LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117566.D
Acq On : 28 Oct 2019 17:25
Operator : JU
Sample : K5501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 185-56-(0-2.2)

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-BF101819.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	5.351	552	555	579	rBV	844079	978599	82.89%	10.112%
2	6.381	726	730	747	rBV	977638	1093364	92.61%	11.298%
3	6.504	747	751	770	rVB	1187234	1127749	95.52%	11.653%
4	6.728	785	789	802	rBV	234431	238430	20.20%	2.464%
5	6.881	811	815	827	rBV	943229	819300	69.40%	8.466%
6	7.292	881	885	902	rBV	616760	649723	55.03%	6.714%
7	8.010	1003	1007	1022	rBV	253669	300778	25.48%	3.108%
8	9.080	1185	1189	1209	rBV	1329936	1180591	100.00%	12.199%
9	9.480	1253	1257	1270	rBB	120007	127726	10.82%	1.320%
10	9.757	1301	1304	1321	rBB	352935	344237	29.16%	3.557%
11	10.551	1436	1439	1456	rBV	589472	616054	52.18%	6.366%
12	11.245	1554	1557	1566	rBV	304244	314611	26.65%	3.251%
13	11.774	1644	1647	1660	rBV	63941	65040	5.51%	0.672%
14	12.463	1761	1764	1769	rBV	20531	20362	1.72%	0.210%
15	12.557	1778	1780	1789	rBV	11201	15238	1.29%	0.157%
16	12.692	1798	1803	1806	rBV	19336	21649	1.83%	0.224%
17	12.827	1822	1826	1829	rBV	1038029	848674	71.89%	8.769%
18	13.051	1855	1864	1868	rBV4	7972	12814	1.09%	0.132%
19	13.727	1975	1979	1991	rBV2	92802	166050	14.06%	1.716%
20	13.892	2003	2007	2016	rBV	210907	225023	19.06%	2.325%
21	14.039	2028	2032	2036	rBV2	13838	14863	1.26%	0.154%
22	14.339	2080	2083	2086	rBV	16243	15424	1.31%	0.159%
23	14.410	2093	2095	2106	rBV2	13398	18075	1.53%	0.187%
24	14.639	2129	2134	2137	rVB2	25320	23500	1.99%	0.243%
25	14.704	2142	2145	2149	rVB	25521	24343	2.06%	0.252%
26	14.951	2184	2187	2192	rVB	29867	32635	2.76%	0.337%
27	15.321	2244	2250	2262	rVB	169535	250354	21.21%	2.587%
28	15.709	2312	2316	2321	rVB3	27374	33379	2.83%	0.345%
29	15.798	2324	2331	2340	rBV9	16186	45674	3.87%	0.472%
30	16.174	2391	2395	2408	rVB6	15642	32687	2.77%	0.338%
31	17.362	2590	2597	2602	rBV8	8439	20729	1.76%	0.214%

