LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

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-BF012218.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	4.934	479	484	492	rBV	90999	143859	2.95%	0.377%
2	5.340	548	553	556	rBV	4124085	4367083	89.52%	11.459%
3	6.375	723	729	740	rBV	3888998	4878583	100.00%	12.801%
4	6.498	745	750	753	rBV	4505353	4384551	89.87%	11.505%
5	6.722	784	788	795	rBV	1215800	1011937	20.74%	2.655%
6	6.875	810	814	818	rBV	3258957	3140584	64.37%	8.241%
7	7.292	880	885	888	rBV	2729393	2651342	54.35%	6.957%
8	7.386	898	901	910	rVB	51236	63517	1.30%	0.167%
9	8.004	1002	1006	1012	rBV	1565855	1314315	26.94%	3.449%
10	9.080	1184	1189	1192	rBV	4195404	3659457	75.01%	9.602%
11	9.475	1252	1256	1264	rVB	479887	419871	8.61%	1.102%
12	9.757	1300	1304	1307	rBV	1483763	1279547	26.23%	3.357%
13	9.786	1307	1309	1316	rVB	140106	137668	2.82%	0.361%
14	10.469	1422	1425	1430	rBV	110336	101451	2.08%	0.266%
15	10.551	1435	1439	1447	rBV	2048401	1983129	40.65%	5.203%
16	11.245	1553	1557	1562	rBV	1193807	1058953	21.71%	2.779%
17	12.645	1792	1795	1799	rBV2	130576	101609	2.08%	0.267%
18	12.721	1806	1808	1815	rVB3	62138	62451	1.28%	0.164%
19	12.833	1822	1827	1830	rBV	2547891	2555823	52.39%	6.706%
20	13.051	1858	1864	1868	rBV2	158499	226837	4.65%	0.595%
21	13.351	1912	1915	1918	rVB	74086	65495	1.34%	0.172%
22	13.392	1918	1922	1925	rBV2	54241	72961	1.50%	0.191%
23	13.721	1974	1978	1985	rBV	608818	731028	14.98%	1.918%
24	13.774	1985	1987	1991	rVB2	63169	64059	1.31%	0.168%
25	13.886	2002	2006	2012	rBV	942473	878133	18.00%	2.304%
26	14.039	2030	2032	2035	rBV2	66004	71445	1.46%	0.187%
27	14.162	2051	2053	2057	rBV3	55684	50699	1.04%	0.133%
28	14.357	2081	2086	2092	rBV2	566505	890140	18.25%	2.336%
29	14.404	2092	2094	2099	rVB	124854	107014	2.19%	0.281%
30	14.962	2186	2189	2192	rBV	274859	272583	5.59%	0.715%
31	14.998	2192	2195	2200	rVV3	156270	241741	4.96%	0.634%
32	15.039	2200	2202	2207	rVB	153301	174023	3.57%	0.457%
33	15.321	2245	2250	2258	rBV	519843	710185	14.56%	1.863%
34	15.733	2317	2320	2326	rVB	174685	239447	4.91%	0.628%

LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

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-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 38111520

