LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119826.D
Acq On : 7 Apr 2020 17:03
Operator : MA/SJ
Sample : L2102-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-46-MEDIAN

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-BF031820.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	2.116	3	5	12	rVB2	63919	75117	1.35%	0.198%
2	4.998	487	495	506	rBV	199996	296807	5.33%	0.784%
3	5.404	558	564	567	rBV	5078460	5425490	97.39%	14.333%
4	6.428	732	738	741	rBV	4555353	5500954	98.74%	14.532%
5	6.786	795	799	802	rBV	692676	522498	9.38%	1.380%
6	6.945	821	826	829	rBV	4410304	3998991	71.78%	10.565%
7	7.357	889	896	899	rBV	3074635	3288053	59.02%	8.686%
8	8.069	1013	1017	1021	rBV	725005	644702	11.57%	1.703%
9	9.157	1196	1202	1205	rBV	5848696	5571003	100.00%	14.718%
10	9.545	1264	1268	1271	rBV	576911	425595	7.64%	1.124%
11	9.827	1310	1316	1320	rBV	809534	707881	12.71%	1.870%
12	10.621	1446	1451	1454	rBV	3297867	2981876	53.52%	7.878%
13	11.316	1566	1569	1572	rBV	773162	620329	11.13%	1.639%
14	11.851	1657	1660	1669	rBV	427986	438135	7.86%	1.157%
15	12.027	1687	1690	1693	rBV2	46582	61284	1.10%	0.162%
16	12.415	1752	1756	1760	rBV3	45637	59751	1.07%	0.158%
17	12.533	1771	1776	1778	rBV	91007	106596	1.91%	0.282%
18	12.633	1790	1793	1798	rBV	166177	222230	3.99%	0.587%
19	12.733	1807	1810	1812	rBV	143440	115654	2.08%	0.306%
20	12.786	1817	1819	1822	rVB	89567	75120	1.35%	0.198%
21	12.910	1836	1840	1844	rBV	4572266	4776780	85.74%	12.619%
22	13.439	1928	1930	1933	rVB2	106494	80945	1.45%	0.214%
23	13.815	1991	1994	2001	rVB	508909	566793	10.17%	1.497%
24	13.962	2015	2019	2021	rBV	515636	510586	9.17%	1.349%
25	15.074	2205	2208	2213	rVB2	153737	184804	3.32%	0.488%
26	15.409	2262	2265	2270	rBV	319893	453747	8.14%	1.199%
27	16.374	2426	2429	2432	rBV4	87653	141073	2.53%	0.373%

Sum of corrected areas: 37852794

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
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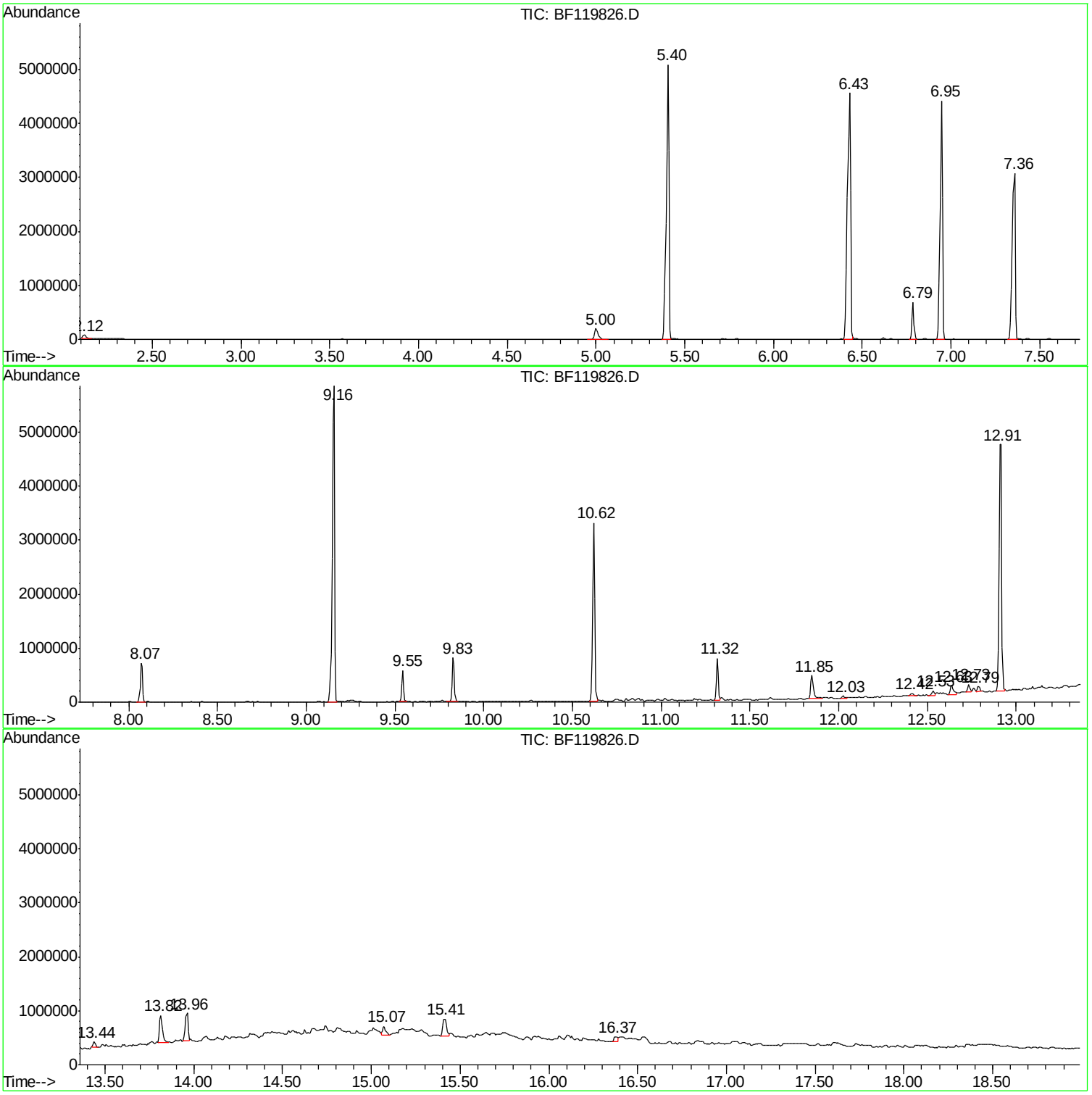
Operator : MA/SJ
Sample : L2102-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-46-MEDIAN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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\BF040620\
Data File : BF119826.D
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Operator : MA/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : RT-46-MEDIAN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

