LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
Data File : BF119757.D
Acq On : 4 Apr 2020 10:45
Operator : MA/SJ
Sample : L2100-07
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 239-105060708-0-6

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	2.193	13	18	25	rBV	100744	129344	2.10%	0.262%
2	5.034	496	501	509	rVB	187455	290774	4.72%	0.588%
3	5.428	562	568	571	rBV	5539808	6157468	100.00%	12.462%
4	6.445	734	741	744	rBV	5187227	5970815	96.97%	12.084%
5	6.804	798	802	806	rBV	1314419	1031838	16.76%	2.088%
6	6.963	825	829	832	rBV	5238406	4685069	76.09%	9.482%
7	7.369	891	898	901	rBV	3572240	3934179	63.89%	7.962%
8	8.086	1016	1020	1024	rBV	1445089	1264353	20.53%	2.559%
9	9.169	1199	1204	1207	rBV	6341434	5671814	92.11%	11.479%
10	9.557	1267	1270	1274	rBV	662853	586625	9.53%	1.187%
11	9.704	1292	1295	1299	rBV	91413	80454	1.31%	0.163%
12	9.845	1312	1319	1322	rBV	1527544	1271911	20.66%	2.574%
13	9.874	1322	1324	1328	rVB	118057	99913	1.62%	0.202%
14	10.392	1409	1412	1417	rBV	97005	82861	1.35%	0.168%
15	10.633	1448	1453	1457	rBV	3328796	3338606	54.22%	6.757%
16	11.333	1568	1572	1574	rBV	1289553	1105472	17.95%	2.237%
17	11.357	1574	1576	1579	rVB	862709	634454	10.30%	1.284%
18	11.404	1579	1584	1587	rBV	279086	265792	4.32%	0.538%
19	11.563	1605	1611	1613	rBV2	132446	131661	2.14%	0.266%
20	11.833	1654	1657	1659	rBV	75429	66466	1.08%	0.135%
21	11.863	1659	1662	1667	rBV	756529	662256	10.76%	1.340%
22	11.945	1673	1676	1679	rBV	127784	137514	2.23%	0.278%
23	12.151	1709	1711	1716	rVB	94311	72628	1.18%	0.147%
24	12.386	1748	1751	1753	rBV	59305	66172	1.07%	0.134%
25	12.545	1775	1778	1781	rBV	1182845	982326	15.95%	1.988%
26	12.651	1792	1796	1801	rBV4	285806	390458	6.34%	0.790%
27	12.745	1809	1812	1813	rBV	206986	176232	2.86%	0.357%
28	12.774	1814	1817	1820	rVV	1010228	920320	14.95%	1.863%
29	12.821	1823	1825	1831	rVB2	60863	71877	1.17%	0.145%
30	12.921	1838	1842	1848	rVB	4294442	4067194	66.05%	8.231%
31	13.104	1871	1873	1876	rVB	133611	105415	1.71%	0.213%
32	13.210	1888	1891	1893	rVB2	93174	81023	1.32%	0.164%
33	13.404	1921	1924	1929	rVB	205897	188042	3.05%	0.381%
34	13.451	1930	1932	1935	rBV	123723	99830	1.62%	0.202%

LSC Area Percent Report

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Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 239-105060708-0-6

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

35	13.609	1956	1959	1963	rVB	135609	134207	2.18%	0.272%
36	13.751	1981	1983	1985	rBV	83910	77597	1.26%	0.157%
37	13.821	1992	1995	2001	rVB2	488382	519633	8.44%	1.052%
38	13.974	2016	2021	2024	rBV2	1183724	1443062	23.44%	2.921%
39	13.998	2024	2025	2030	rVB	456524	342534	5.56%	0.693%
40	14.451	2100	2102	2106	rBV5	118216	118291	1.92%	0.239%
41	15.009	2193	2197	2200	rBV	435124	631119	10.25%	1.277%
42	15.303	2245	2247	2253	rVB	252114	338627	5.50%	0.685%
43	15.368	2255	2258	2264	rVB	254346	291609	4.74%	0.590%
44	15.433	2265	2269	2272	rBV	565995	693021	11.25%	1.403%