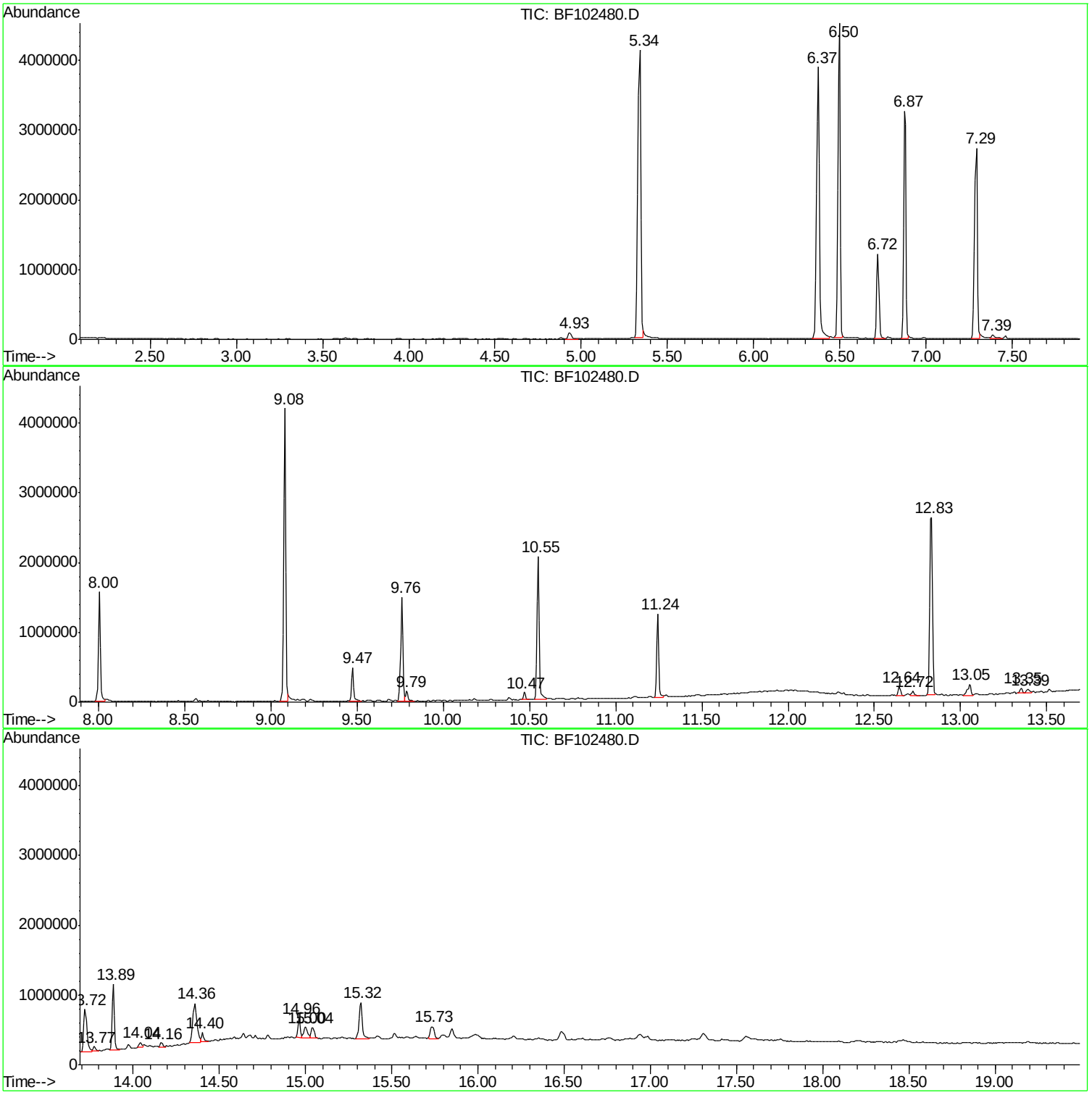
LSC Report - Integrated Chromatogram

Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

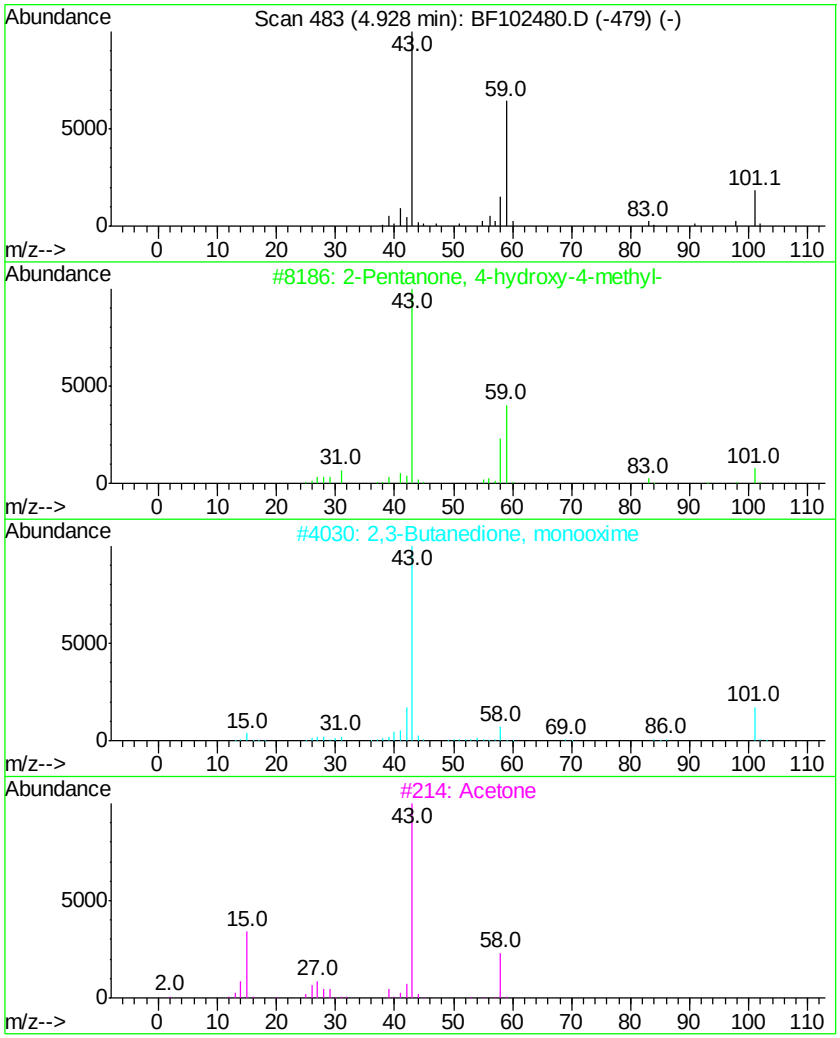
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

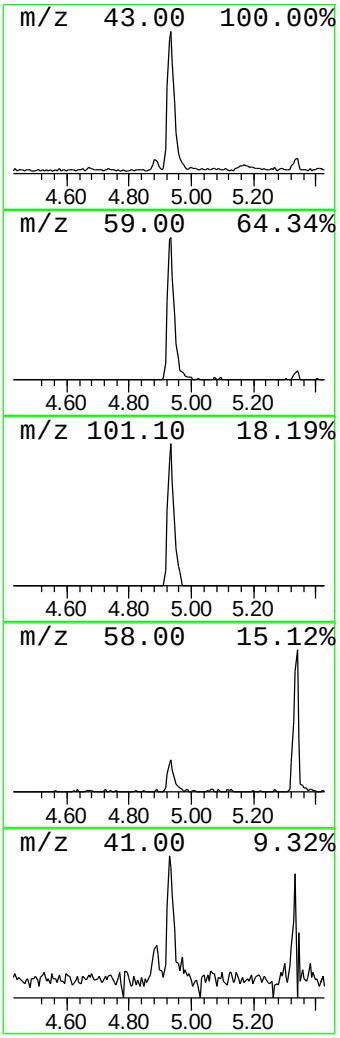
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.84 ng	143859	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetone	58	C3H6O	000067-64-1	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

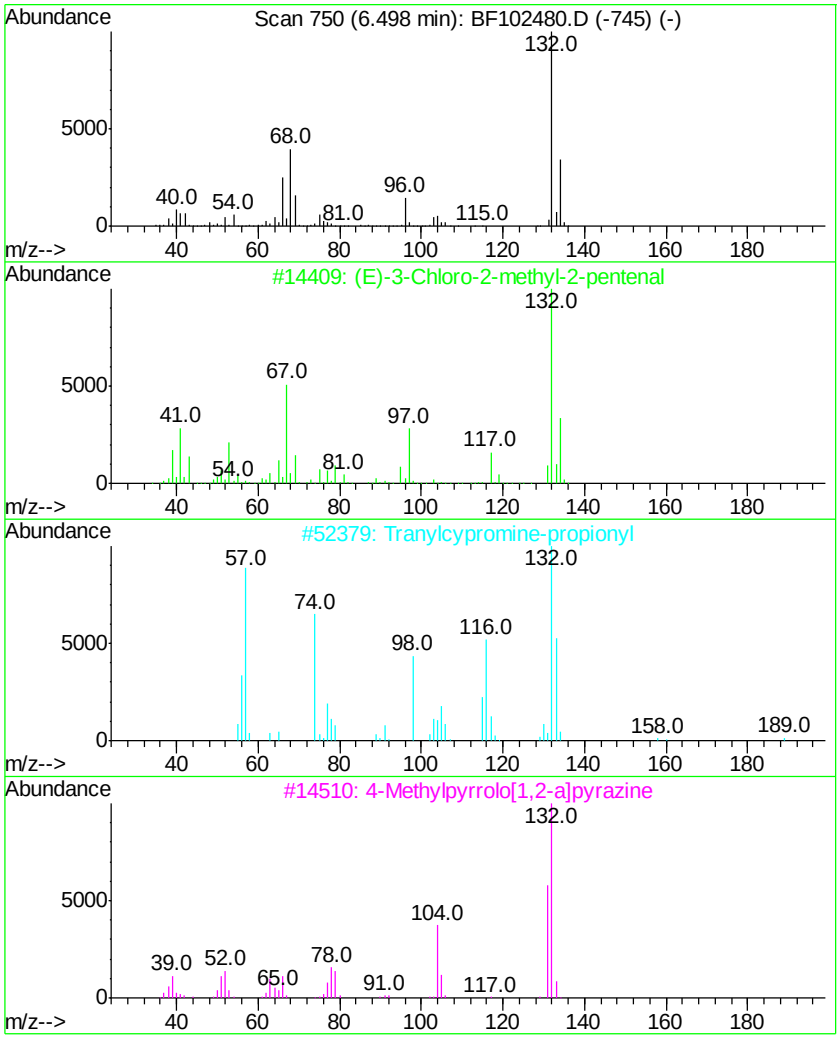
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

