LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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	2.210	17	21	28	rBV	112632	137044	2.12%	0.262%
2	5.040	498	502	509	rVB	112010	140713	2.17%	0.269%
3	5.446	565	571	574	rBV	5161123	5359400	82.73%	10.257%
4	6.345	721	724	732	rBV	73159	86828	1.34%	0.166%
5	6.451	737	742	745	rBV	4888066	5412523	83.55%	10.359%
6	6.834	803	807	810	rBV	1817512	1595777	24.63%	3.054%
7	6.987	829	833	836	rBV	5066039	4363241	67.36%	8.351%
8	7.392	897	902	905	rBV	3906428	3526196	54.43%	6.749%
9	8.116	1020	1025	1028	rBV	2605472	2154531	33.26%	4.123%
10	9.198	1203	1209	1212	rBV	6573306	6477963	100.00%	12.398%
11	9.586	1270	1275	1278	rBV	237566	181664	2.80%	0.348%
12	9.633	1281	1283	1292	rVB	48009	68870	1.06%	0.132%
13	9.875	1315	1324	1327	rBV	3218520	2681992	41.40%	5.133%
14	10.663	1453	1458	1461	rBV	4346020	3791721	58.53%	7.257%
15	11.363	1573	1577	1580	rBV	2690327	2355161	36.36%	4.507%
16	11.892	1664	1667	1676	rBV	588702	621074	9.59%	1.189%
17	12.569	1778	1782	1785	rBV2	90644	119122	1.84%	0.228%
18	12.674	1797	1800	1808	rBV2	204169	318706	4.92%	0.610%
19	12.804	1819	1822	1824	rBV2	72164	66383	1.02%	0.127%
20	12.951	1842	1847	1850	rBV	6317198	6116492	94.42%	11.706%
21	13.186	1884	1887	1891	rBV2	96088	107009	1.65%	0.205%
22	13.310	1906	1908	1911	rBV2	56353	65034	1.00%	0.124%
23	13.433	1926	1929	1933	rVB2	159200	155398	2.40%	0.297%
24	13.527	1943	1945	1948	rVB2	91769	85937	1.33%	0.164%
25	13.645	1963	1965	1972	rVB5	57505	73883	1.14%	0.141%
26	13.857	1994	2001	2016	rBV2	519033	1241970	19.17%	2.377%
27	14.004	2022	2026	2029	rVB	1957310	1821789	28.12%	3.487%
28	14.174	2052	2055	2059	rBV	187261	162556	2.51%	0.311%
29	14.280	2070	2073	2080	rVB3	67739	91811	1.42%	0.176%
30	14.480	2104	2107	2109	rBV	286983	247718	3.82%	0.474%
31	14.786	2156	2159	2164	rVB	283269	274708	4.24%	0.526%
32	15.127	2213	2217	2223	rVB	271826	299332	4.62%	0.573%
33	15.463	2269	2274	2278	rBV	1158564	1426902	22.03%	2.731%
34	15.510	2278	2282	2290	rVB	203812	279295	4.31%	0.535%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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	15.945	2352	2356	2364	rVB2	143955	221878	3.43%	0.425%
36	16.457	2438	2443	2454	rVB3	58513	119750	1.85%	0.229%