Sum of corrected areas: 49410856

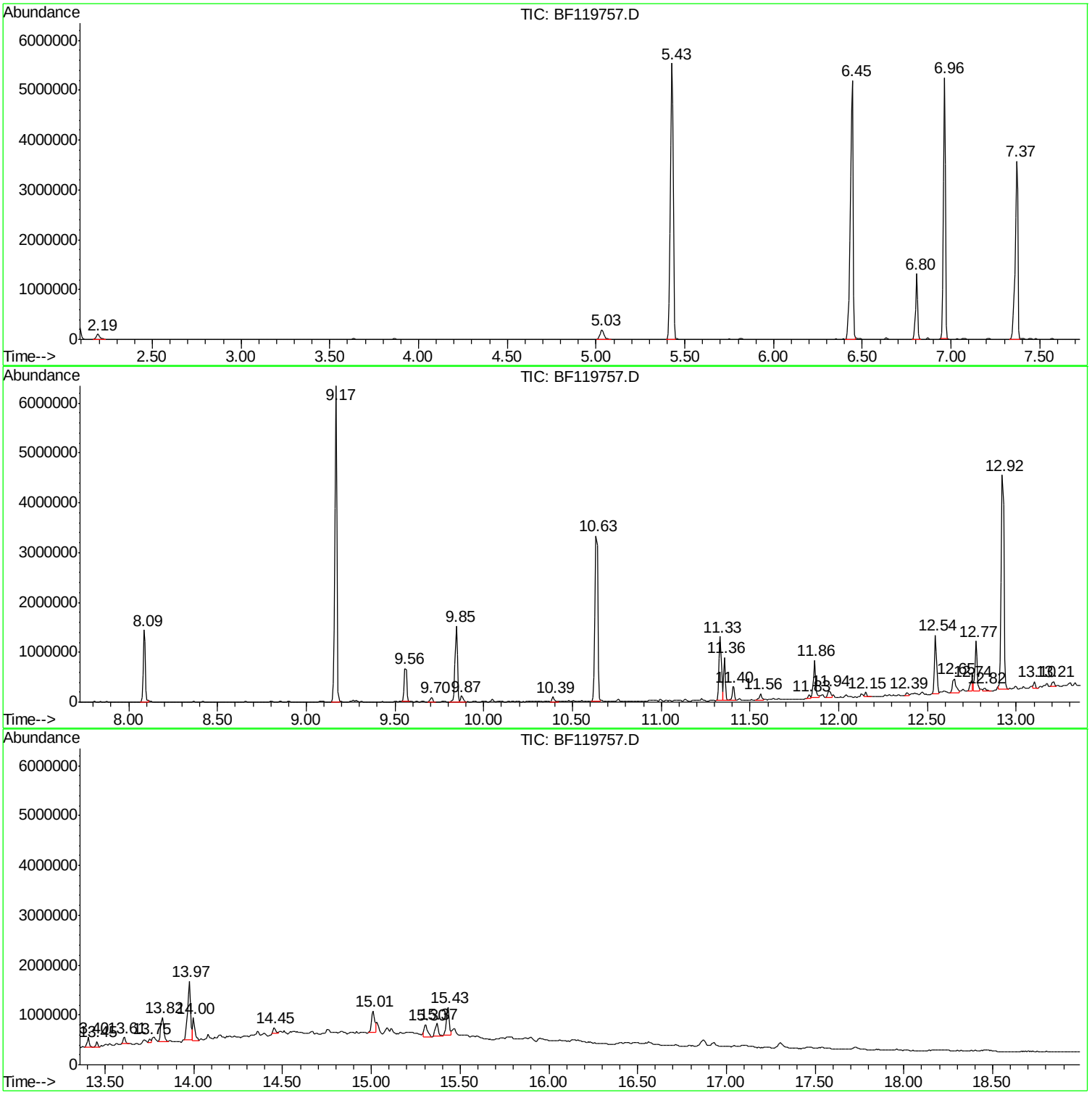
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
Data File : BF119757.D
Acq On : 4 Apr 2020 10:45
Operator : MA/SJ
Sample : L2100-07
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 239-105060708-0-6

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\BF040320\
Data File : BF119757.D
Acq On : 4 Apr 2020 10:45
Operator : MA/SJ
Sample : L2100-07
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 239-105060708-0-6

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

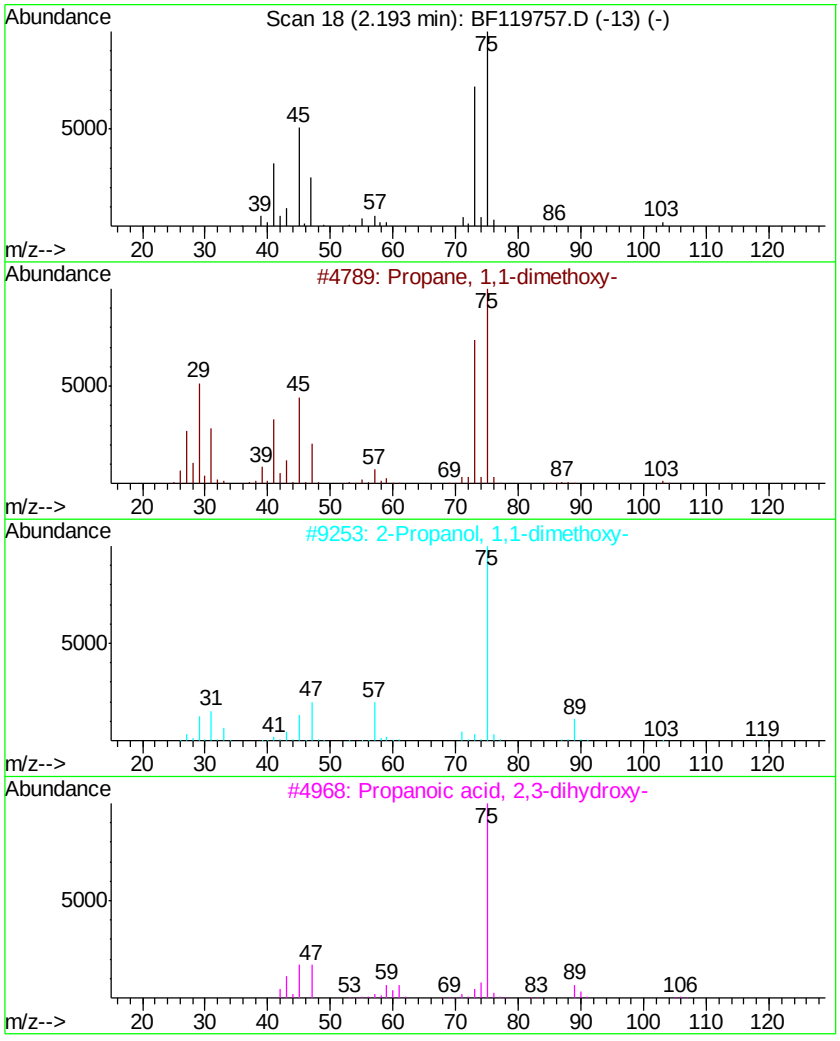
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