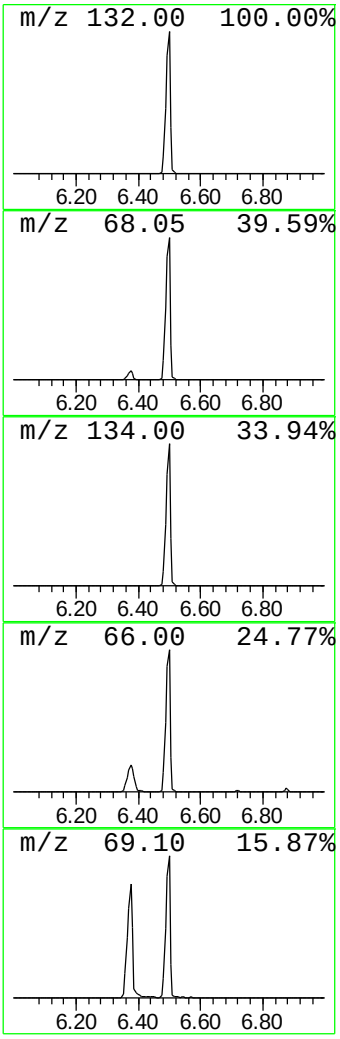
****

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	86.66 ng	4384550	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

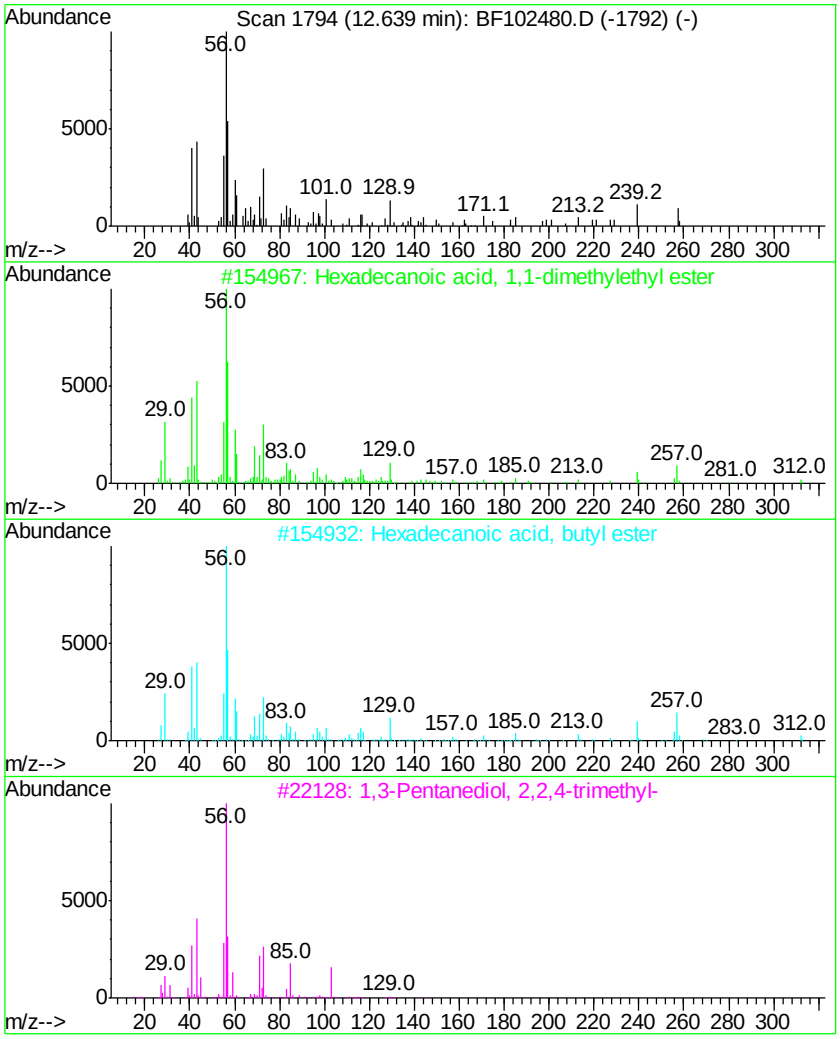
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

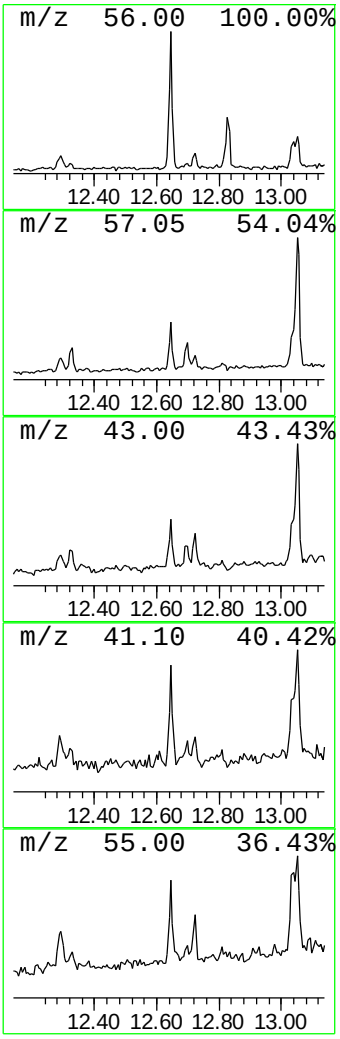
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexadecanoic acid, 1,1-dime... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.31 ng	101609	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
3	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	47
4	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	38
5	Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	35