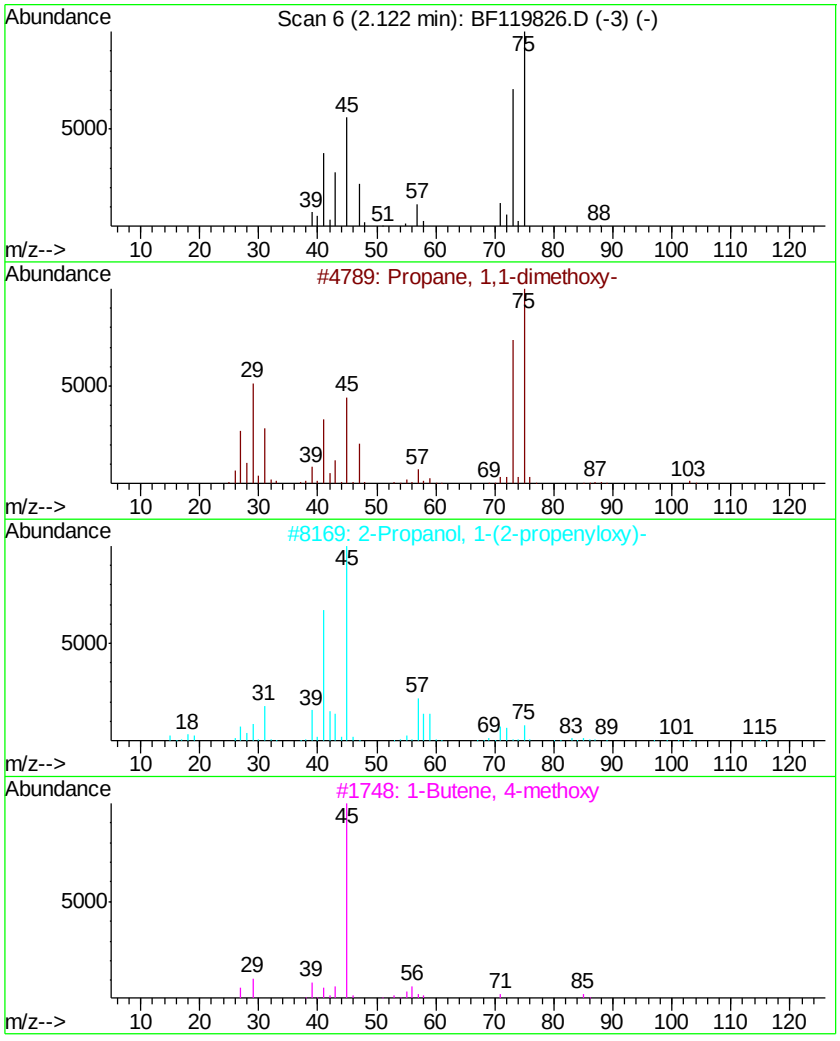
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

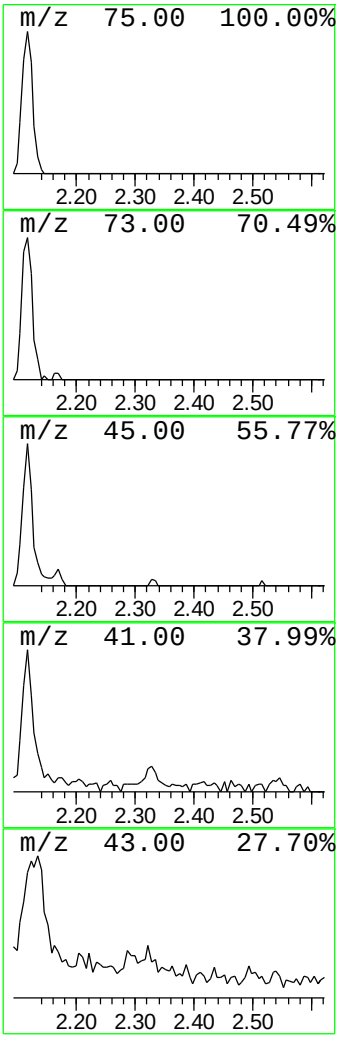
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	2.88 ng	75117	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	2-Propanol, 1-(2-propenyloxy)-	116	C6H12O2	021460-36-6	10
3	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	9
4	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
5	1,2,4-Butanetriol	106	C4H10O3	003068-00-6	9