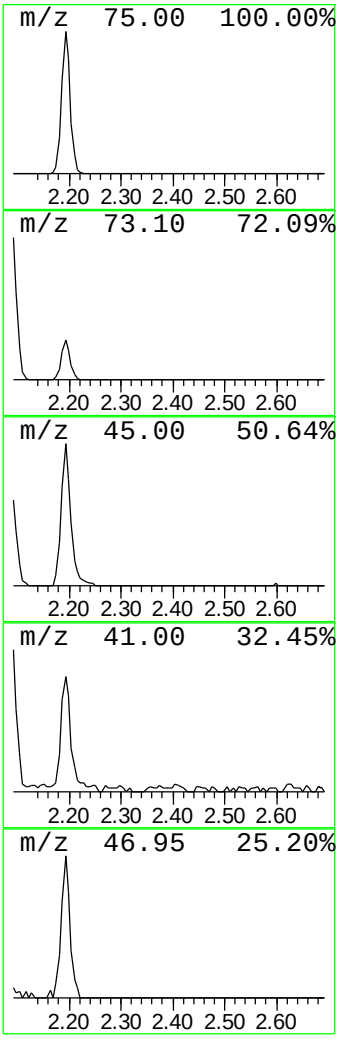
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	2.51 ng	129344	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	50
3	Propanoic acid, 2,3-dihydroxy-	106	C3H6O4	000473-81-4	36
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
5	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
Data File : BF119757.D
Acq On : 4 Apr 2020 10:45
Operator : MA/SJ
Sample : L2100-07
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 239-105060708-0-6

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

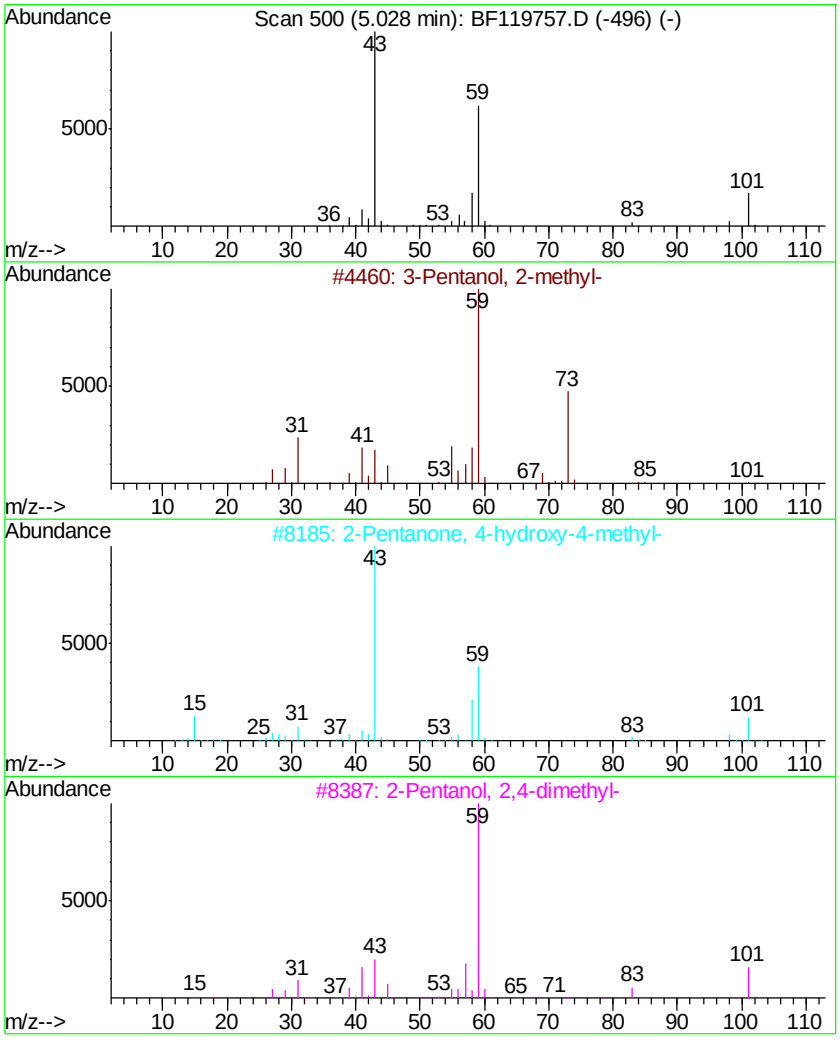
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

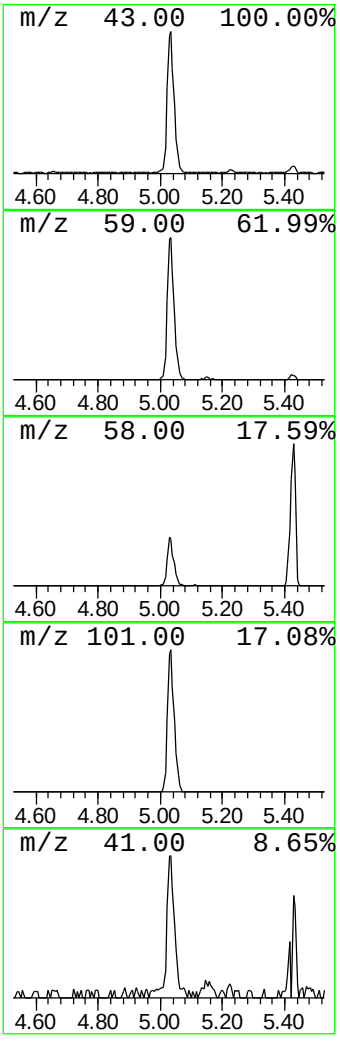
****

Peak Number 2 3-Pentanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	5.64 ng	290774	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	37
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
Data File : BF119757.D
Acq On : 4 Apr 2020 10:45
Operator : MA/SJ
Sample : L2100-07
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 239-105060708-0-6

