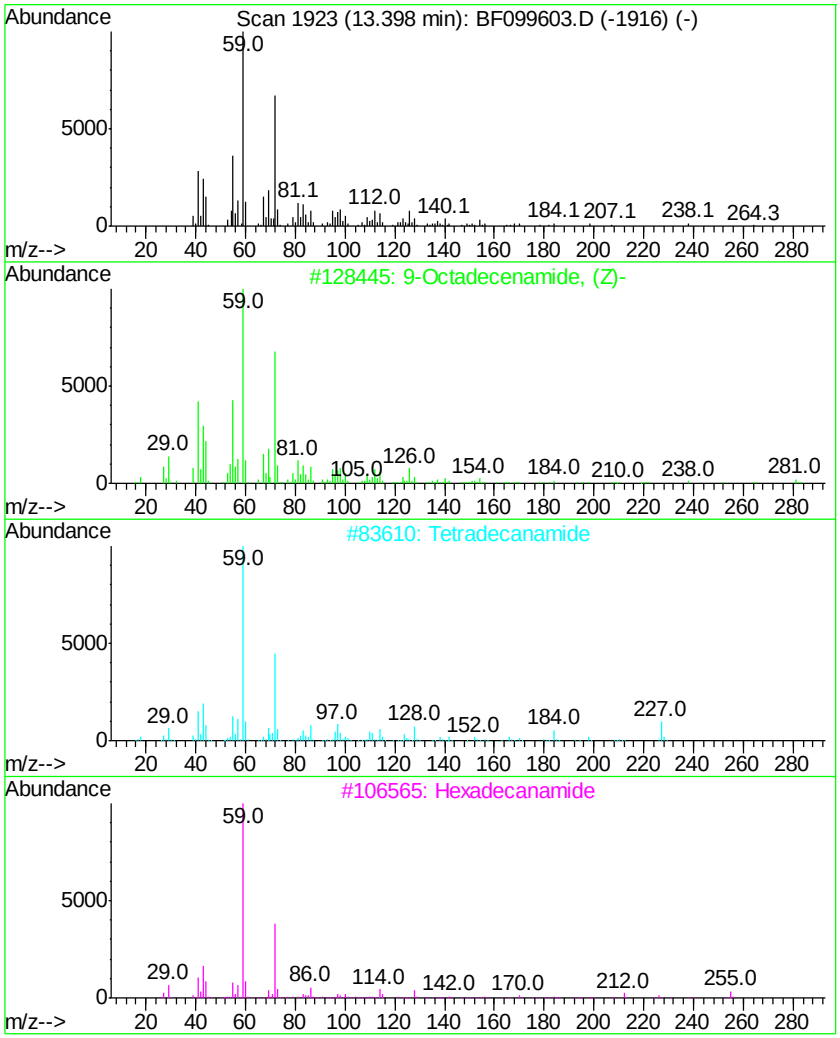
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

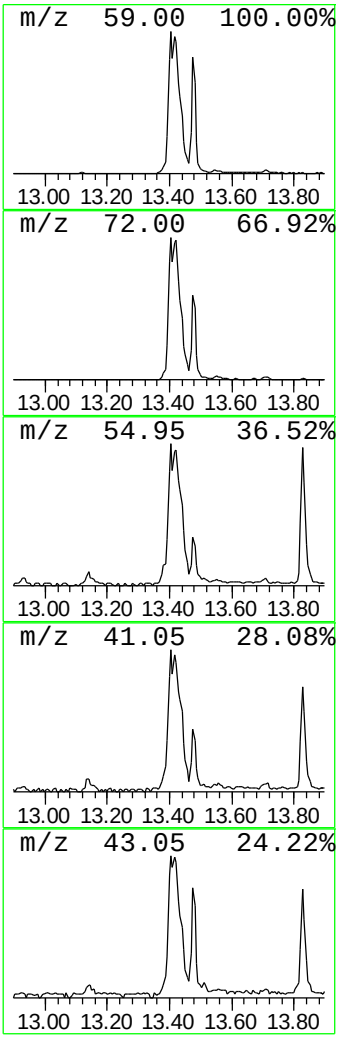
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	15.49 ng	405368	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Tetradecanamide	227	C14H29NO	000638-58-4	72
3	Hexadecanamide	255	C16H33NO	000629-54-9	59
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Pentanamide	101	C5H11NO	000626-97-1	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