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

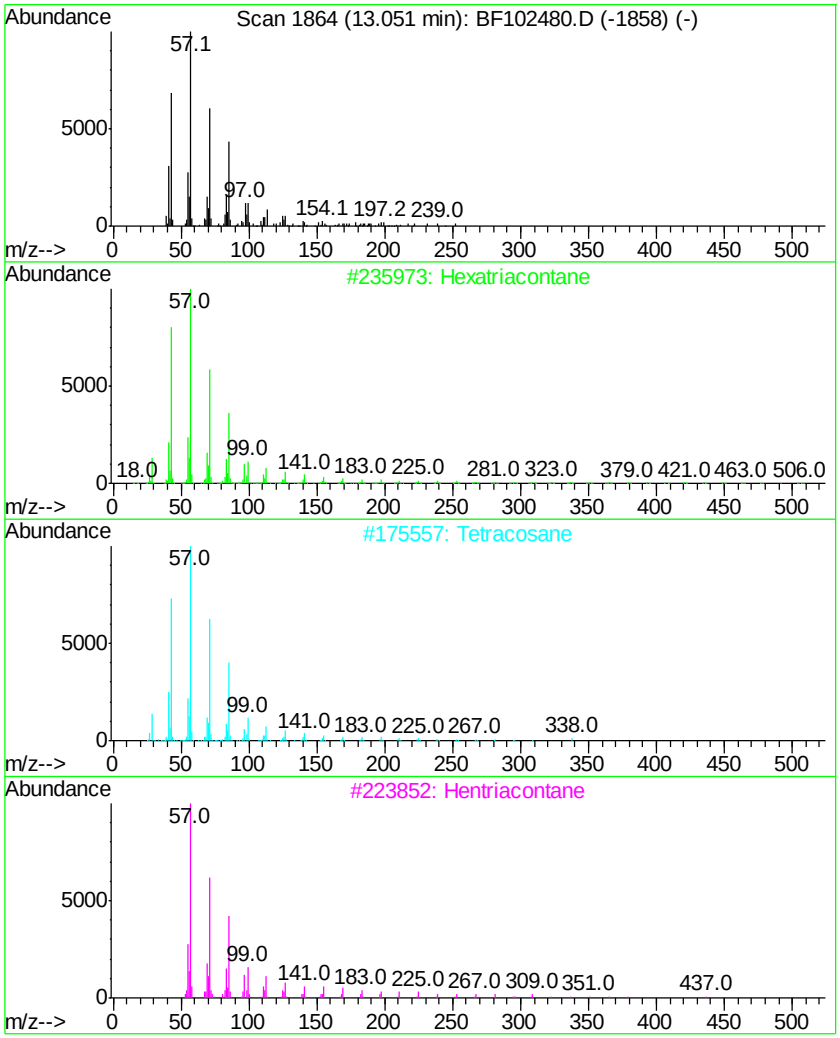
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

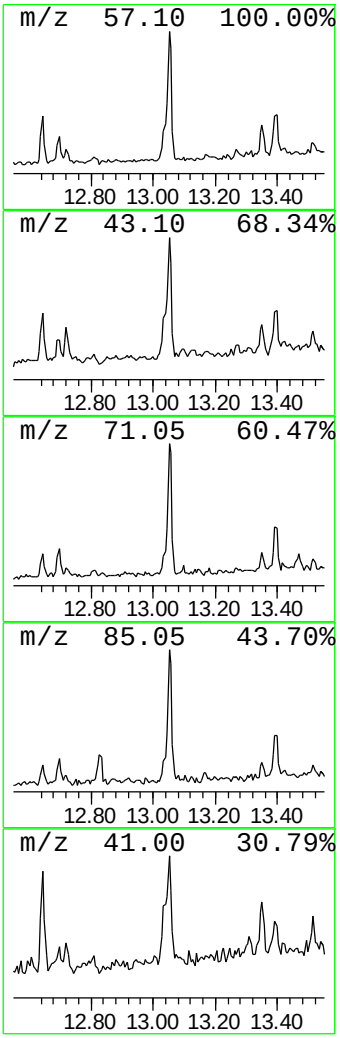
****

Peak Number 5 Hexatriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.05	5.17 ng	226837	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	87
2	Tetracosane	338	C24H50	000646-31-1	87
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Octacosane	394	C28H58	000630-02-4	87





Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

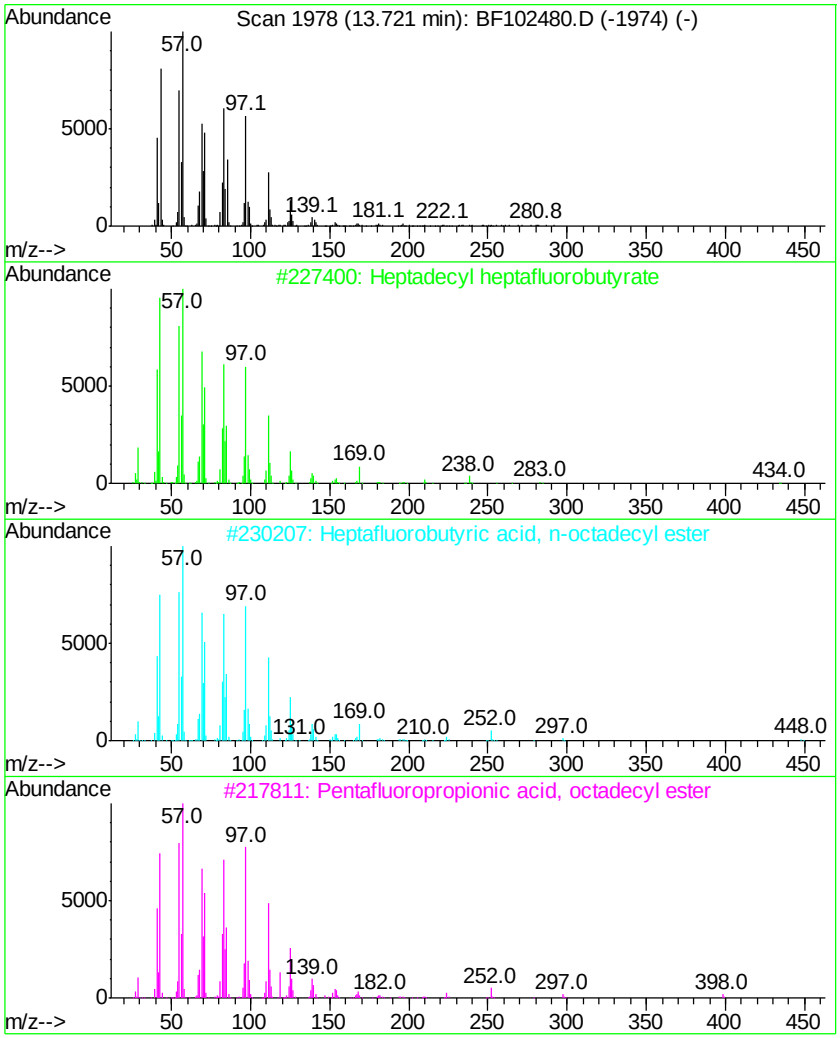
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

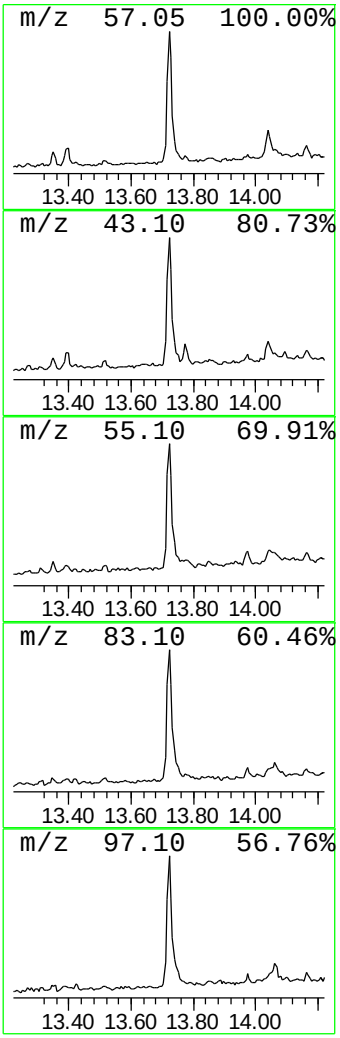
****

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	16.65 ng	731028	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

