LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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	573	rBV	749626	833404	71.31%	8.145%
2	6.381	726	730	747	rBV	935798	967903	82.82%	9.459%
3	6.504	747	751	764	rVB	1123207	971099	83.10%	9.491%
4	6.733	787	790	799	rBV	262282	260605	22.30%	2.547%
5	6.886	812	816	830	rBV	821067	688707	58.93%	6.731%
6	7.298	882	886	910	rBV	545720	577364	49.40%	5.643%
7	8.010	1004	1007	1020	rBV	357260	337834	28.91%	3.302%
8	9.086	1186	1190	1193	rBV	1346189	1073717	91.88%	10.494%
9	9.480	1254	1257	1267	rBV	136831	113379	9.70%	1.108%
10	9.763	1301	1305	1317	rBV	486400	409587	35.05%	4.003%
11	10.551	1436	1439	1457	rVB	671654	652283	55.82%	6.375%
12	11.245	1554	1557	1561	rBV2	399262	391647	33.51%	3.828%
13	11.780	1641	1648	1657	rBV	110051	129424	11.07%	1.265%
14	12.468	1762	1765	1771	rBV	31959	36356	3.11%	0.355%
15	12.557	1777	1780	1787	rBV	33913	40561	3.47%	0.396%
16	12.692	1799	1803	1807	rBV	27700	31054	2.66%	0.303%
17	12.833	1822	1827	1830	rBV	1232363	1168635	100.00%	11.421%
18	13.727	1975	1979	1992	rBV	144095	236201	20.21%	2.308%
19	13.892	2003	2007	2015	rBV	375104	394911	33.79%	3.860%
20	14.045	2029	2033	2043	rVB3	14493	21343	1.83%	0.209%
21	14.345	2080	2084	2086	rBV	27201	26774	2.29%	0.262%
22	14.374	2086	2089	2095	rVB5	13739	23109	1.98%	0.226%
23	14.645	2131	2135	2138	rBV	34915	33051	2.83%	0.323%
24	14.715	2144	2147	2152	rVB	19765	17838	1.53%	0.174%
25	14.921	2178	2182	2185	rBV	12326	17775	1.52%	0.174%
26	14.962	2185	2189	2192	rVB2	57725	63753	5.46%	0.623%
27	15.004	2192	2196	2199	rBV4	10045	17469	1.49%	0.171%
28	15.321	2245	2250	2265	rBV	273129	370024	31.66%	3.616%
29	15.503	2277	2281	2285	rVB3	9662	14156	1.21%	0.138%
30	15.721	2313	2318	2323	rVB	77793	105060	8.99%	1.027%
31	15.792	2323	2330	2335	rBV5	29851	77595	6.64%	0.758%
32	16.186	2391	2397	2401	rBV3	18262	28953	2.48%	0.283%
33	16.456	2437	2443	2447	rBV6	16665	28738	2.46%	0.281%
34	16.733	2485	2490	2498	rBV6	10608	22593	1.93%	0.221%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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