Sum of corrected areas: 52250371

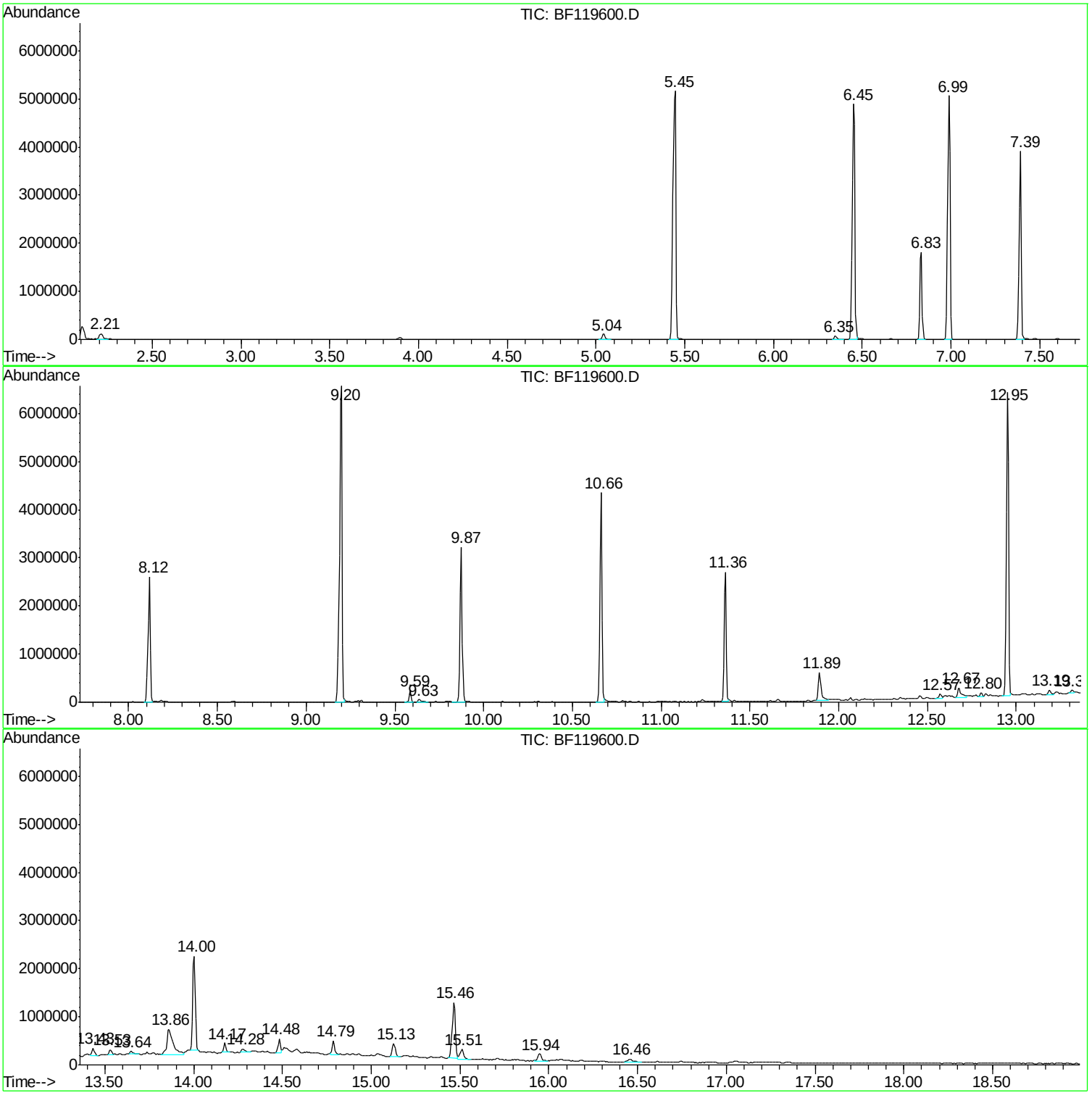
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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

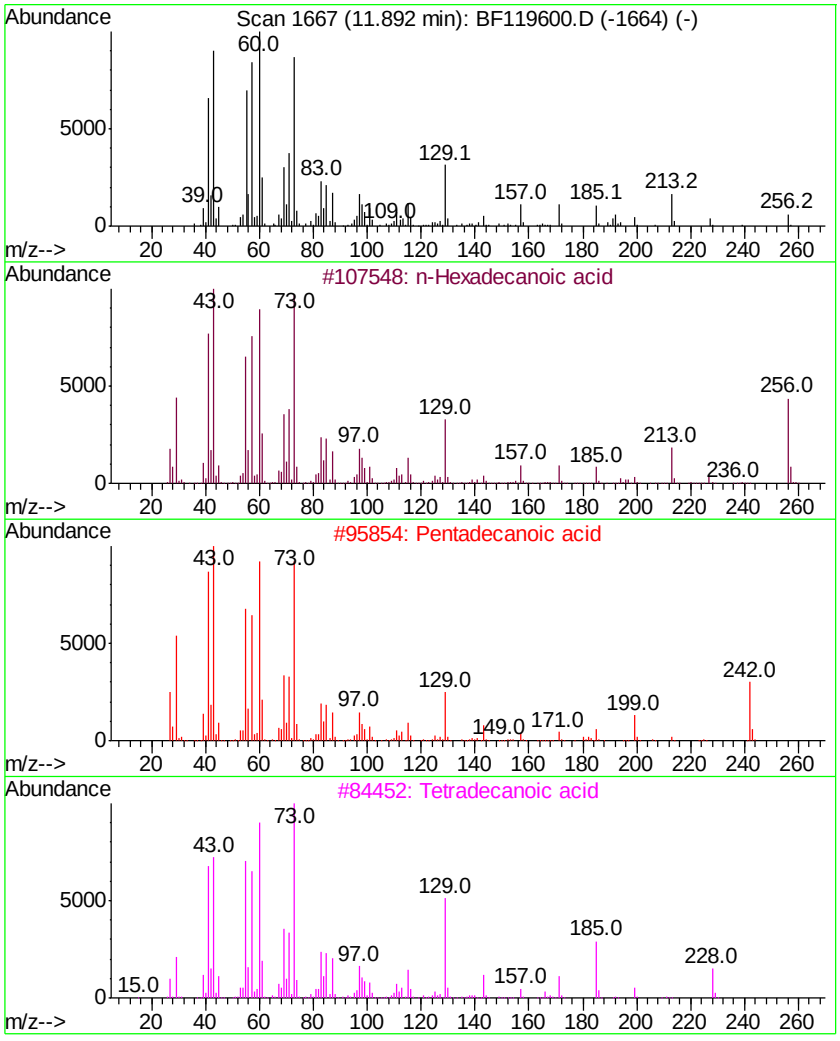
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