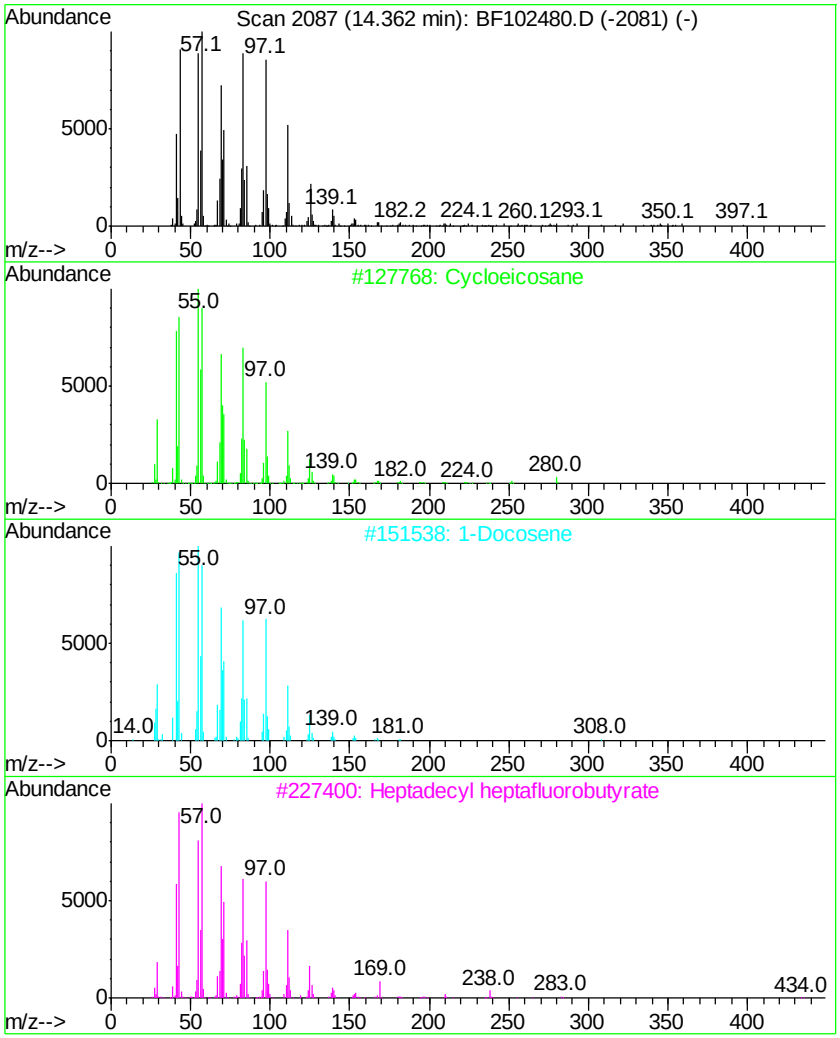
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

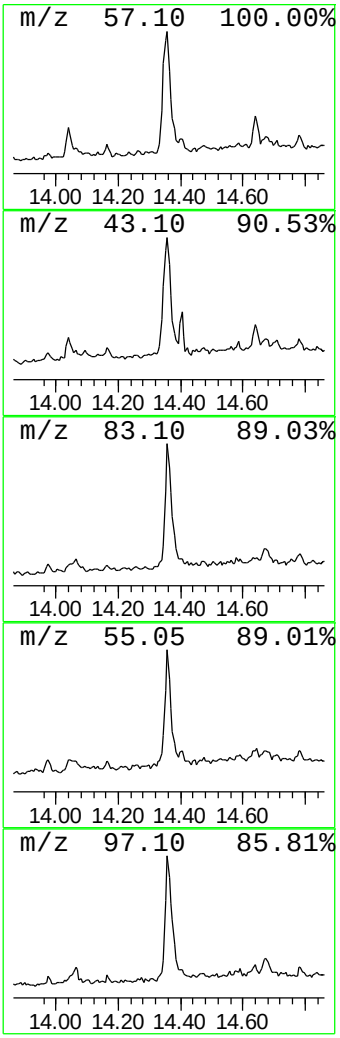
****

Peak Number 7 Cycloeicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	20.27 ng	890140	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	95
2	1-Docosene	308	C22H44	001599-67-3	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

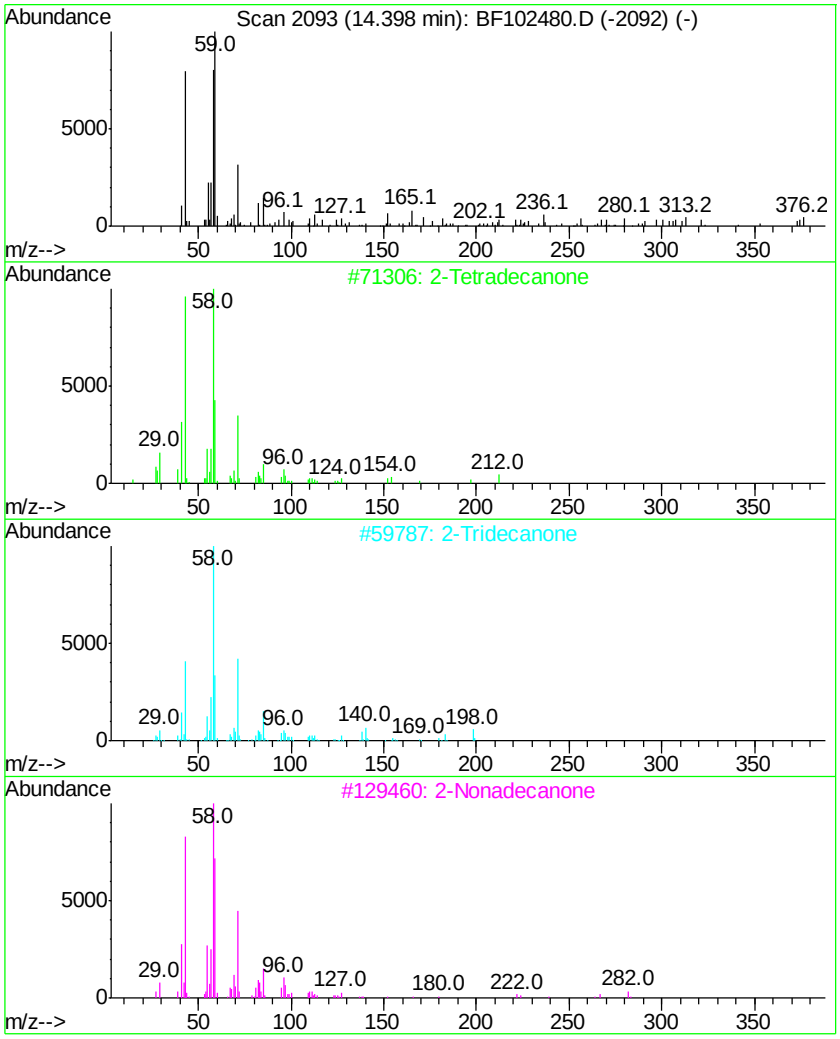
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