Library Search Compound Report

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Data File : BF119826.D
Acq On : 7 Apr 2020 17:03
Operator : MA/SJ
Sample : L2102-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-46-MEDIAN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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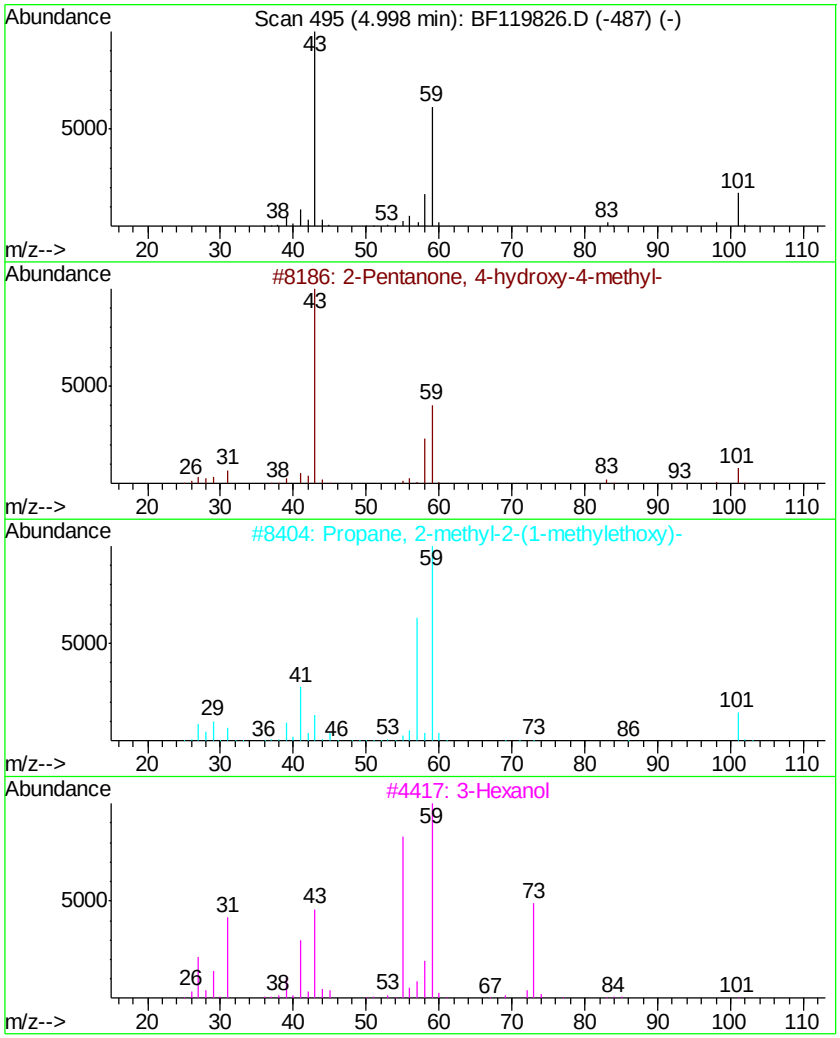
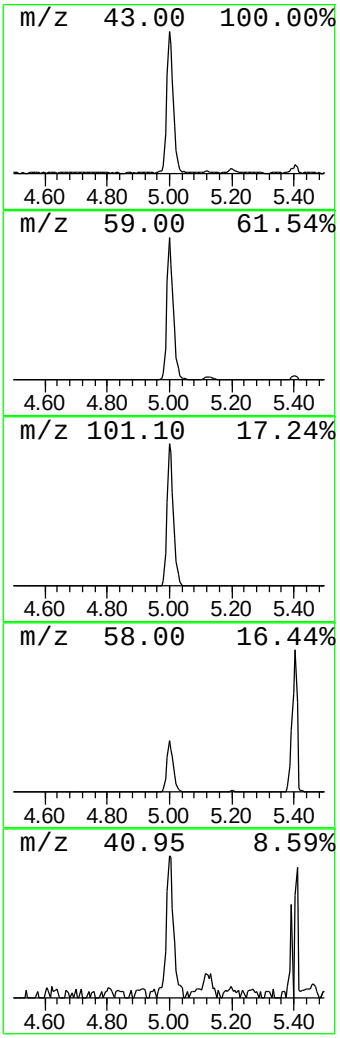
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	11.36 ng	296807	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol	102	C6H14O	000623-37-0	36
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119826.D
Acq On : 7 Apr 2020 17:03
Operator : MA/SJ
Sample : L2102-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-46-MEDIAN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