Sum of corrected areas: 9677675

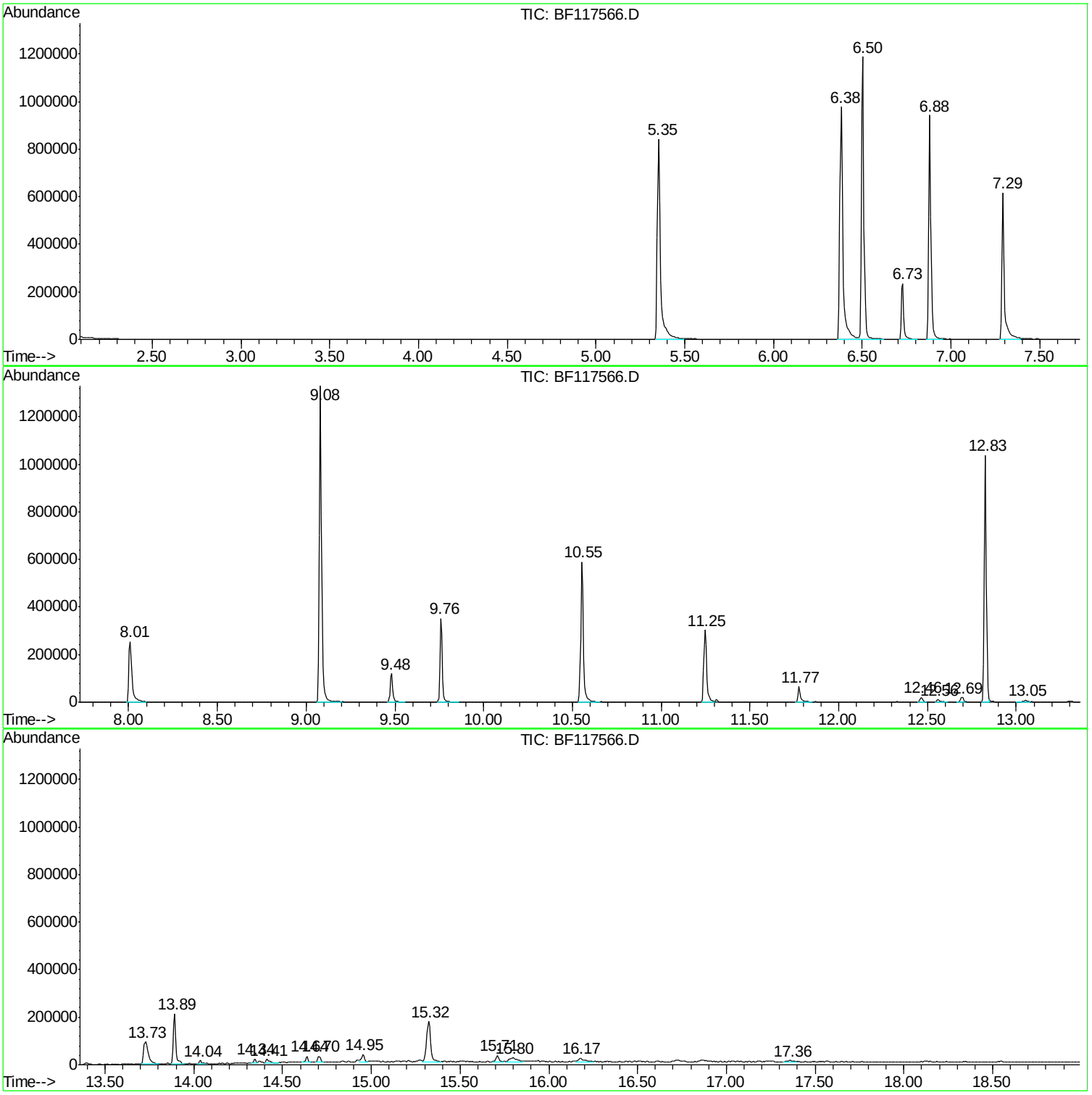
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117566.D
Acq On : 28 Oct 2019 17:25
Operator : JU
Sample : K5501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 185-56-(0-2.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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\BF102819\
Data File : BF117566.D
Acq On : 28 Oct 2019 17:25
Operator : JU
Sample : K5501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 185-56-(0-2.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

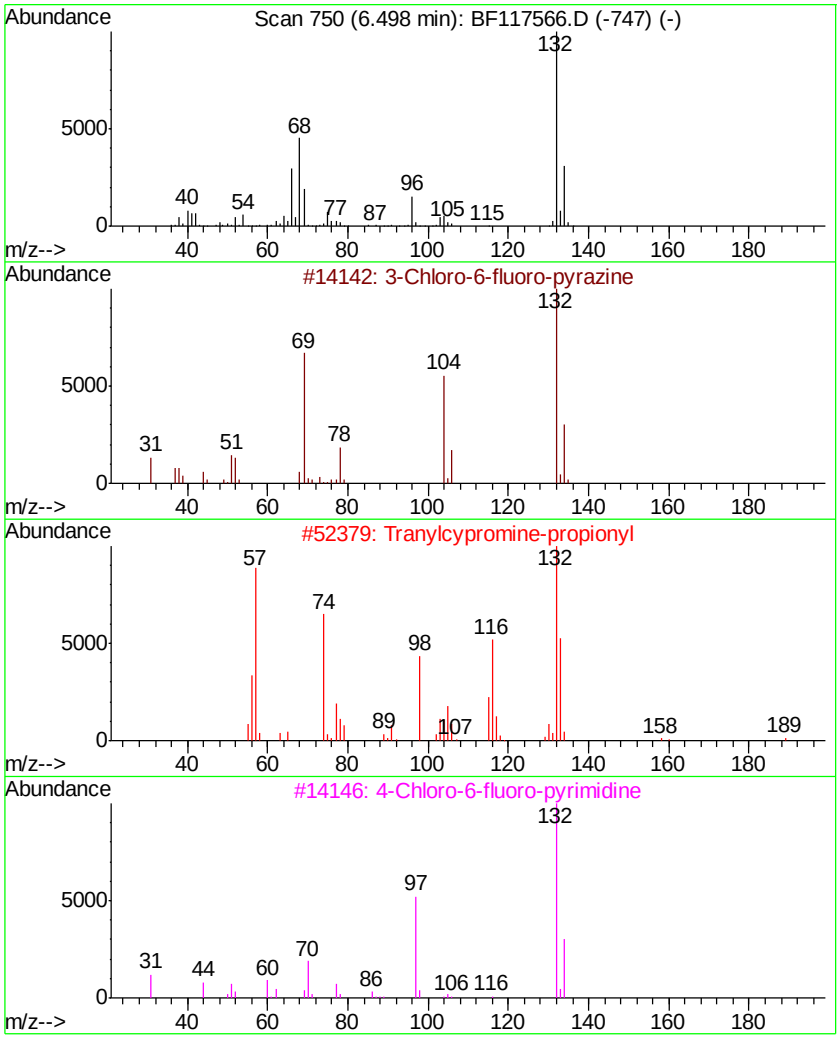
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