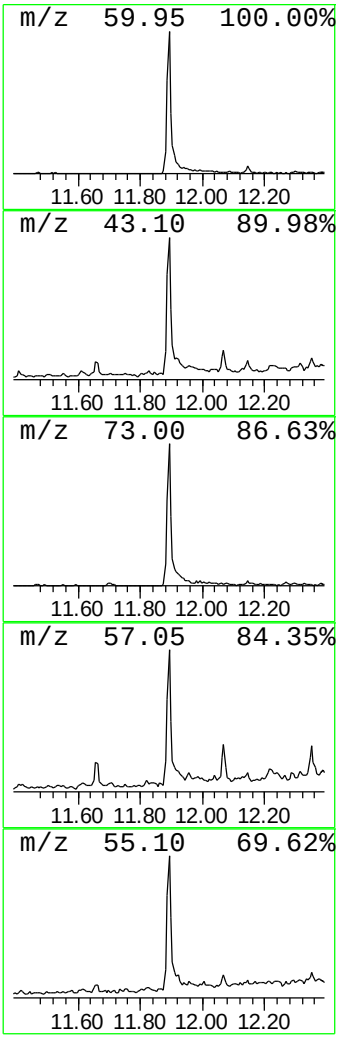
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	5.27 ng	621074	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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

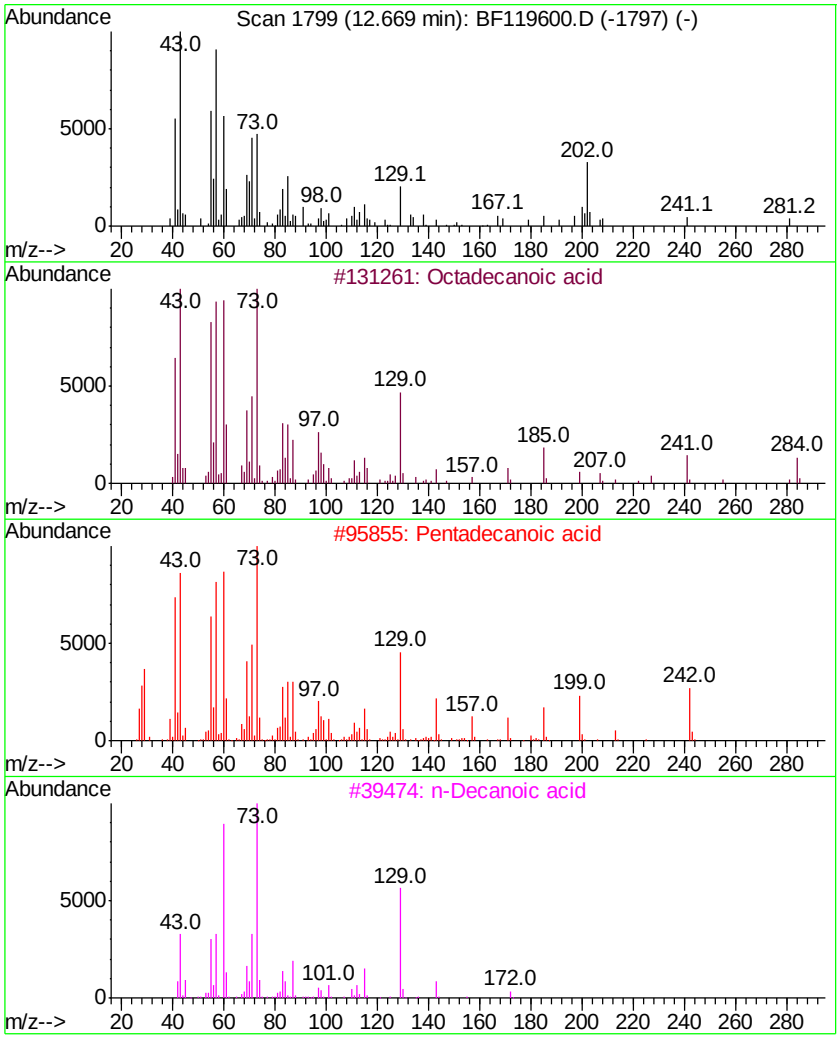
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