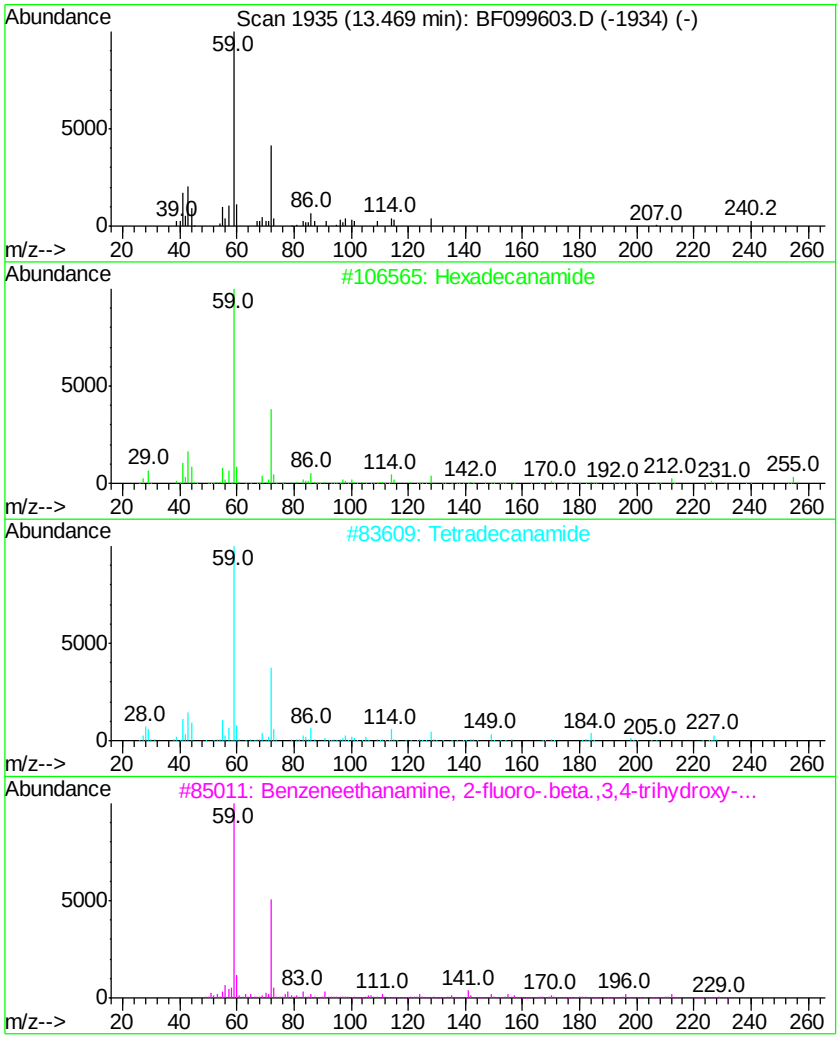
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

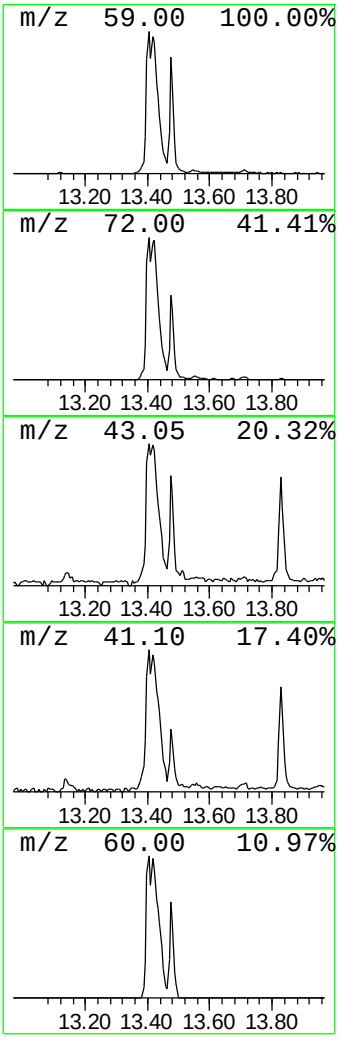
****

Peak Number 10 Hexadecanamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	5.80 ng	151637	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	86
2	Tetradecanamide	227	C14H29NO	000638-58-4	86
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	72
4	Dodecanamide	199	C12H25NO	001120-16-7	64
5	Decanamide-	171	C10H21NO	002319-29-1	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