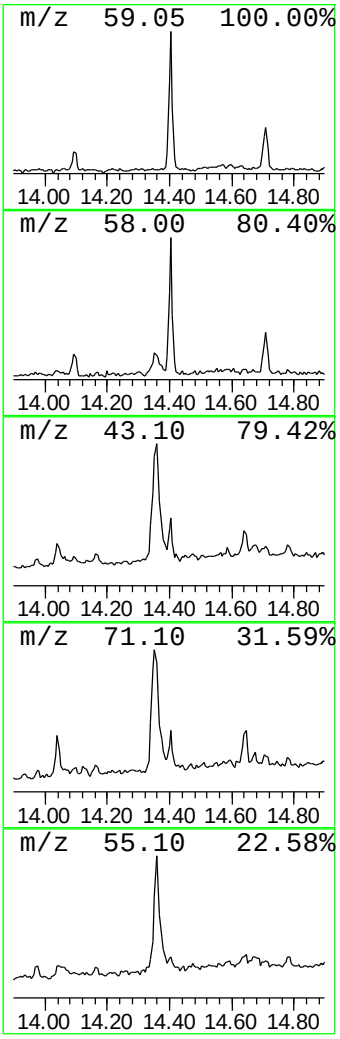
****

Peak Number 8 2-Tetradecanone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	2.44 ng	107014	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Tetradecanone	212	C14H28O	002345-27-9	59
2	2-Tridecanone	198	C13H26O	000593-08-8	50
3	2-Nonadecanone	282	C19H38O	000629-66-3	45
4	2-Pentadecanone	226	C15H30O	002345-28-0	45
5	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	43





Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

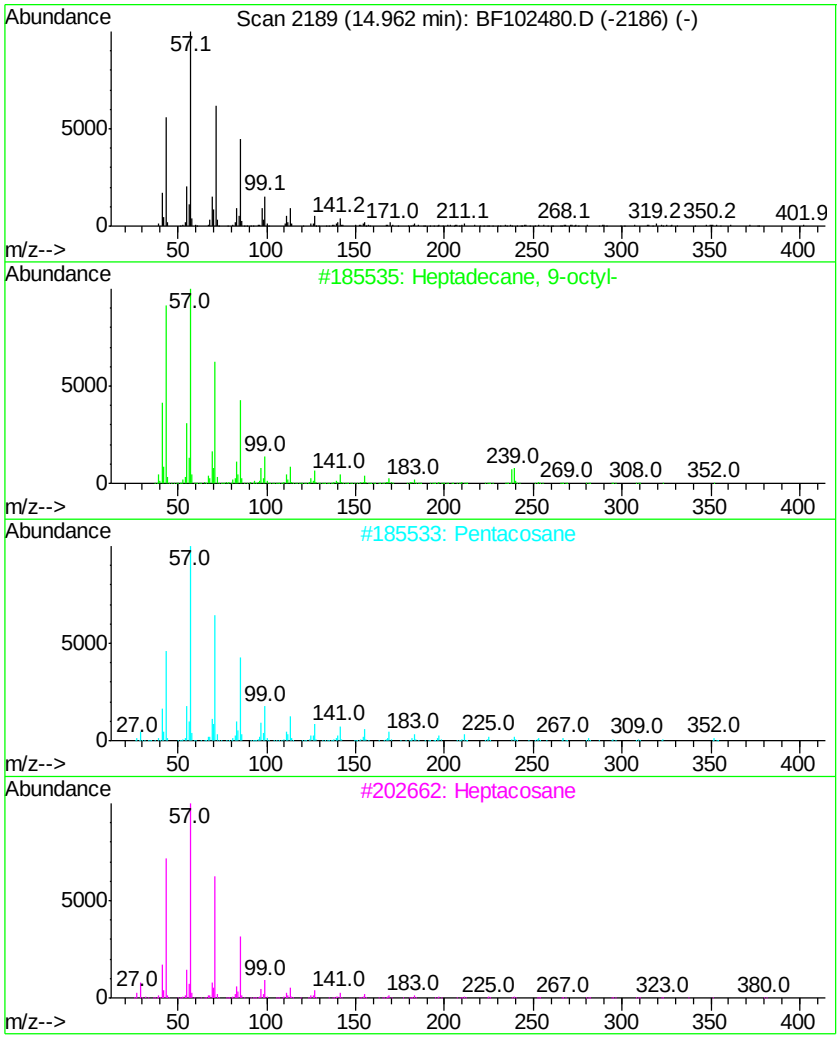
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

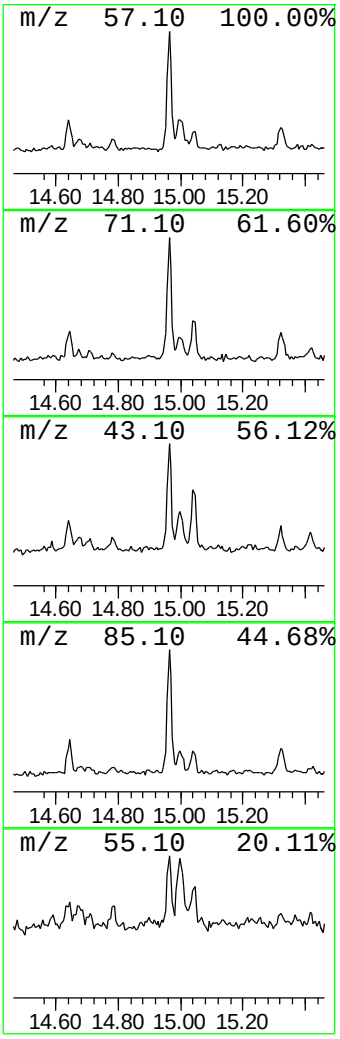
****

Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	7.68 ng	272583	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heptacosane	380	C27H56	000593-49-7	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Triacontane	422	C30H62	000638-68-6	90





Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

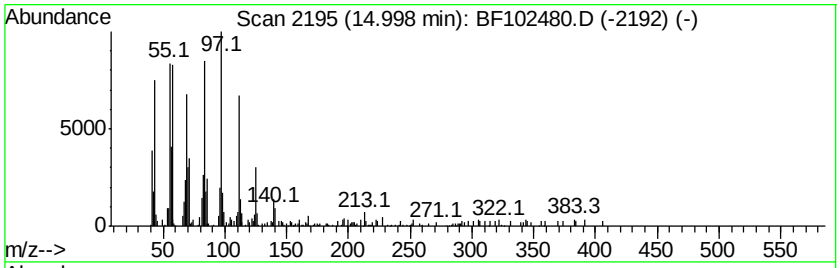
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