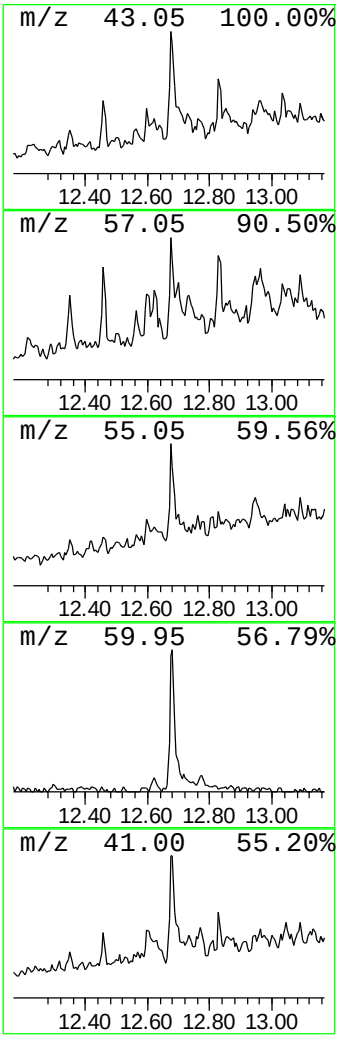
****

Peak Number 3 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	2.71 ng	318706	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	n-Decanoic acid	172	C10H20O2	000334-48-5	55
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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

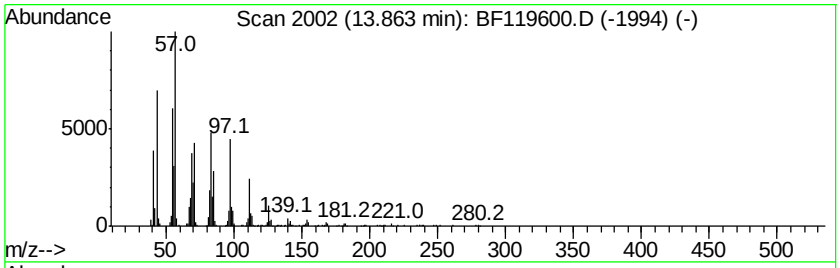
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

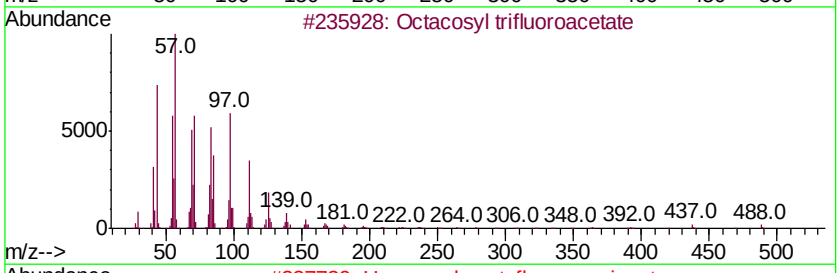
****

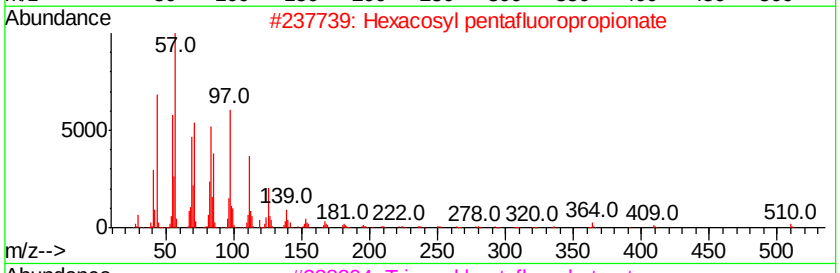
Peak Number 4 Octacosyl trifluoroacetate Concentration Rank 2

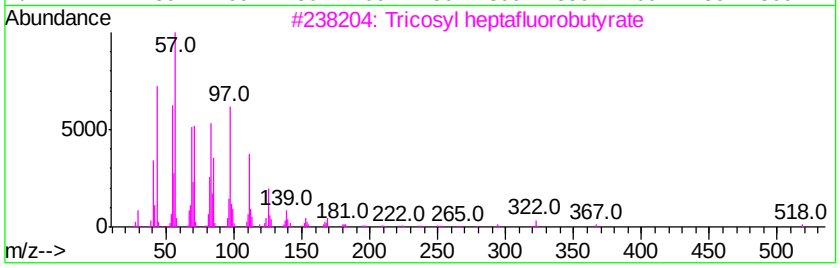
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	13.63 ng	1241970	Chrysene-d12	14.00

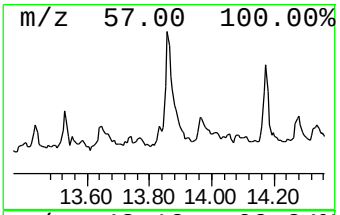
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
4	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91
5	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91