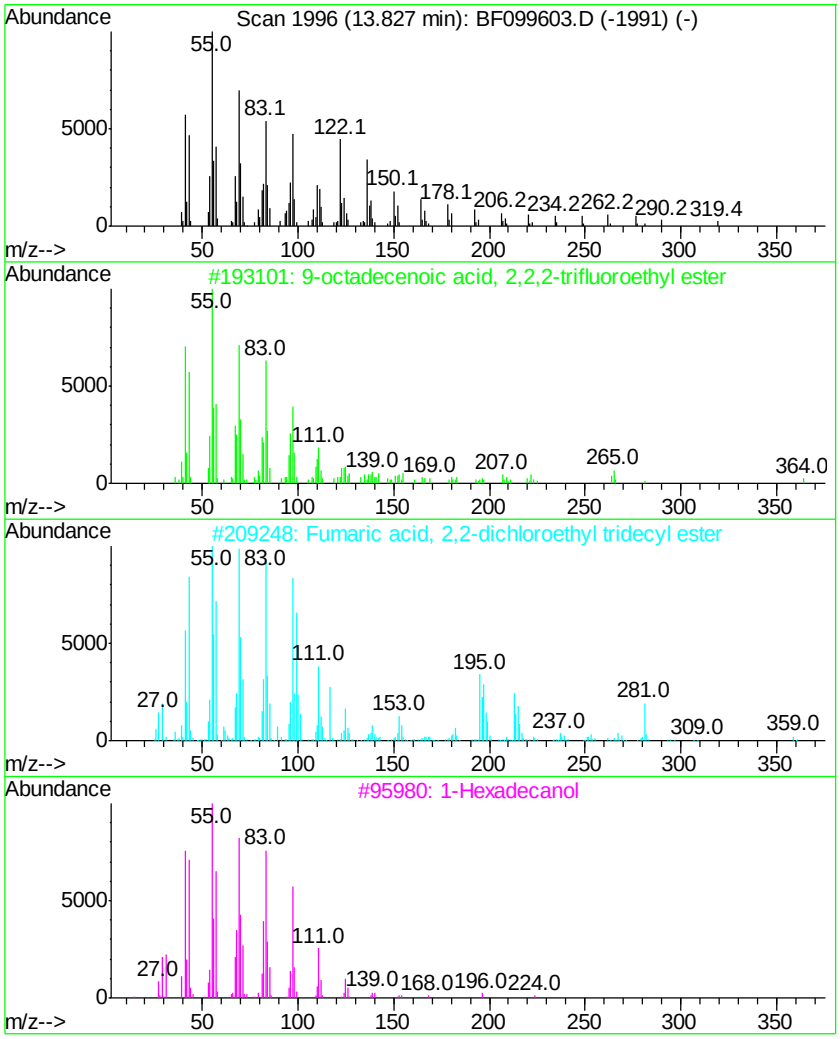
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

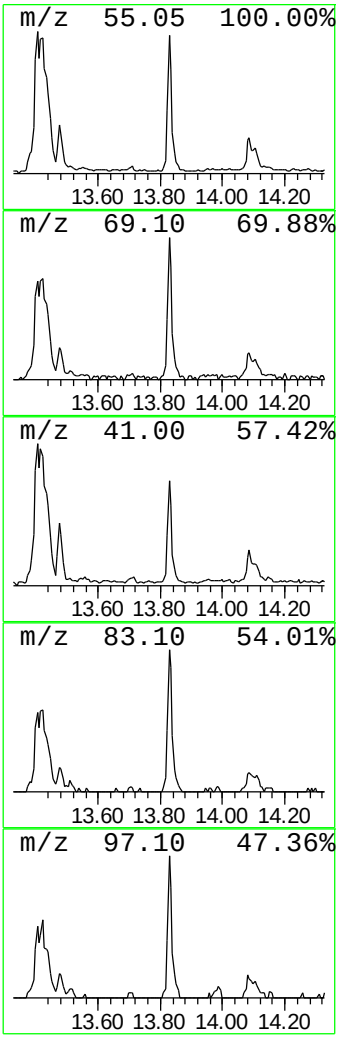
****

Peak Number 11 unknown13.83 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	10.01 ng	261827	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	45
2	Fumaric acid, 2,2-dichloroethyl ...	394	C19H32Cl2O4	1000348-58-1	43
3	1-Hexadecanol	242	C16H34O	036653-82-4	41
4	1-Tetradecene, 14-bromo-	274	C14H27Br	074646-31-4	38
5	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