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

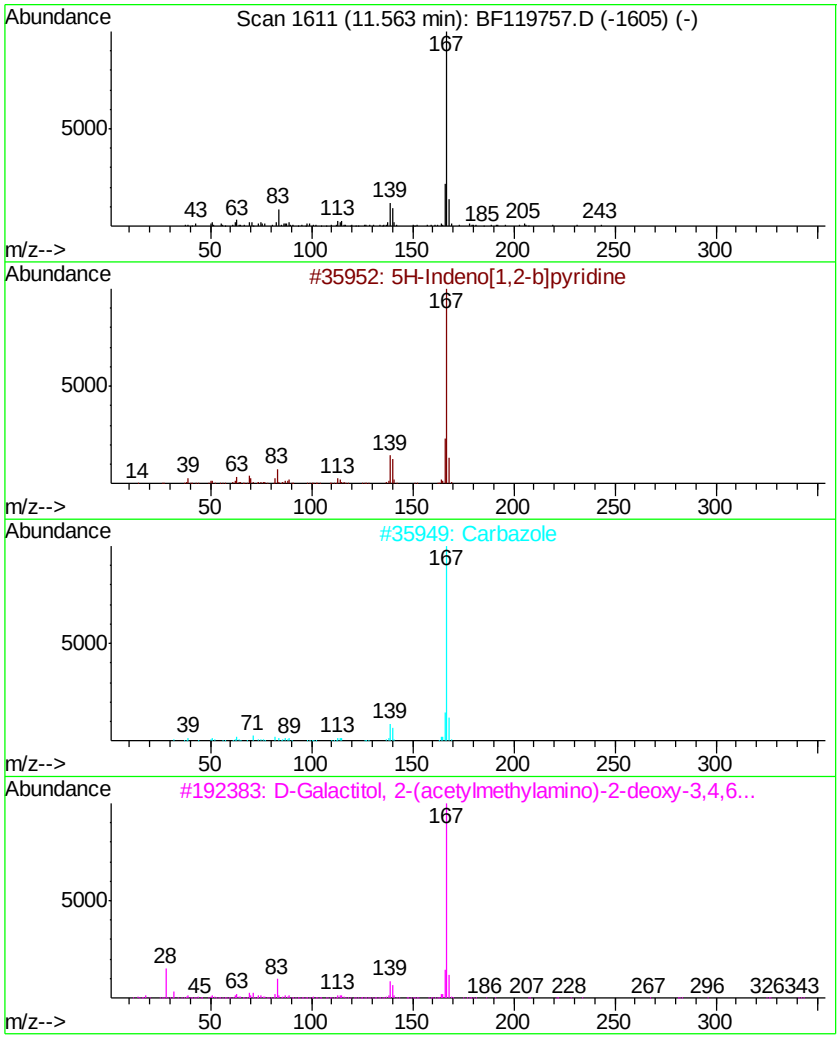
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

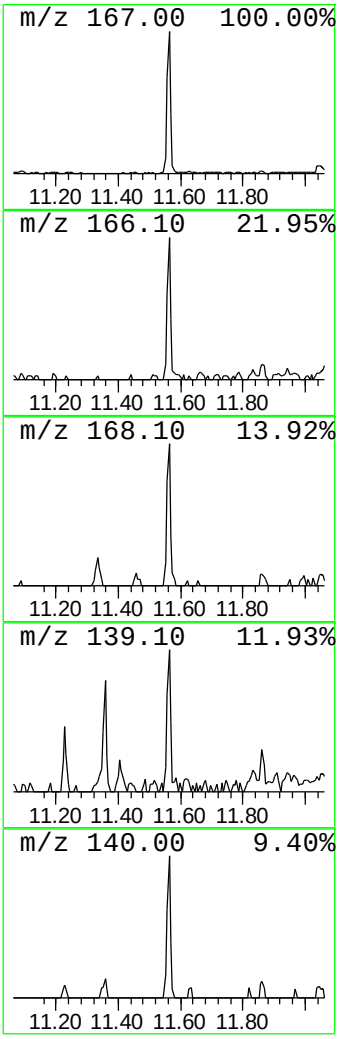
****

Peak Number 4 5H-Indeno[1,2-b]pyridine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	2.38 ng	131661	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	91
2	Carbazole	167	C12H9N	000086-74-8	87
3	D-Galactitol, 2-(acetylmethylami...	363	C16H29NO8	074410-42-7	80
4	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	78
5	9H-Carbazole-9-methanol	197	C13H11NO	002409-36-1	72





Library Search Compound Report

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Acq On : 4 Apr 2020 10:45
Operator : MA/SJ
Sample : L2100-07
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 239-105060708-0-6