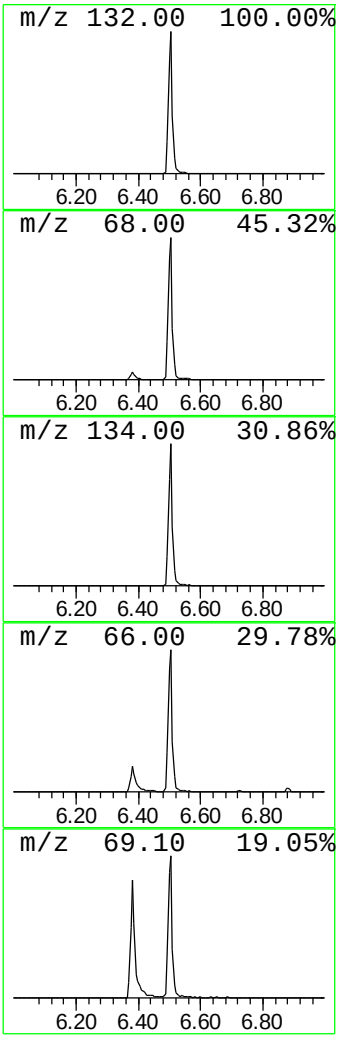
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	94.60 ng	1127750	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117566.D
Acq On : 28 Oct 2019 17:25
Operator : JU
Sample : K5501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 185-56-(0-2.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

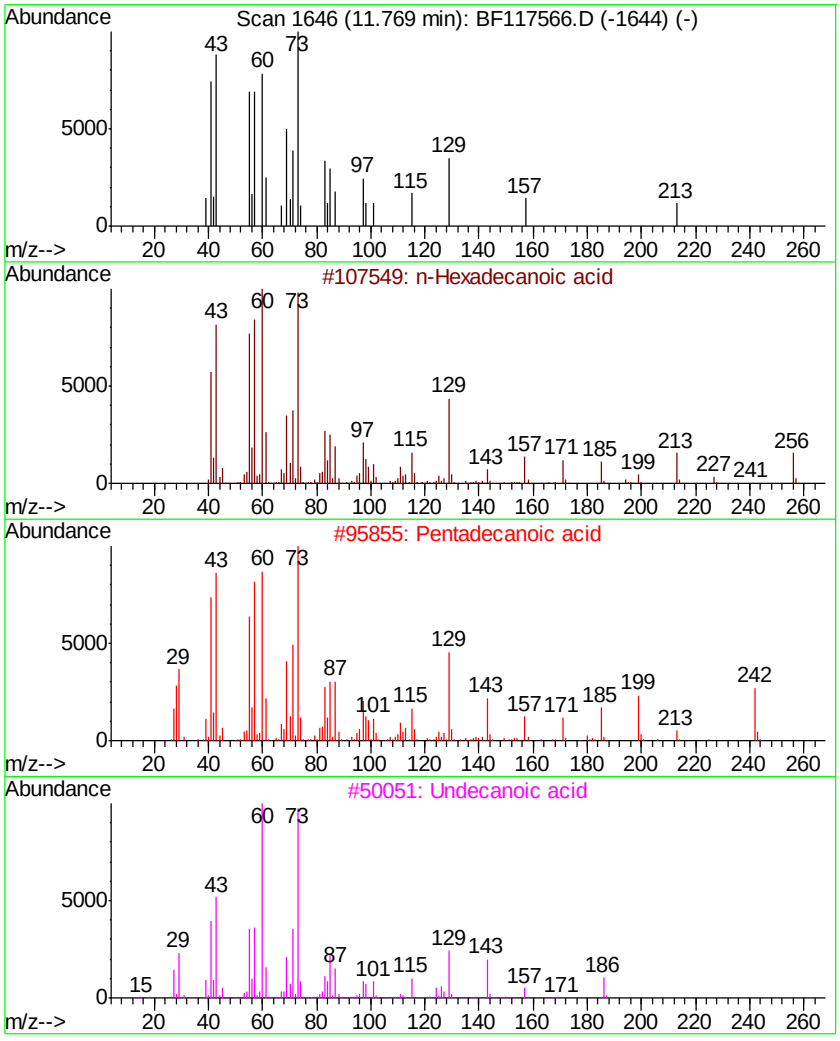
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