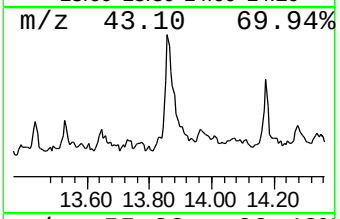


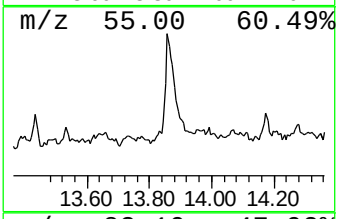


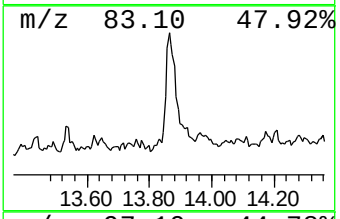


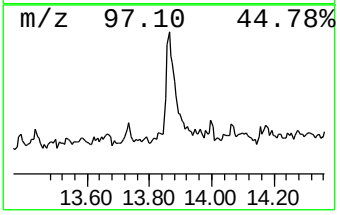












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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

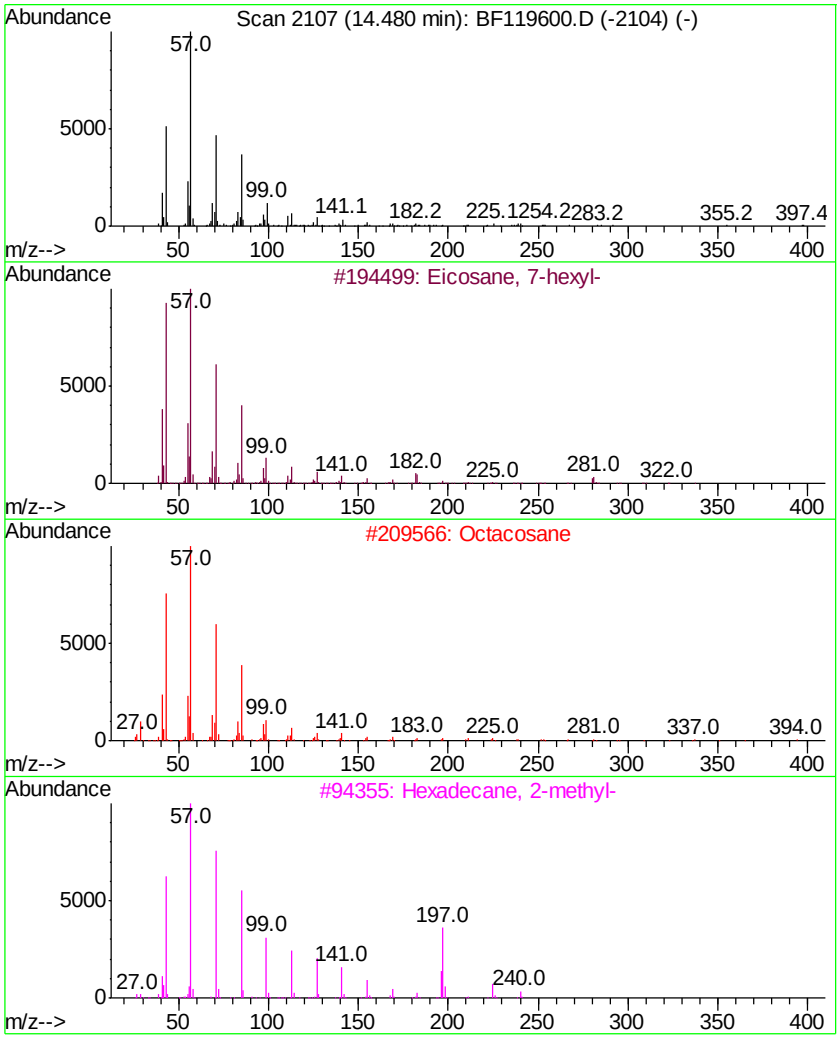
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

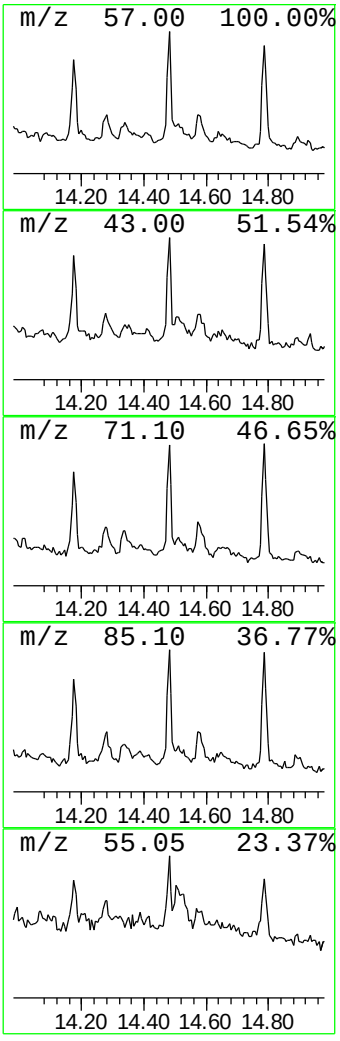
****

Peak Number 5 Eicosane, 7-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	2.72 ng	247718	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Pentacosane	352	C25H52	000629-99-2	86