35	16.856	2503	2511	2516	rBV7	17042	49255	4.21%	0.481%

Sum of corrected areas: 10232157

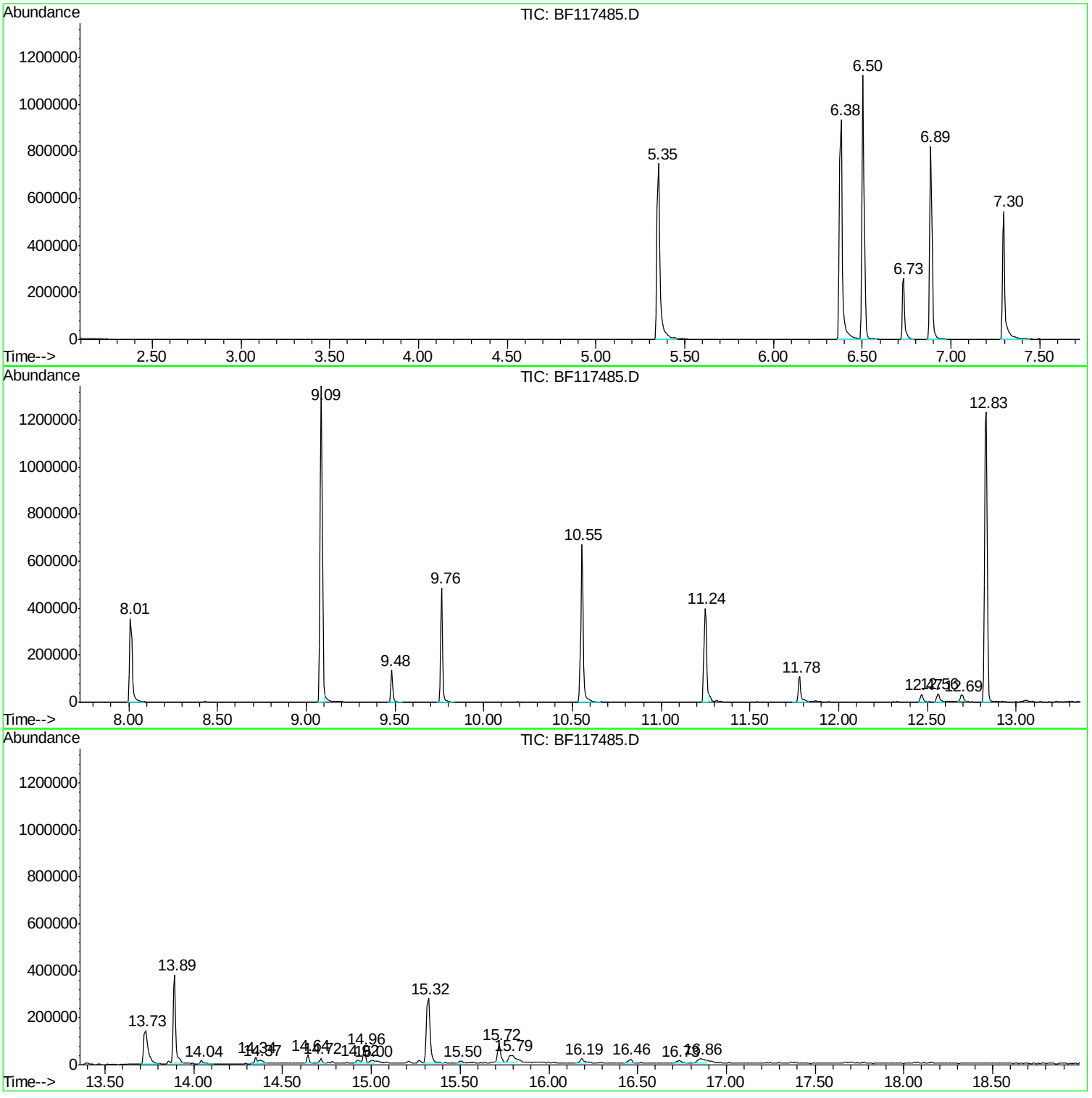
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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

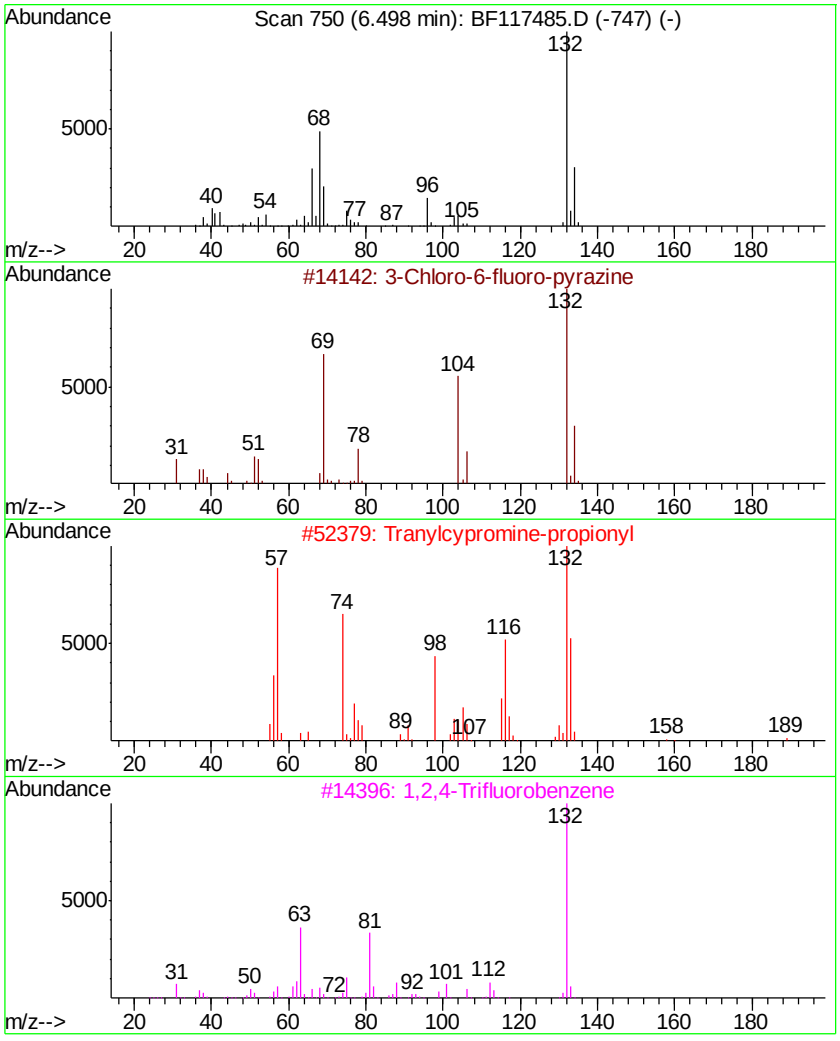
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