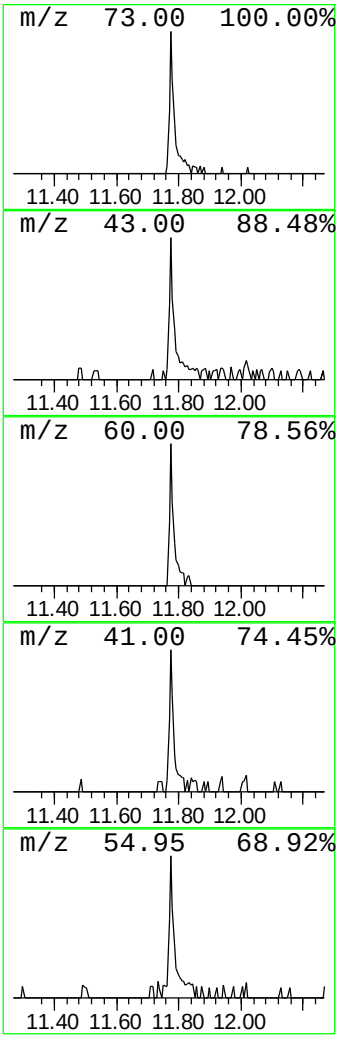
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	4.13 ng	65040	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Undecanoic acid	186	C11H22O2	000112-37-8	59
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117566.D
Acq On : 28 Oct 2019 17:25
Operator : JU
Sample : K5501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 185-56-(0-2.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

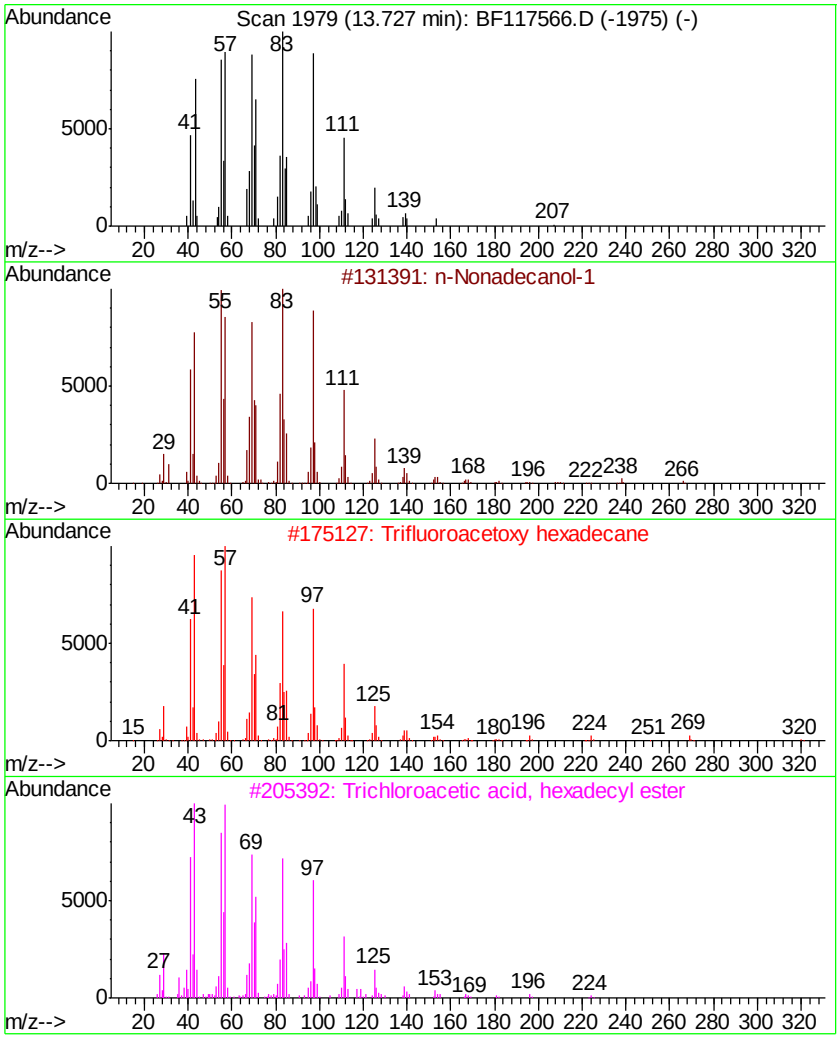
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