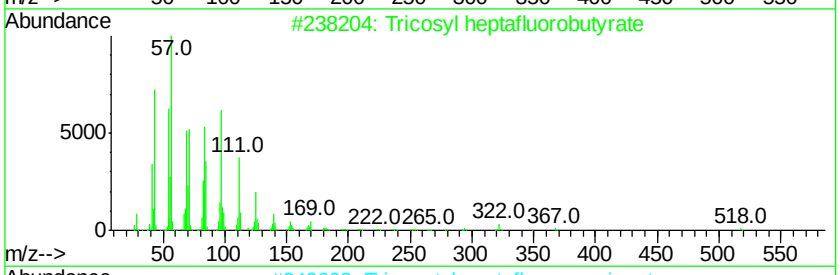
****

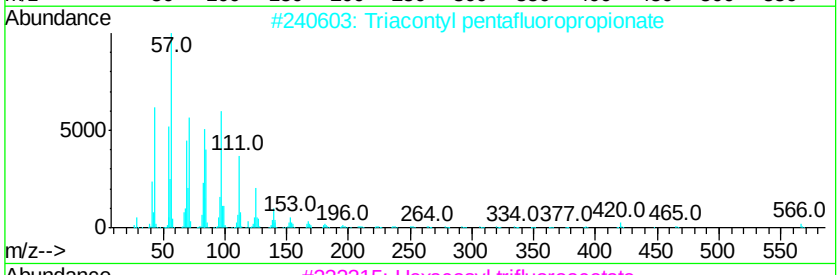
Peak Number 10 Tricosyl heptafluorobutyrate Concentration Rank 6

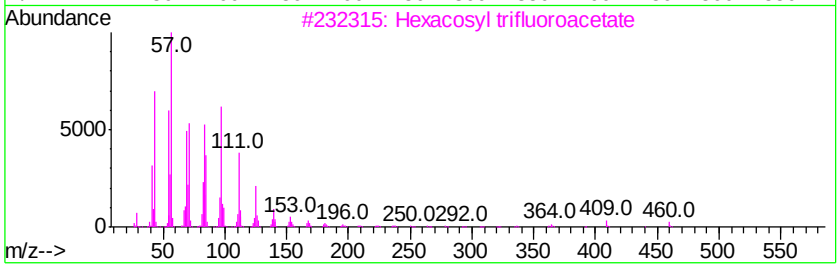
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	6.81 ng	241741	Perylene-d12	15.32

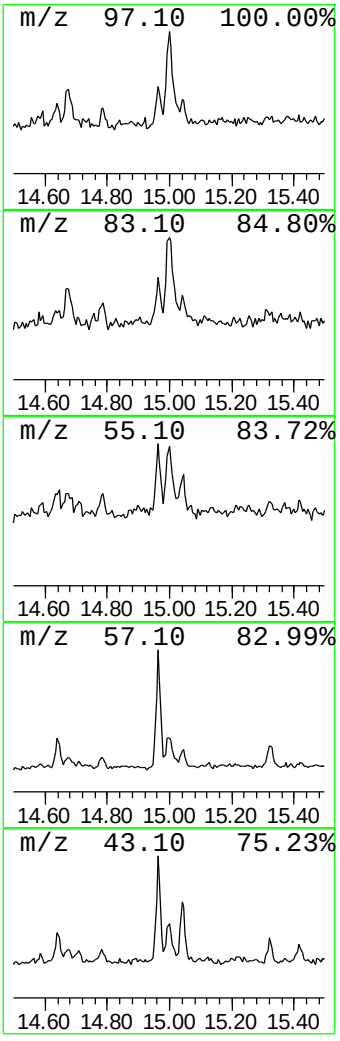
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	87
2	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	87
3	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	87
4	2-Thiopheneacetic acid, oct-3-en...	252	C14H20O2S	1000299-38-6	80
5	1-Octadecene	252	C18H36	000112-88-9	80











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Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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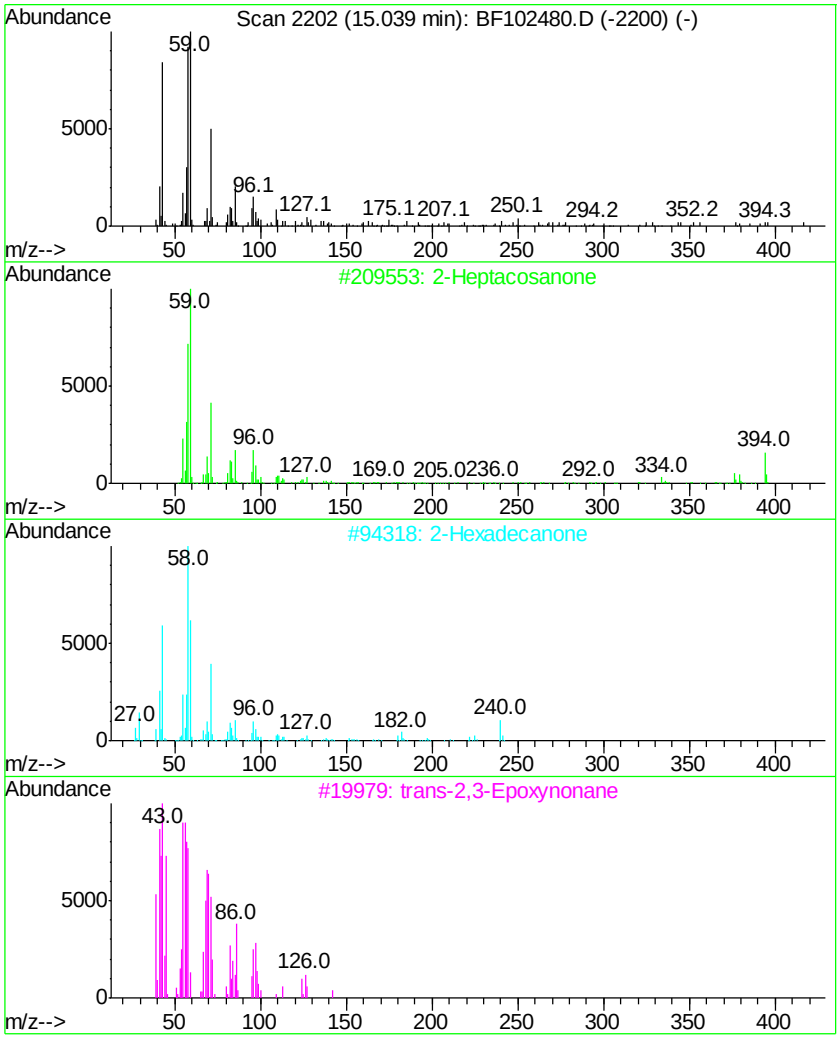
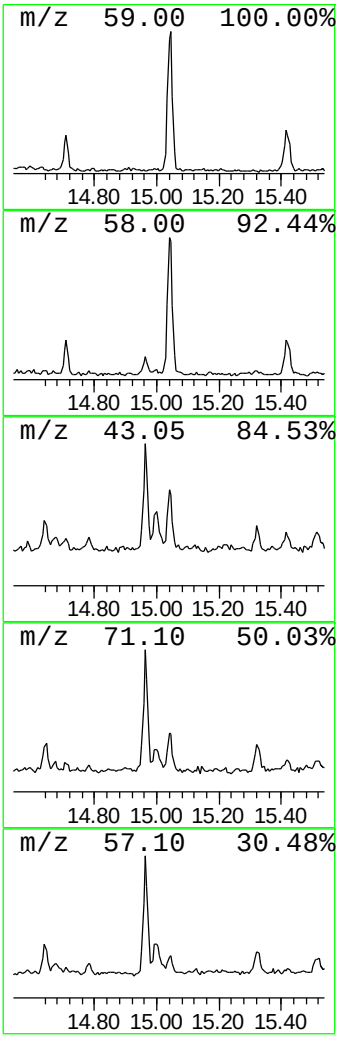
Peak Number 11 2-Heptacosanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	4.90 ng	174023	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptacosanone	394	C27H54O	007796-19-2	93
2	2-Hexadecanone	240	C16H32O	018787-63-8	53
3	trans-2,3-Epoxynonane	142	C9H18O	056820-01-0	50
4	Oxirane, 3-ethyl-2,2-dimethyl-	100	C6H12O	001192-22-9	47
5	2-Tridecanone	198	C13H26O	000593-08-8	47