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

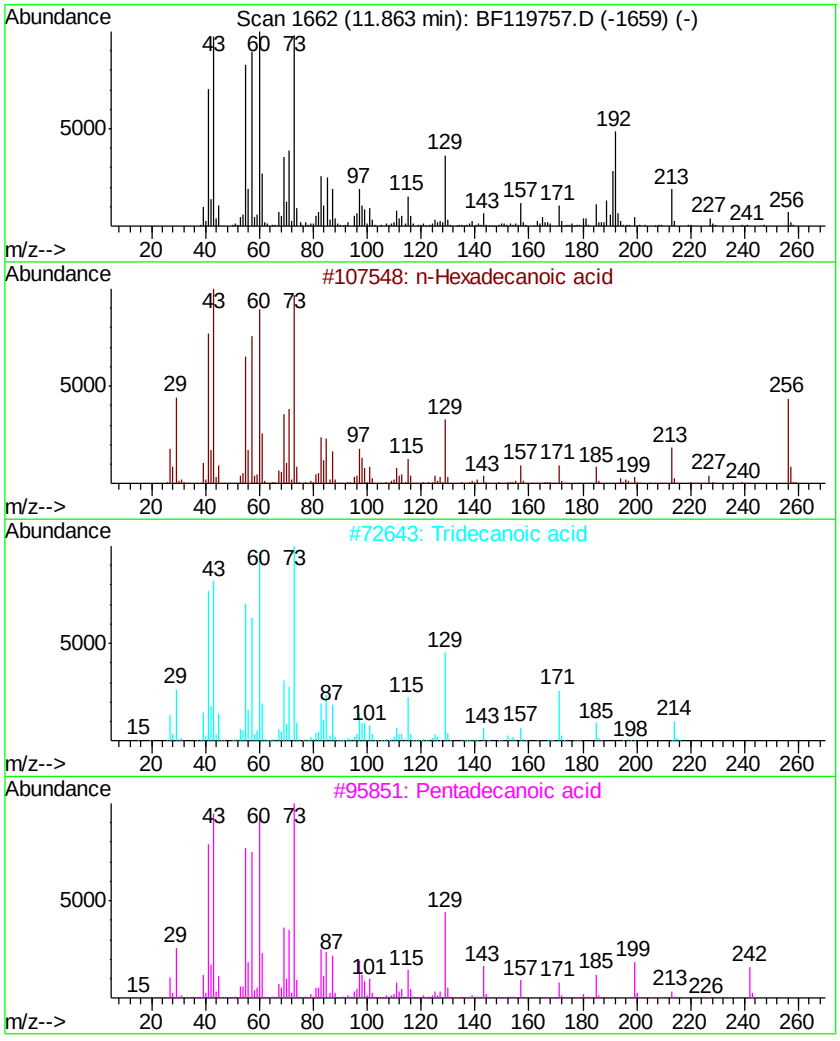
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

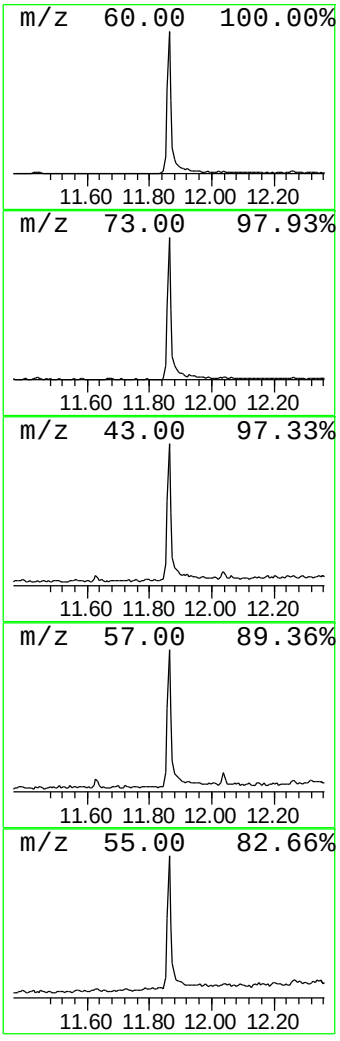
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	11.98 ng	662256	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





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Sample : L2100-07
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 239-105060708-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
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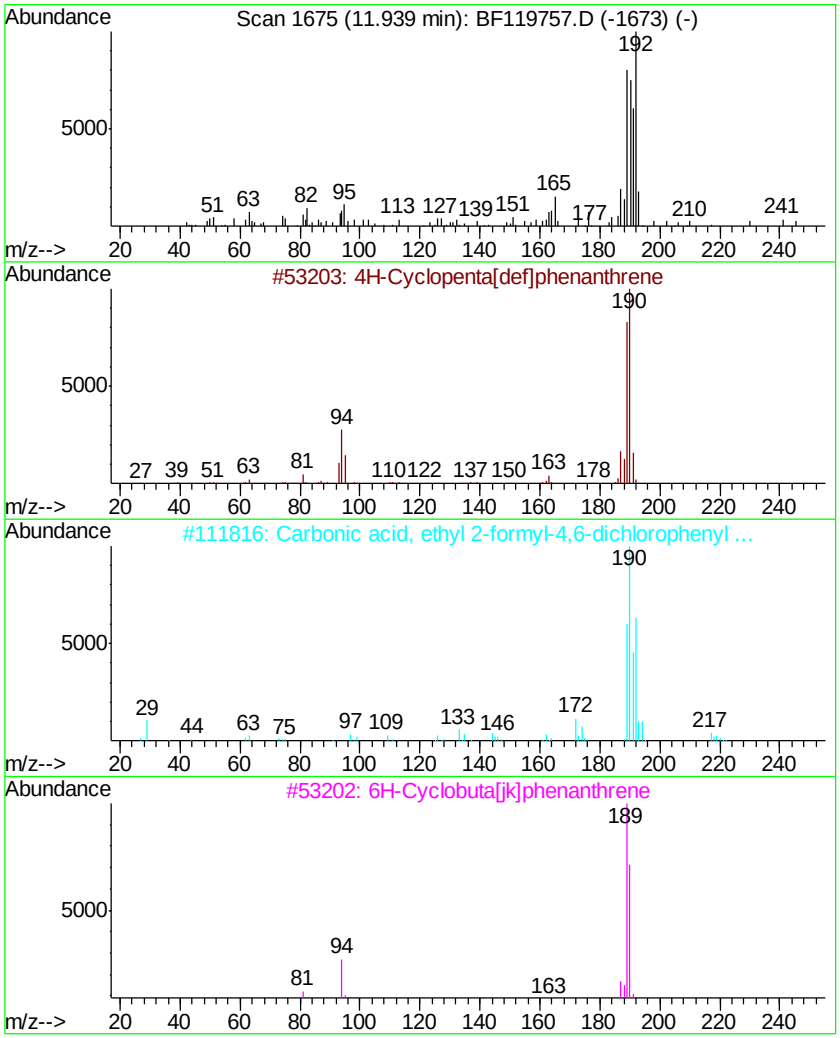
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