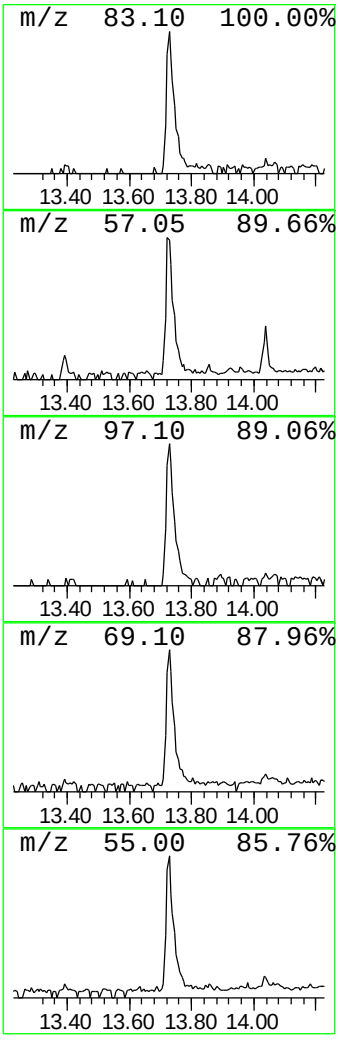
****

Peak Number 4 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	14.76 ng	166050	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117566.D
Acq On : 28 Oct 2019 17:25
Operator : JU
Sample : K5501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 185-56-(0-2.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

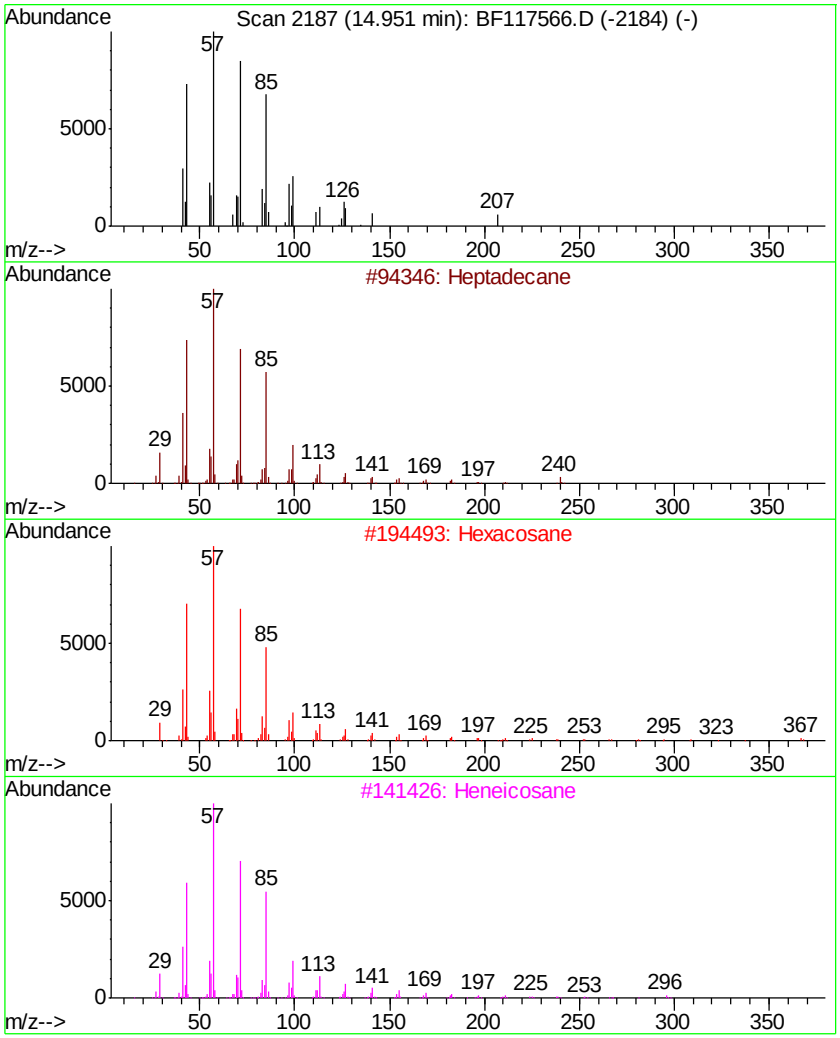
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

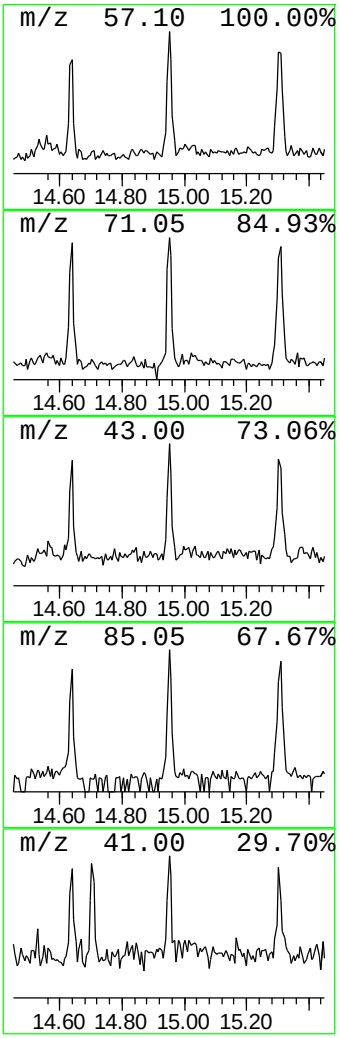
****

Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.61 ng	32635	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Hexacosane	366	C26H54	000630-01-3	80
3	Heneicosane	296	C21H44	000629-94-7	80
4	Tetradecane	198	C14H30	000629-59-4	72
5	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117566.D
Acq On : 28 Oct 2019 17:25
Operator : JU
Sample : K5501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 185-56-(0-2.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