Library Search Compound Report

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Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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

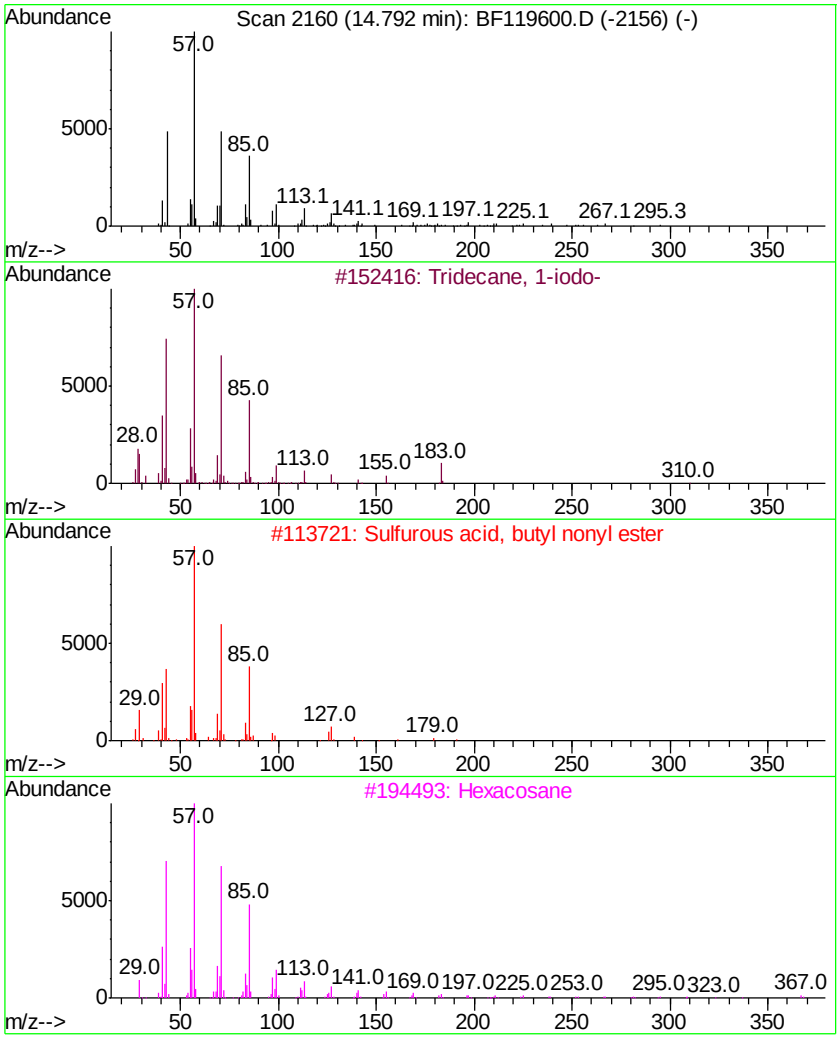
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

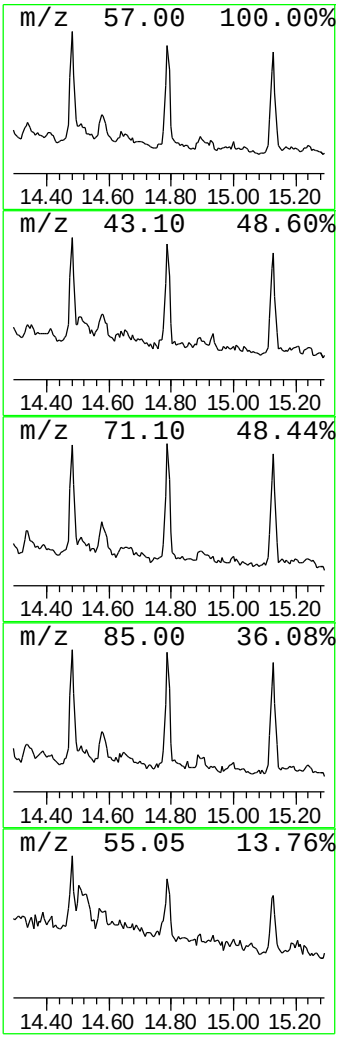
****

Peak Number 6 Tridecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	3.85 ng	274708	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
2	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	80
3	Hexacosane	366	C26H54	000630-01-3	78
4	Heptadecane	240	C17H36	000629-78-7	78
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	78