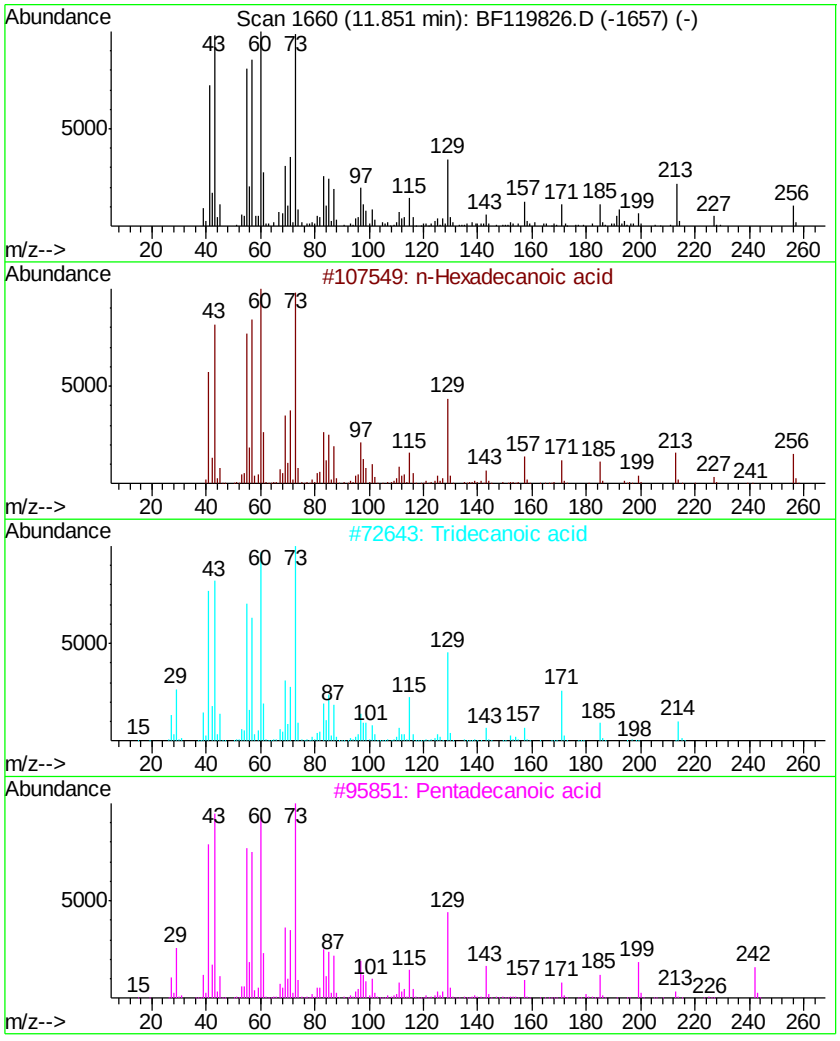
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

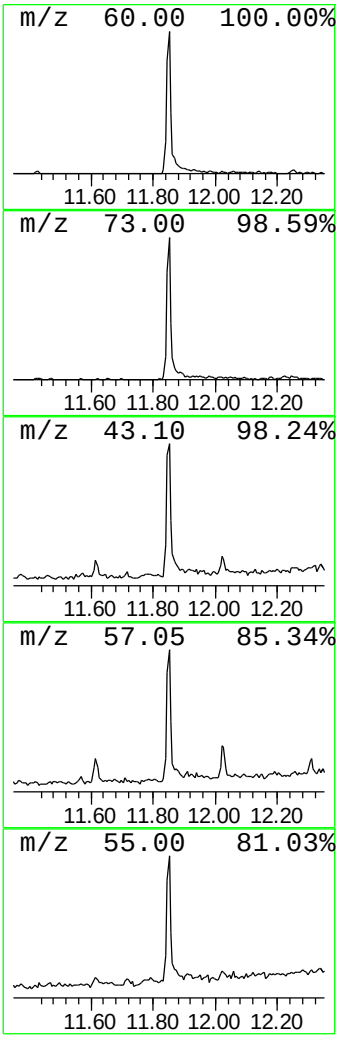
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	14.13 ng	438135	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	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119826.D
Acq On : 7 Apr 2020 17:03
Operator : MA/SJ
Sample : L2102-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-46-MEDIAN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

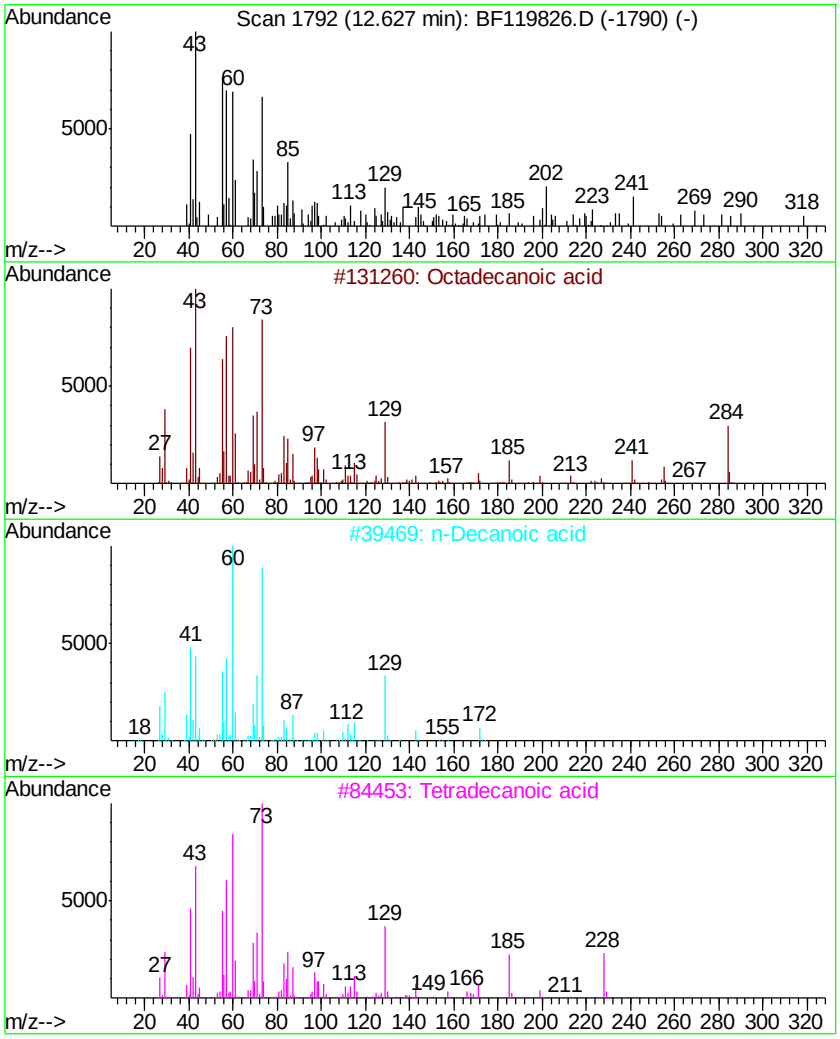
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