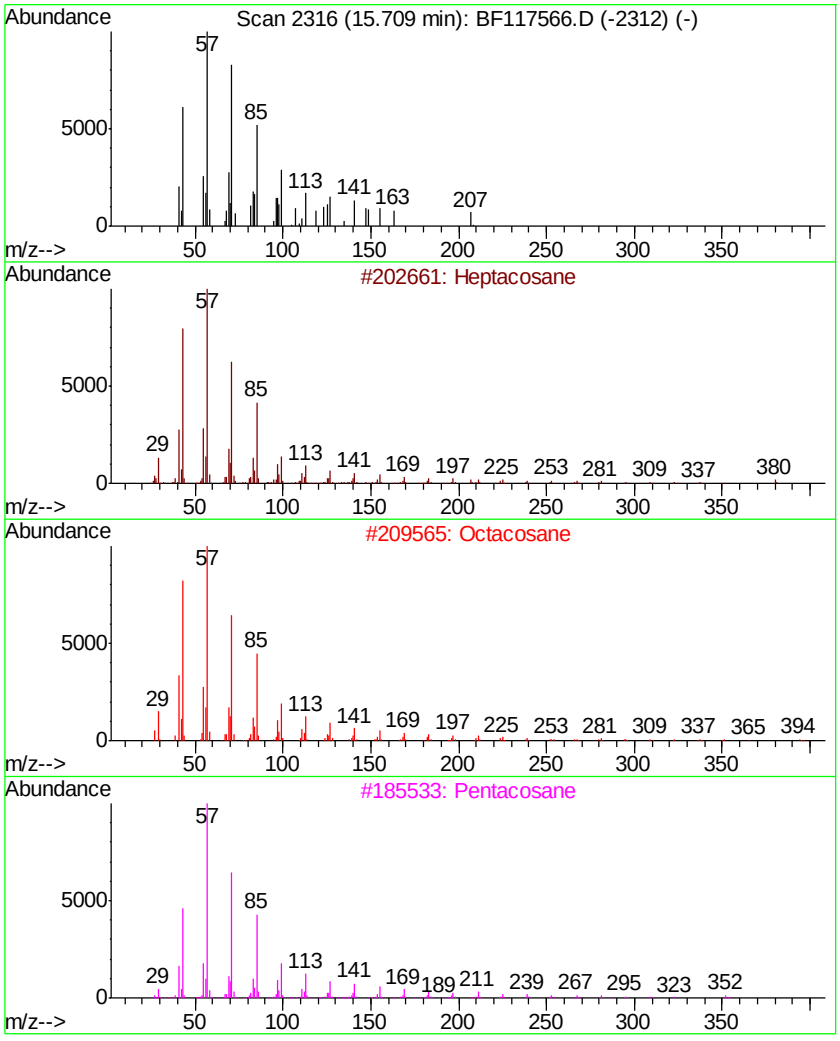
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

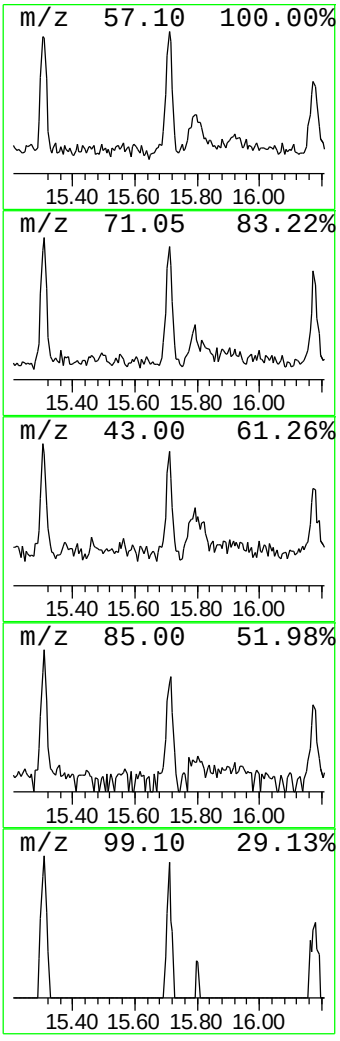
****

Peak Number 6 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.67 ng	33379	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	83
2	Octacosane	394	C28H58	000630-02-4	72
3	Pentacosane	352	C25H52	000629-99-2	72
4	Heneicosane	296	C21H44	000629-94-7	59
5	Tetradecane	198	C14H30	000629-59-4	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117566.D
Acq On : 28 Oct 2019 17:25
Operator : JU
Sample : K5501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 185-56-(0-2.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