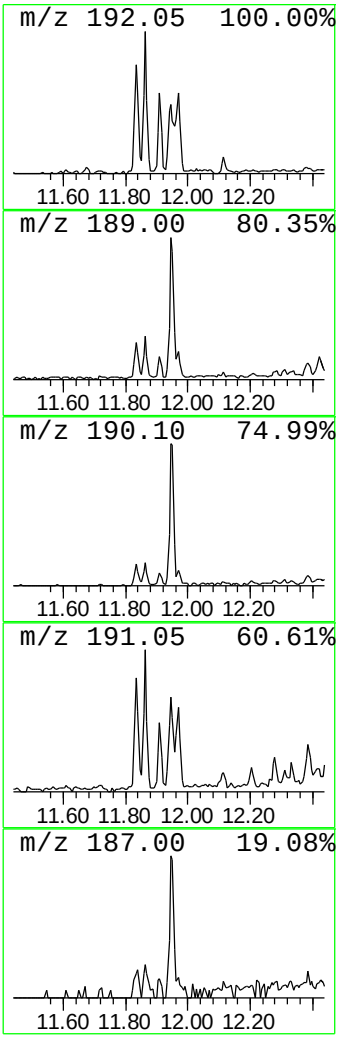
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.49 ng	137514	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	53
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
5	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	42





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ClientSampleId : 239-105060708-0-6

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
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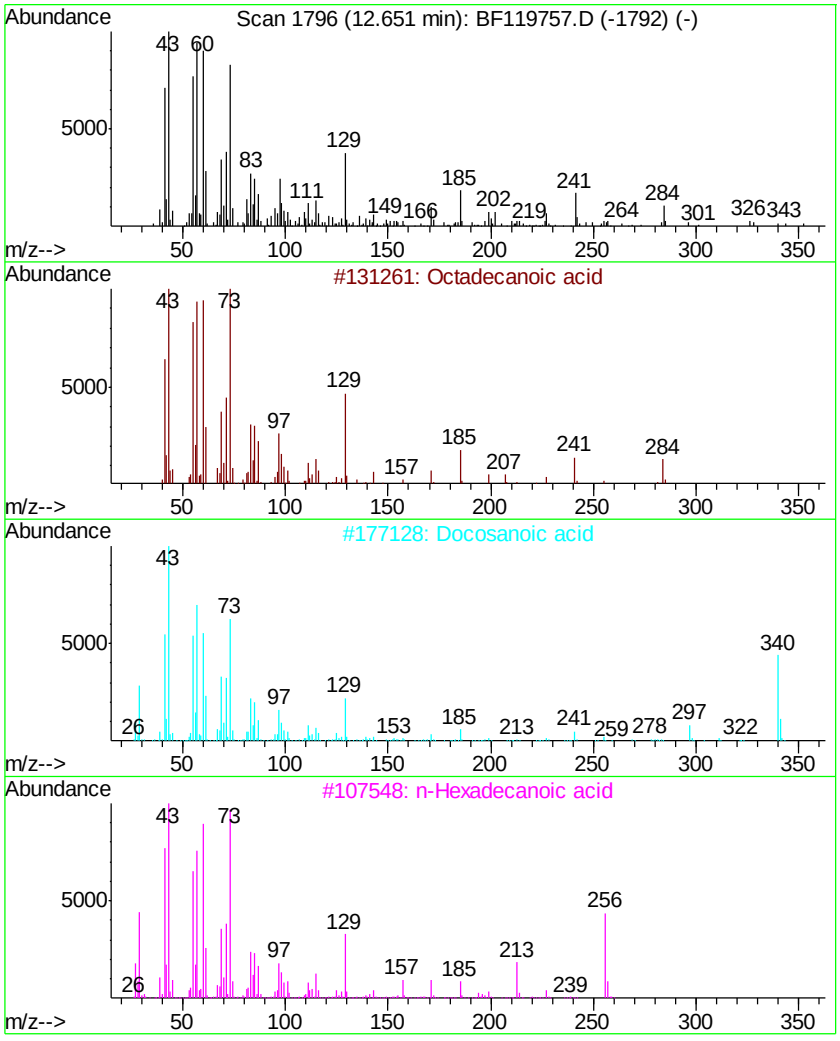
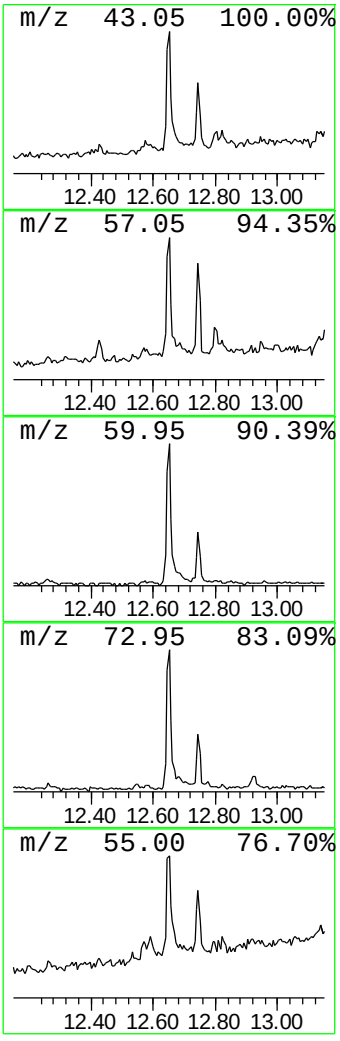
Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	7.06 ng	390458	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Docosanoic acid	340	C22H44O2	000112-85-6	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	78
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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