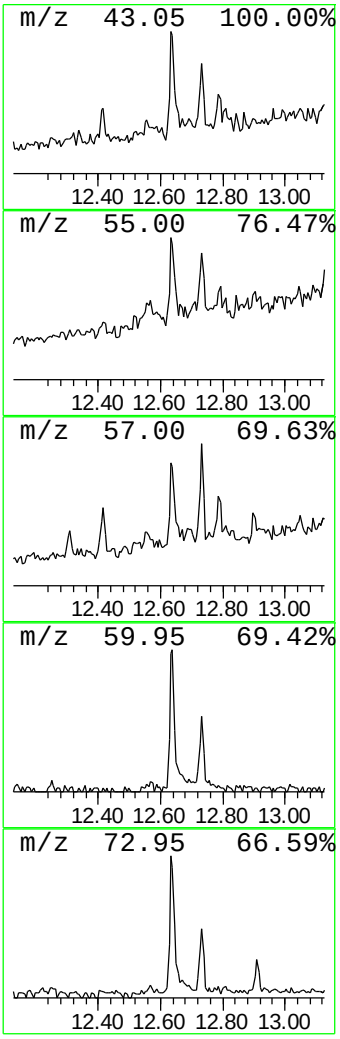
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	7.16 ng	222230	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	n-Decanoic acid	172	C10H20O2	000334-48-5	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	25
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	18





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119826.D
Acq On : 7 Apr 2020 17:03
Operator : MA/SJ
Sample : L2102-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-46-MEDIAN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

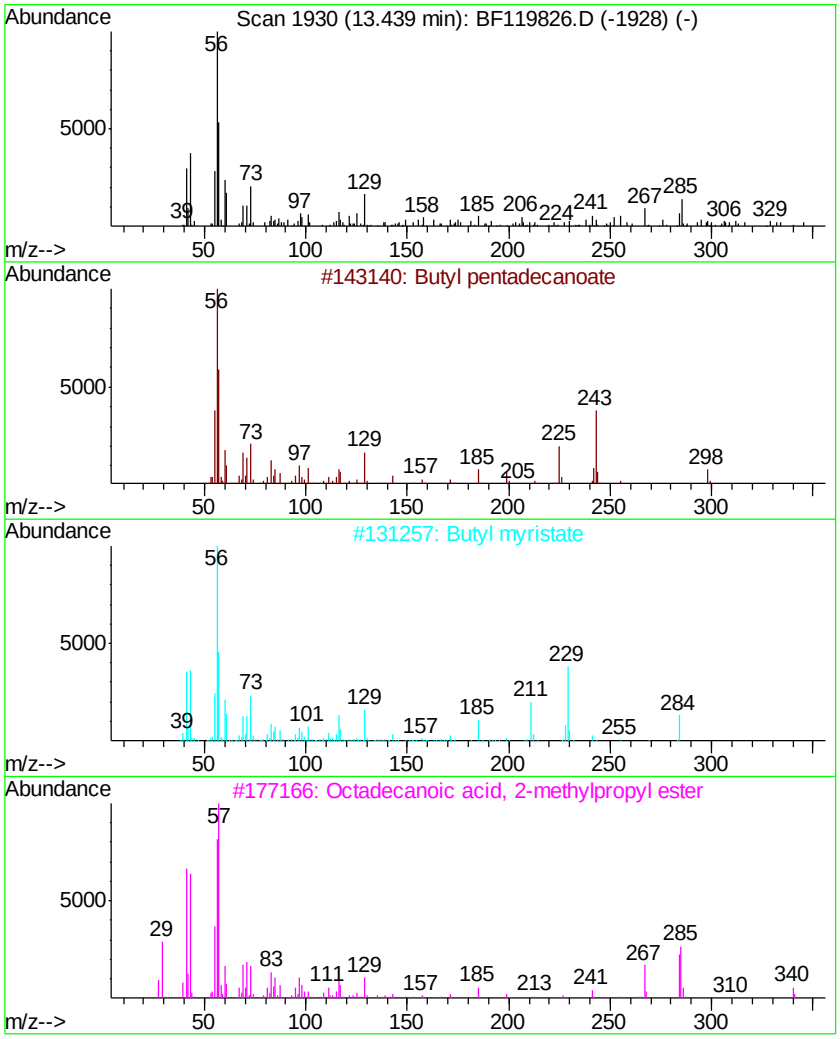
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