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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

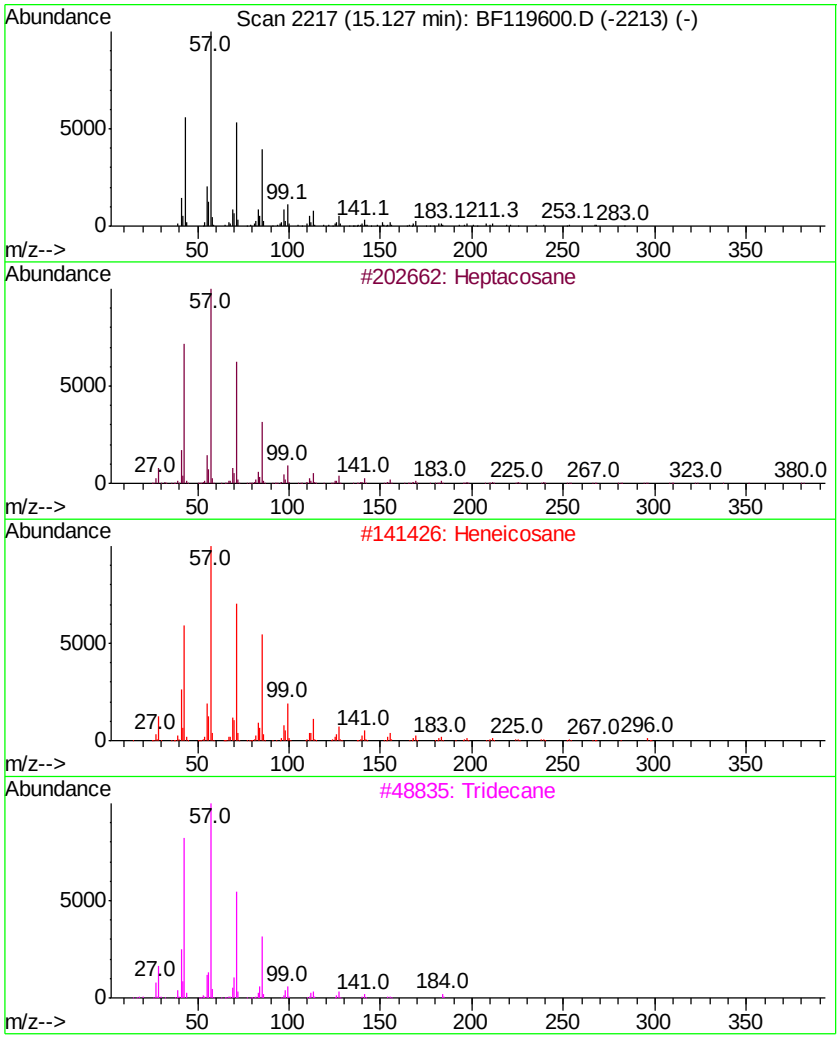
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

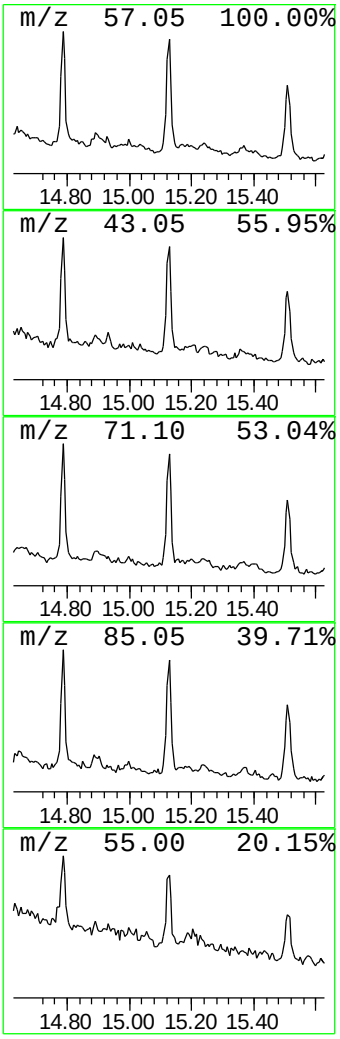
****

Peak Number 7 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	4.20 ng	299332	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	Tridecane	184	C13H28	000629-50-5	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Nonadecane	268	C19H40	000629-92-5	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032720\
Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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