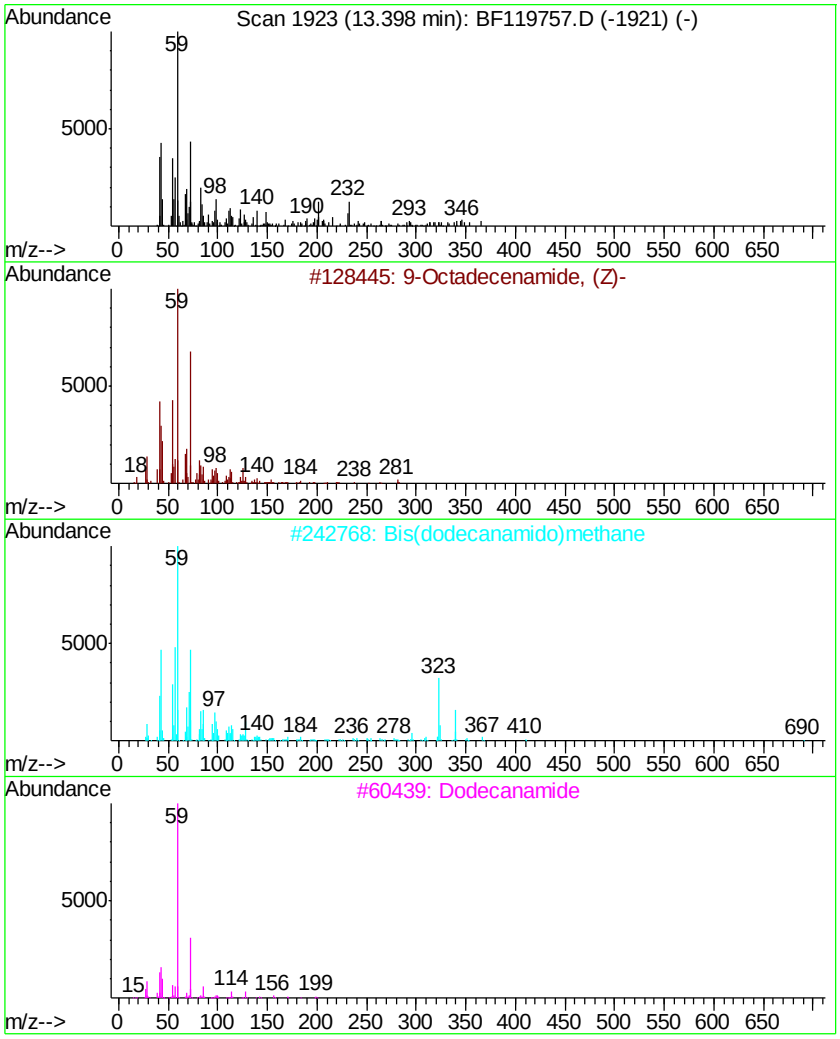
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

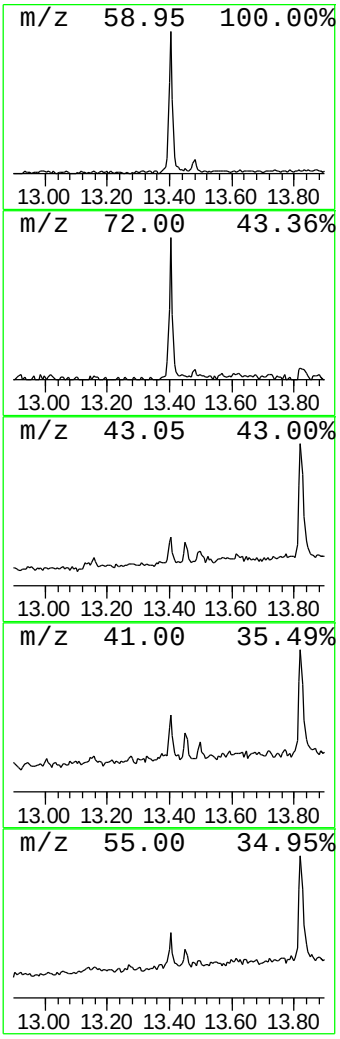
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	2.61 ng	188042	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	Bis(dodecanamido)methane	691	C45H90N2O2	010436-15-4	50
3	Dodecanamide	199	C12H25NO	001120-16-7	47
4	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	47
5	Nonanamide	157	C9H19NO	001120-07-6	46





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
Data File : BF119757.D
Acq On : 4 Apr 2020 10:45
Operator : MA/SJ
Sample : L2100-07
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 239-105060708-0-6