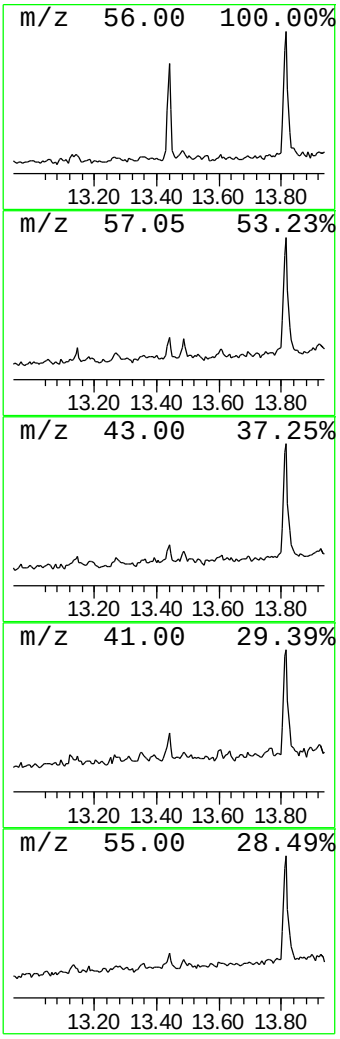
****

Peak Number 7 unknown13.44 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	3.17 ng	80945	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl pentadecanoate	298	C19H38O2	1000336-51-6	42
2	Butyl myristate	284	C18H36O2	000110-36-1	41
3	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	41
4	(n-Butylthio)acetonitrile	129	C6H11NS	071037-08-6	40
5	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38





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Acq On : 7 Apr 2020 17:03
Operator : MA/SJ
Sample : L2102-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-46-MEDIAN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

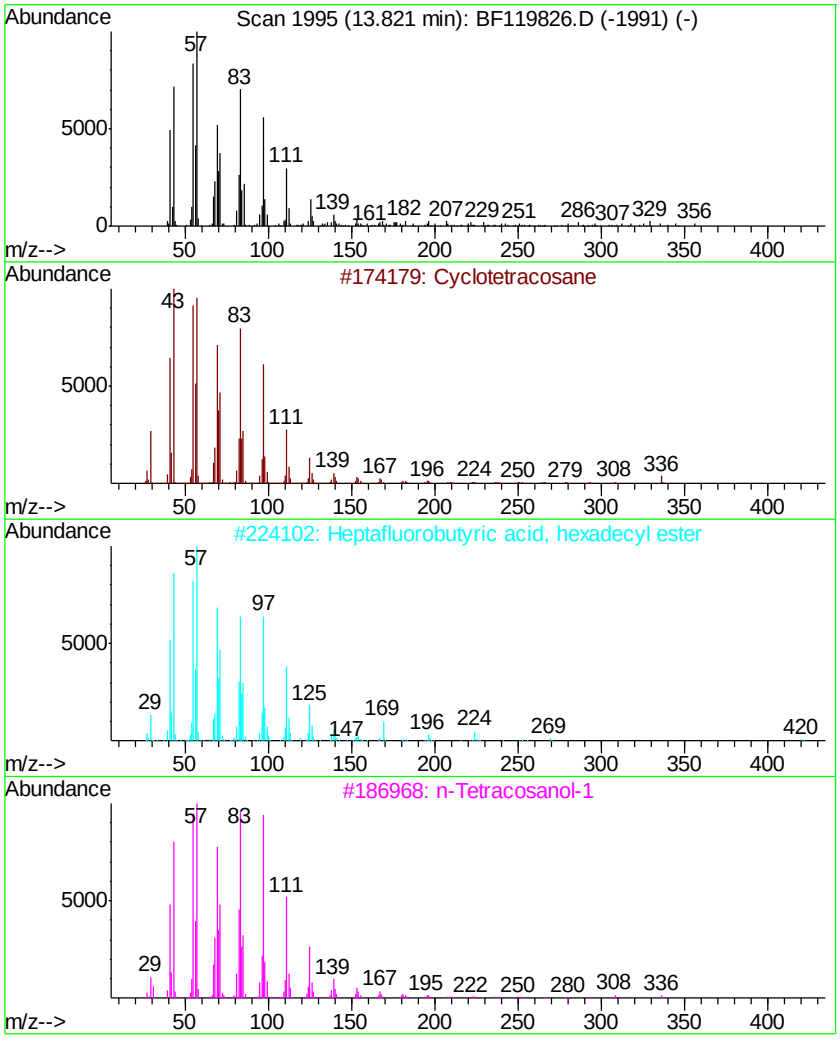
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

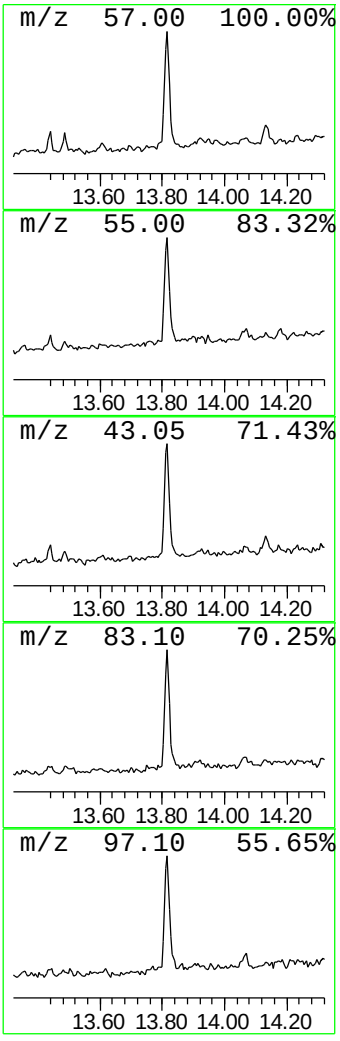
****

Peak Number 8 Cyclotetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	22.20 ng	566793	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	94
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91