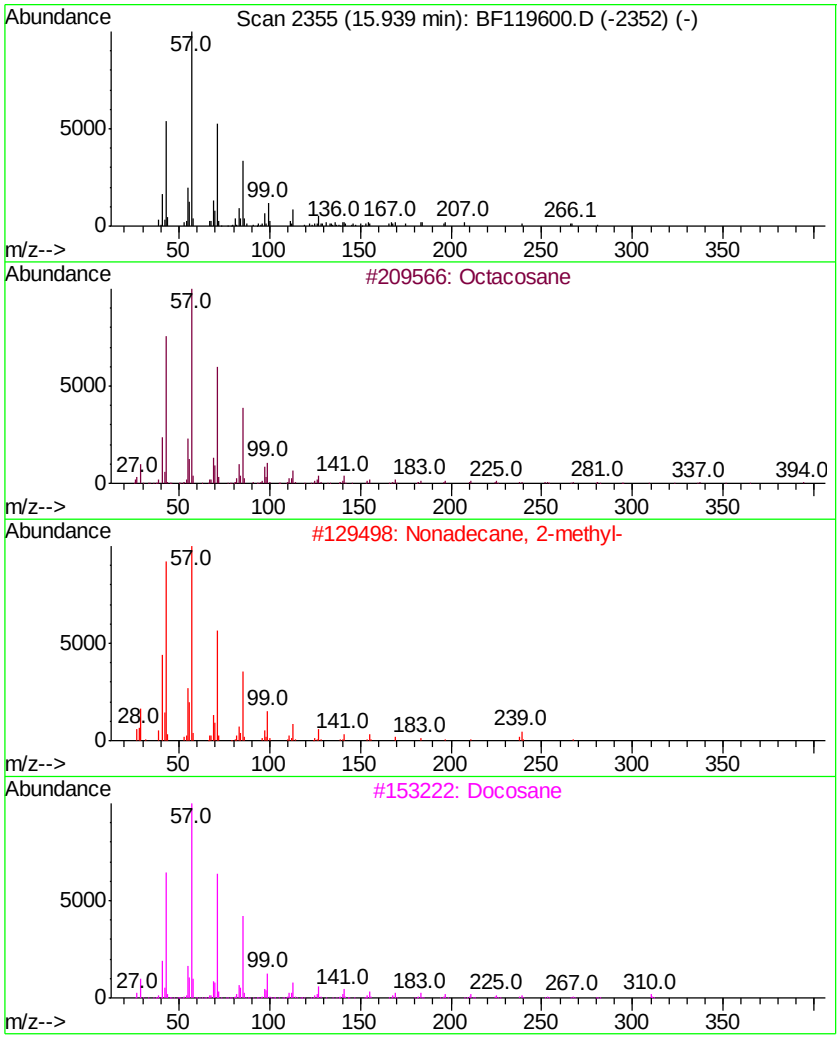
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

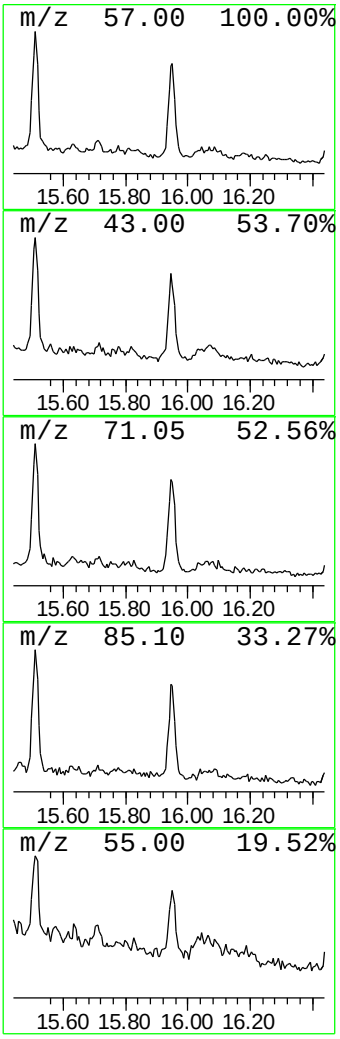
****

Peak Number 8 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	3.11 ng	221878	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
3	Docosane	310	C22H46	000629-97-0	86
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032720\
Data File : BF119600.D
Acq On : 28 Mar 2020 6:54
Operator : CG/JU
Sample : L2051-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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
n-Hexadecanoic acid	11.89	5.3	ng	621074	4	11.36	2355160	20.0
Octadecanoic acid	12.67	2.7	ng	318706	4	11.36	2355160	20.0
Octacosyl trifluo...	13.86	13.6	ng	1241970	5	14.00	1821790	20.0
Eicosane, 7-hexyl-	14.48	2.7	ng	247718	5	14.00	1821790	20.0
Tridecane, 1-iodo-	14.79	3.9	ng	274708	6	15.46	1426900	20.0
Heptacosane	15.13	4.2	ng	299332	6	15.46	1426900	20.0
Octacosane	15.94	3.1	ng	221878	6	15.46	1426900	20.0