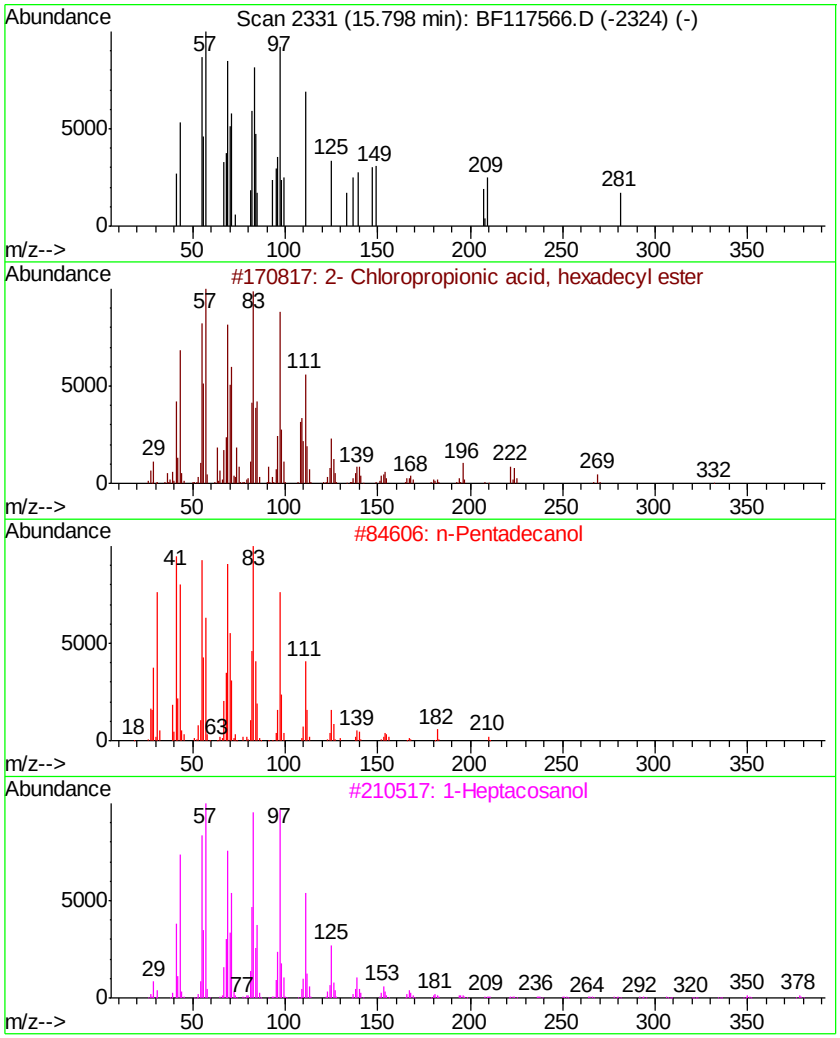
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

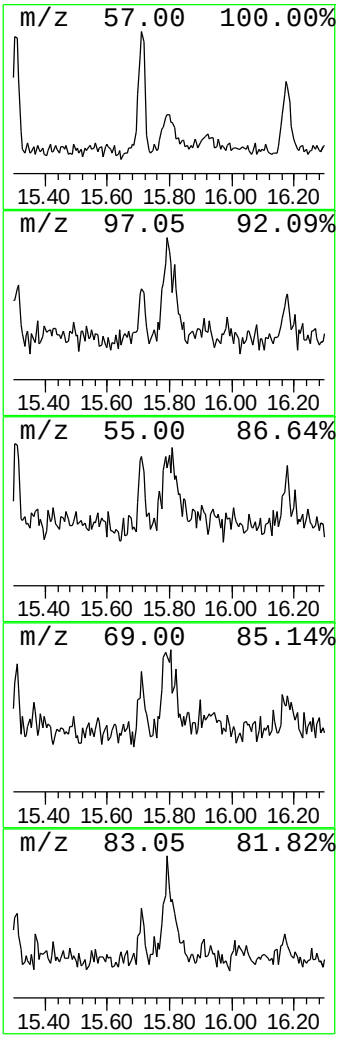
****

Peak Number 7 2- Chloropropionic acid, he... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	3.65 ng	45674	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	64
2	n-Pentadecanol	228	C15H32O	000629-76-5	58
3	1-Heptacosanol	396	C27H56O	002004-39-9	58
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	58
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117566.D
Acq On : 28 Oct 2019 17:25
Operator : JU
Sample : K5501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 185-56-(0-2.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