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Acq On : 7 Apr 2020 17:03
Operator : MA/SJ
Sample : L2102-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-46-MEDIAN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

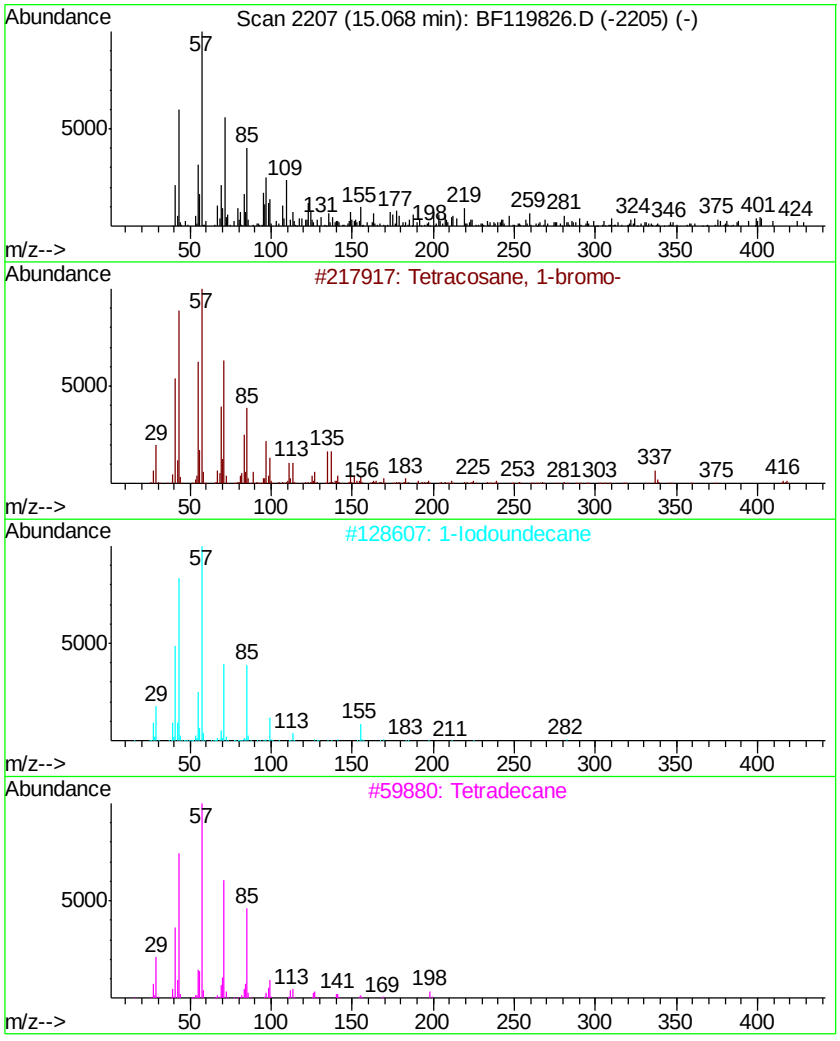
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

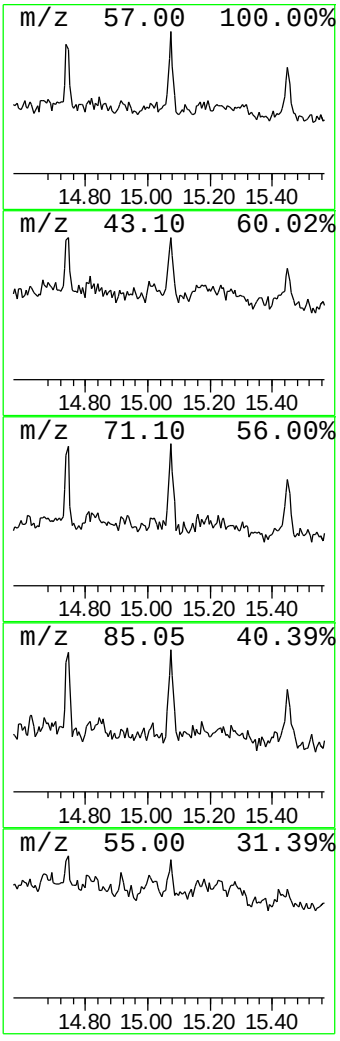
****

Peak Number 9 Tetracosane, 1-bromo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	8.15 ng	184804	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 1-bromo-	416	C24H49Br	006946-24-3	68
2	1-Iodoundecane	282	C11H23I	004282-44-4	68
3	Tetradecane	198	C14H30	000629-59-4	68
4	Docosane	310	C22H46	000629-97-0	59
5	Nonadecane	268	C19H40	000629-92-5	59