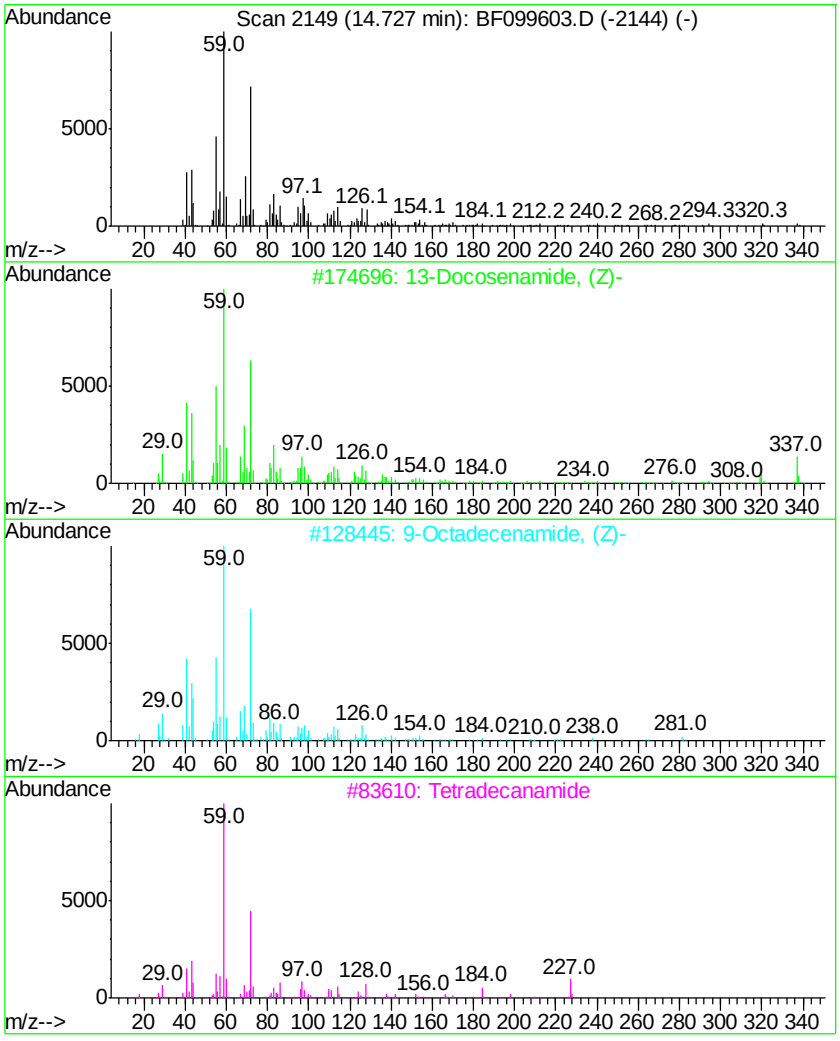
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

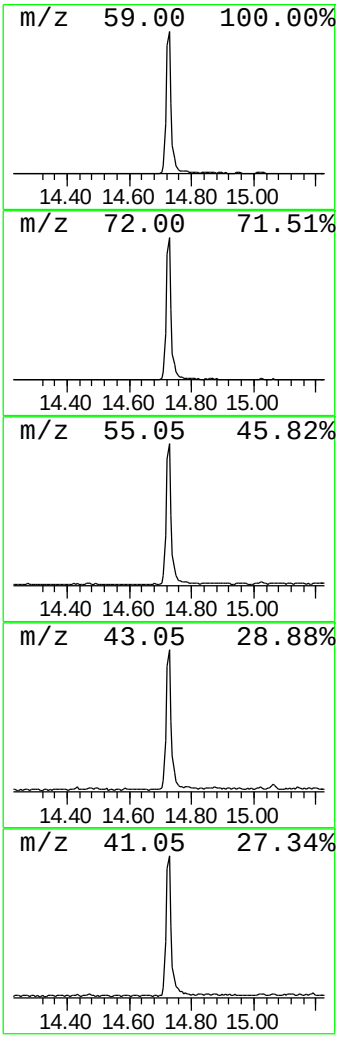
****

Peak Number 13 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	43.70 ng	998852	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	Tetradecanamide	227	C14H29NO	000638-58-4	59
4	2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	43
5	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
Data File : BF099603.D
Acq On : 18 Oct 2017 1:26
Operator : SJ/JU
Sample : I5837-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20170685-FB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
4-Penten-2-one, 4...	3.54	3.4	ng	105507	1	6.83	626180	20.0
3-Hexen-2-one	4.43	53.8	ng	1684060	1	6.83	626180	20.0
2-Pentanone, 4-hy...	5.05	3.8	ng	118323	1	6.83	626180	20.0
unknown6.60	6.60	76.7	ng	2402760	1	6.83	626180	20.0
unknown12.39	12.39	4.7	ng	169776	4	11.35	730010	20.0
9-Octadecenamide,...	13.40	15.5	ng	405368	5	13.99	523227	20.0
Hexadecanamide	13.47	5.8	ng	151637	5	13.99	523227	20.0
unknown13.83	13.83	10.0	ng	261827	5	13.99	523227	20.0
13-Docosenamide, ...	14.73	43.7	ng	998852	6	15.45	457091	20.0