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

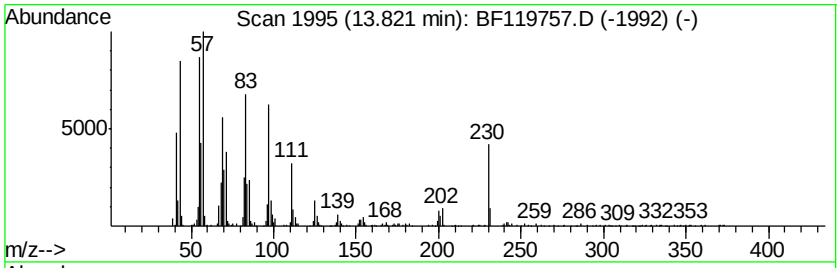
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

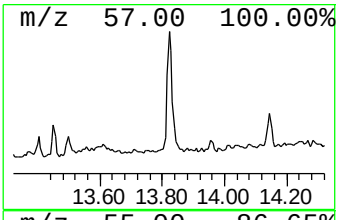
****

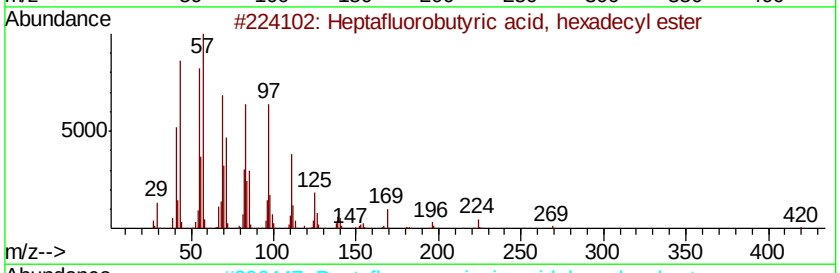
Peak Number 9 Heptafluorobutyric acid, he... Concentration Rank 4

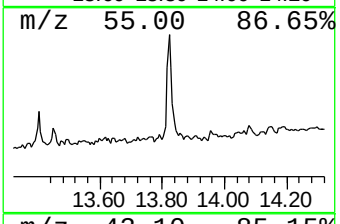
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	7.20 ng	519633	Chrysene-d12	13.97

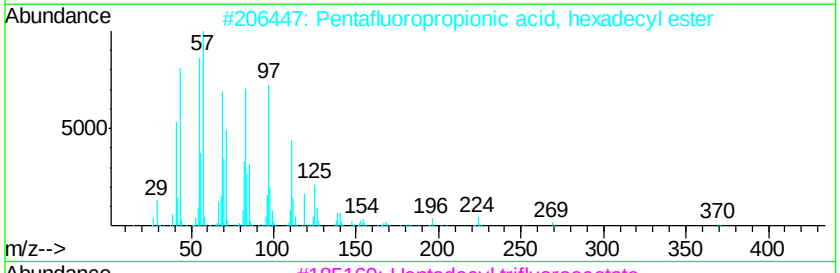
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	89
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87
5	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	83

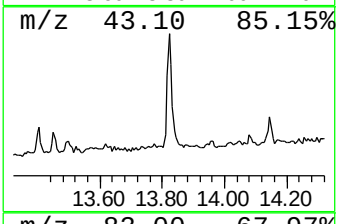


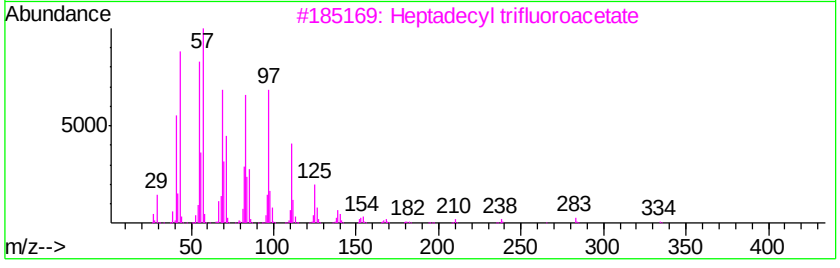


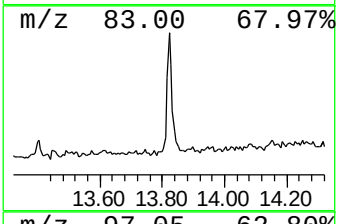


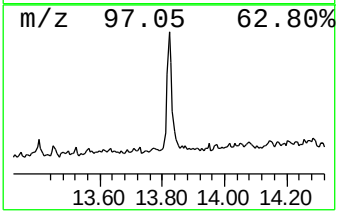












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040320\
Data File : BF119757.D
Acq On : 4 Apr 2020 10:45
Operator : MA/SJ
Sample : L2100-07
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 239-105060708-0-6

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	2.19	2.5	ng	129344	1	6.80	1031840	20.0
3-Pentanol, 2-met...	5.03	5.6	ng	290774	1	6.80	1031840	20.0
5H-Indeno[1,2-b]p...	11.56	2.4	ng	131661	4	11.33	1105470	20.0
n-Hexadecanoic acid	11.86	12.0	ng	662256	4	11.33	1105470	20.0
4H-Cyclopenta[def...	11.94	2.5	ng	137514	4	11.33	1105470	20.0
Octadecanoic acid	12.65	7.1	ng	390458	4	11.33	1105470	20.0
9-Octadecenamide,...	13.40	2.6	ng	188042	5	13.97	1443060	20.0
Heptafluorobutyri...	13.82	7.2	ng	519633	5	13.97	1443060	20.0