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

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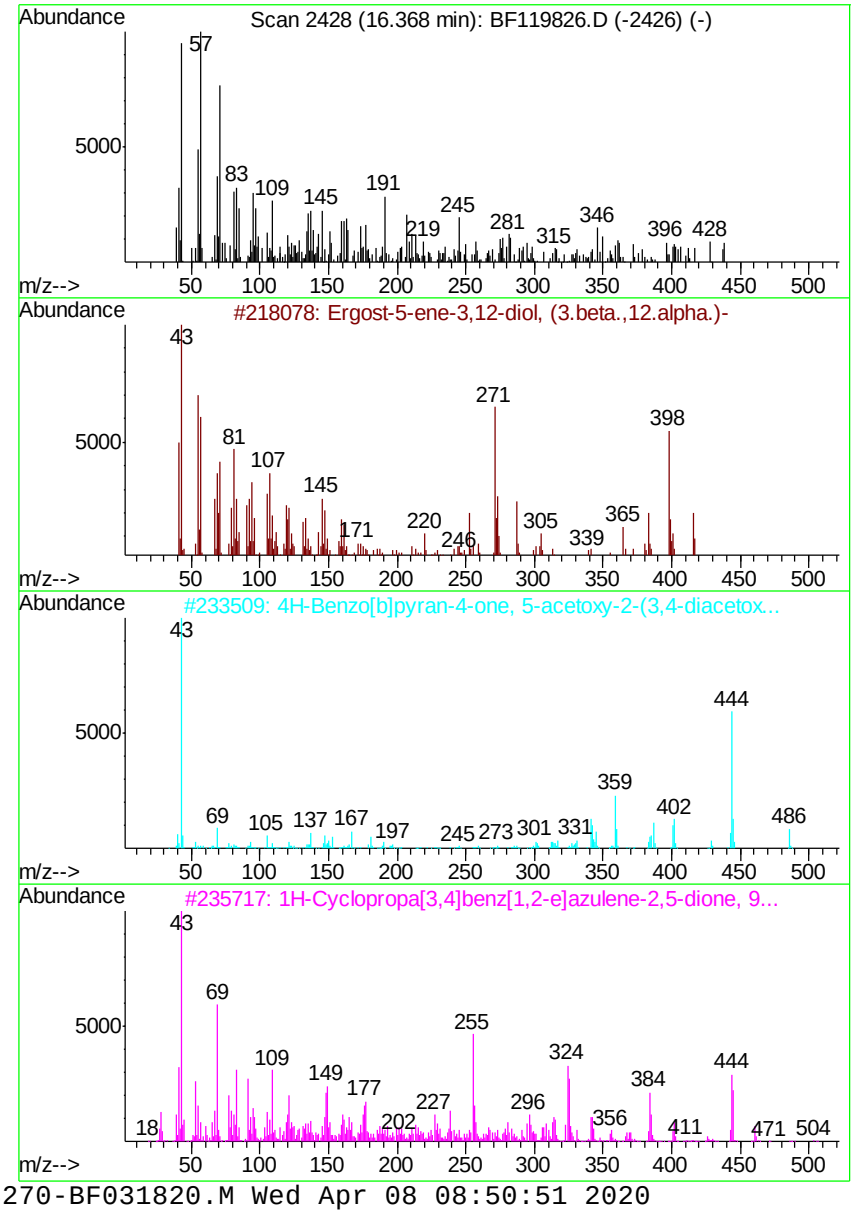
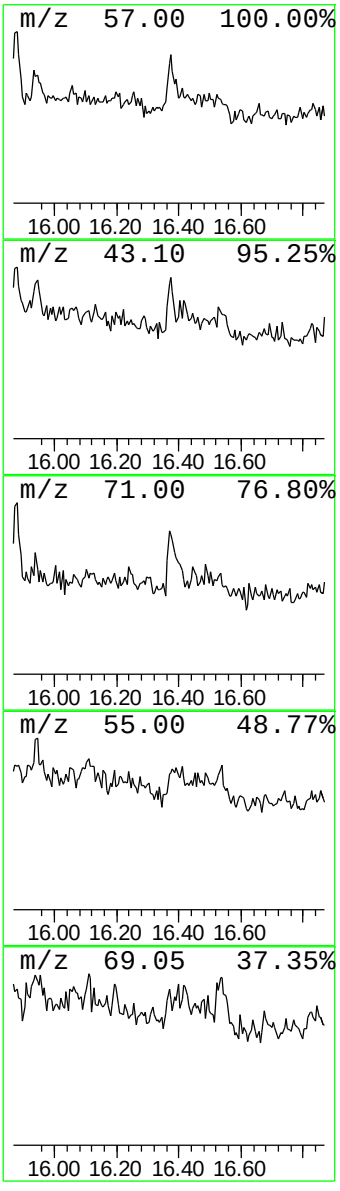
Peak Number 10 unknown16.37 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	6.22 ng	141073	Perylene-d12	15.42

Hit# of 3	Tentative ID	MW	MolForm	CAS#	Qual
1	Ergost-5-ene-3,12-diol, (3.beta....	416	C28H48O2	056052-10-9	9
2	4H-Benzo[b]pyran-4-one, 5-acetox...	486	C24H22O11	014965-19-6	9
3	1H-Cyclopropa[3,4]benz[1,2-e]azu...	504	C26H32O10	077573-14-9	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040620\
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Operator : MA/SJ
Sample : L2102-01
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Instrument : BNA_F
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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
Propane, 1,1-dime...	2.12	2.9	ng	75117	1	6.79	522498	20.0
2-Pentanone, 4-hy...	5.00	11.4	ng	296807	1	6.79	522498	20.0
n-Hexadecanoic acid	11.85	14.1	ng	438135	4	11.32	620329	20.0
Octadecanoic acid	12.63	7.2	ng	222230	4	11.32	620329	20.0
unknown13.44	13.44	3.2	ng	80945	5	13.96	510586	20.0
Cyclotetracosane	13.82	22.2	ng	566793	5	13.96	510586	20.0
Tetracosane, 1-br...	15.07	8.2	ng	184804	6	15.42	453747	20.0
unknown16.37	16.37	6.2	ng	141073	6	15.42	453747	20.0