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Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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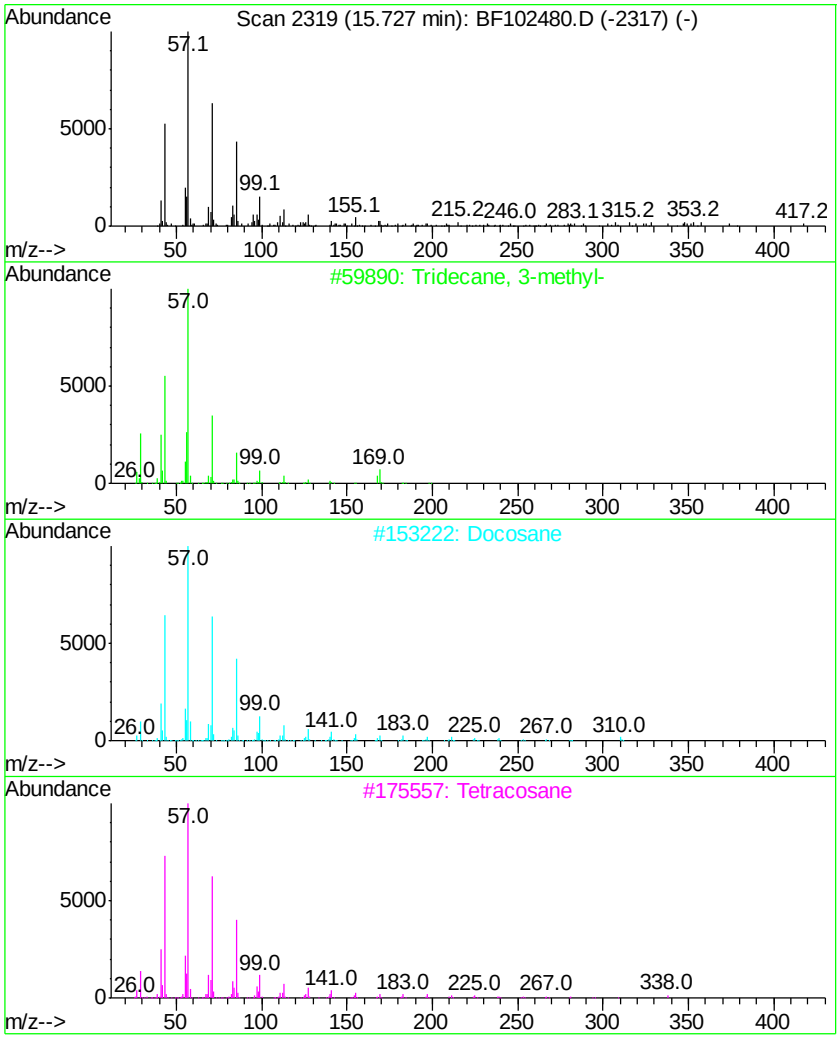
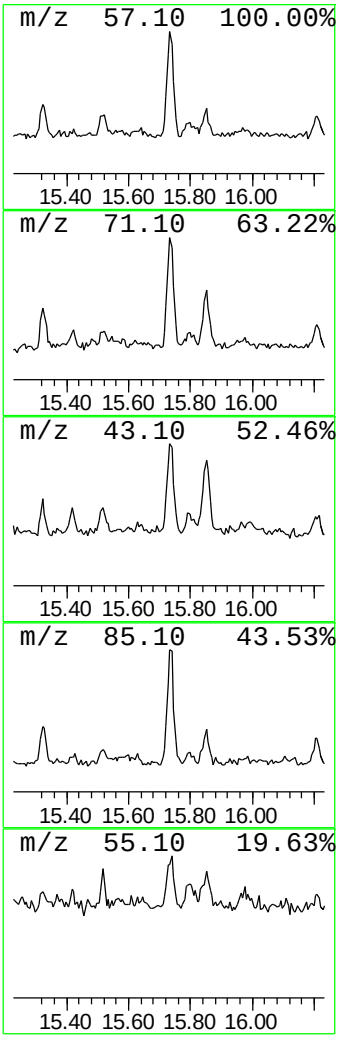
Peak Number 12 Tridecane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	6.74 ng	239447	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 3-methyl-	198	C14H30	006418-41-3	93
2	Docosane	310	C22H46	000629-97-0	86
3	Tetracosane	338	C24H50	000646-31-1	86
4	Tricosane	324	C23H48	000638-67-5	86
5	2-methyltetracosane	352	C25H52	1000376-72-6	86





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF012618\
Data File : BF102480.D
Acq On : 26 Jan 2018 20:29
Operator : SJ/JU
Sample : J1289-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-53-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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...	4.93	2.8	ng	143859	1	6.72	1011940	20.0
unknown6.50	6.50	86.7	ng	4384550	1	6.72	1011940	20.0
Hexadecanoic acid...	12.64	2.3	ng	101609	5	13.89	878133	20.0
Hexatriacontane	13.05	5.2	ng	226837	5	13.89	878133	20.0
Heptadecyl heptaf...	13.72	16.6	ng	731028	5	13.89	878133	20.0
Cycloeicosane	14.36	20.3	ng	890140	5	13.89	878133	20.0
2-Tetradecanone	14.40	2.4	ng	107014	5	13.89	878133	20.0
Heptadecane, 9-oc...	14.96	7.7	ng	272583	6	15.32	710185	20.0
Tricosyl heptaflu...	15.00	6.8	ng	241741	6	15.32	710185	20.0
2-Heptacosanone	15.04	4.9	ng	174023	6	15.32	710185	20.0
Tridecane, 3-methyl-	15.73	6.7	ng	239447	6	15.32	710185	20.0