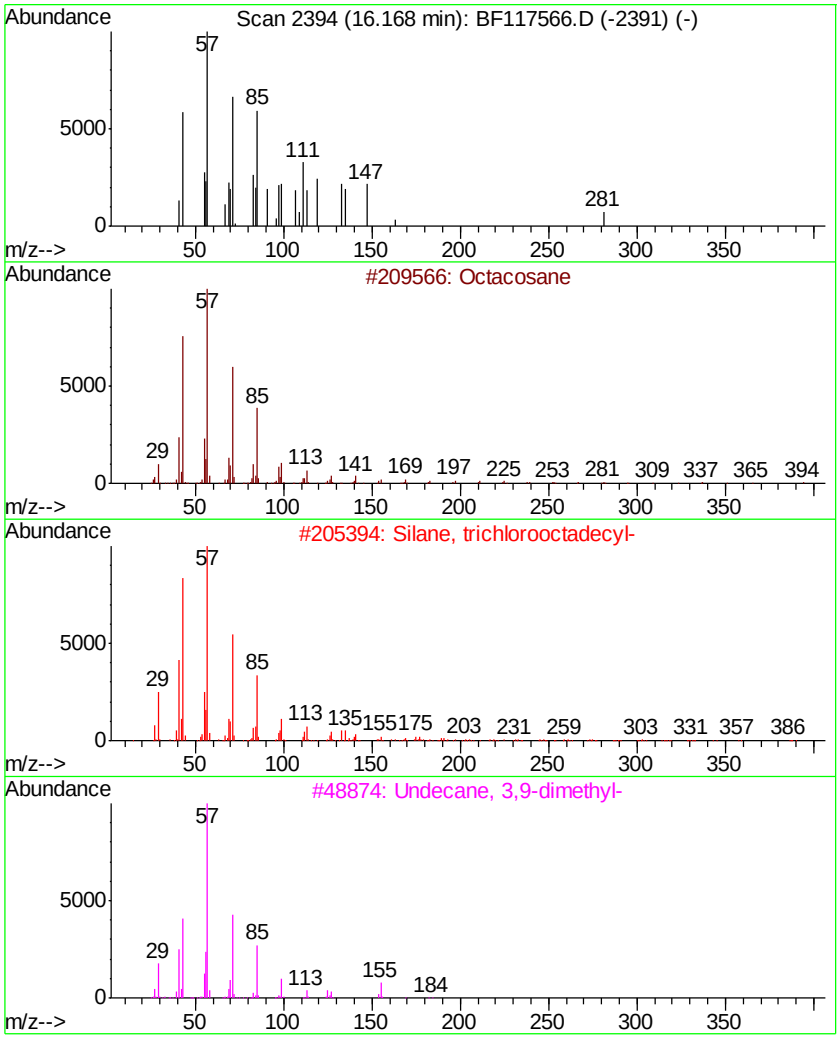
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

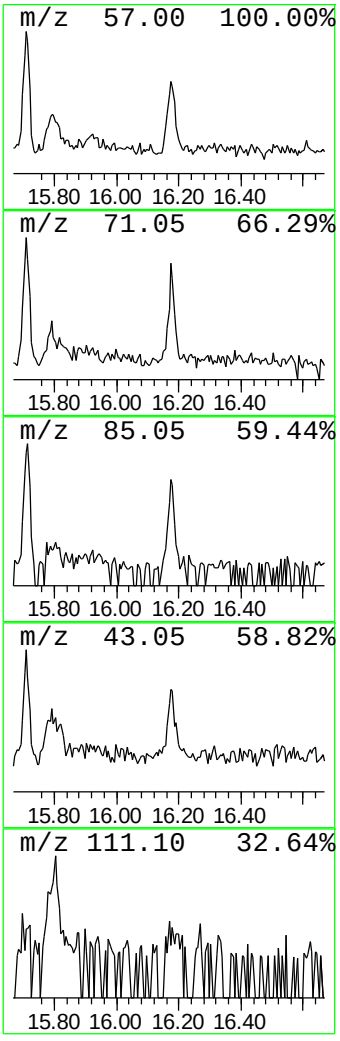
****

Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.61 ng	32687	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	59
2	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	59
3	Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	58
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	50
5	Tetradecane	198	C14H30	000629-59-4	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102819\
Data File : BF117566.D
Acq On : 28 Oct 2019 17:25
Operator : JU
Sample : K5501-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 185-56-(0-2.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown6.50	6.50	94.6	ng	1127750	1	6.73	238430	20.0
n-Hexadecanoic acid	11.77	4.1	ng	65040	4	11.25	314611	20.0
n-Nonadecanol-1	13.73	14.8	ng	166050	5	13.89	225023	20.0
Heptadecane	14.95	2.6	ng	32635	6	15.32	250354	20.0
Heptacosane	15.71	2.7	ng	33379	6	15.32	250354	20.0
2- Chloropropioni...	15.80	3.6	ng	45674	6	15.32	250354	20.0
Octacosane	16.17	2.6	ng	32687	6	15.32	250354	20.0