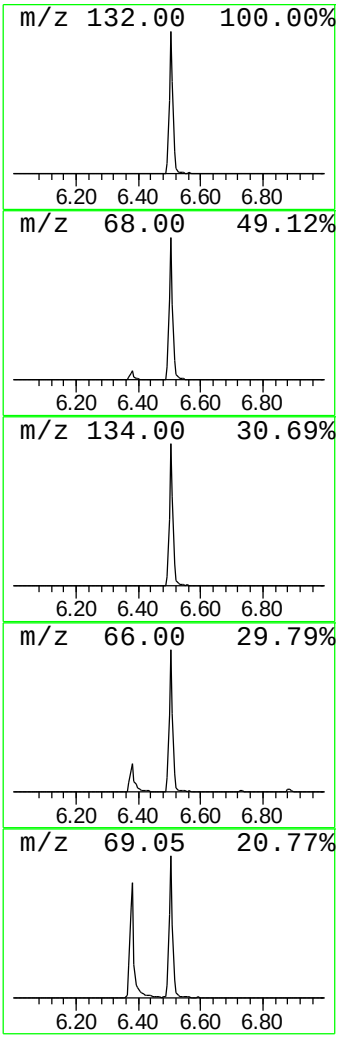
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	74.53 ng	971099	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	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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

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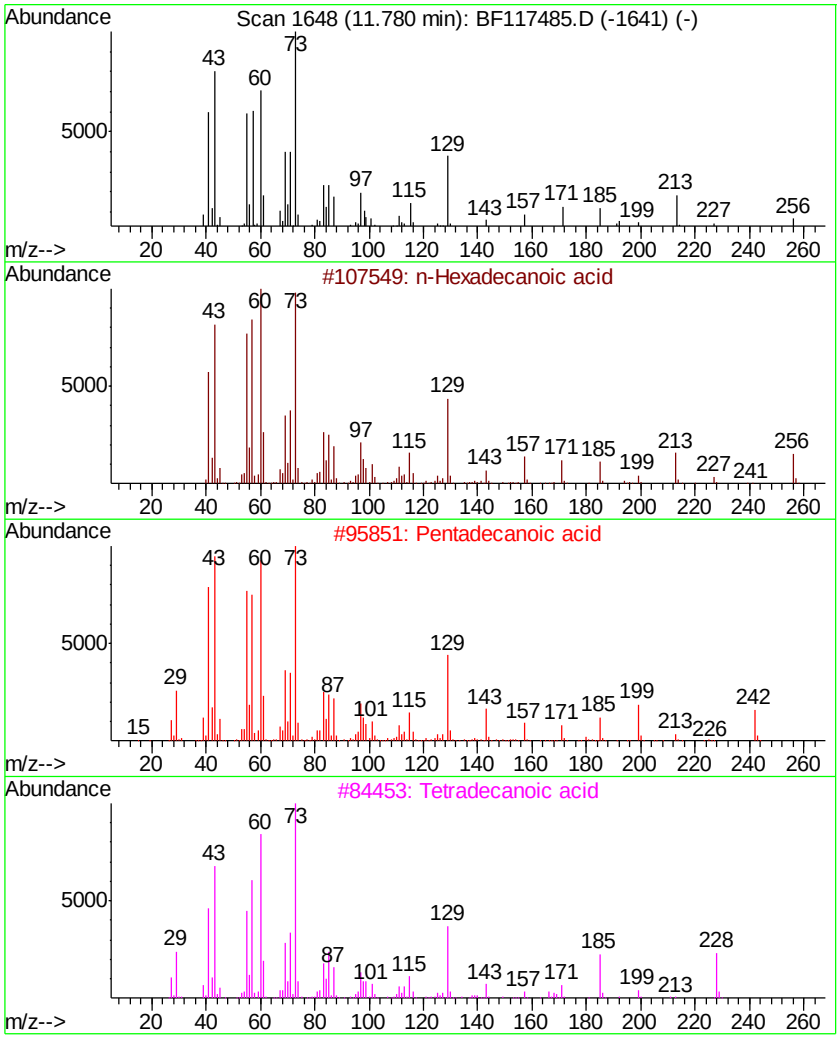
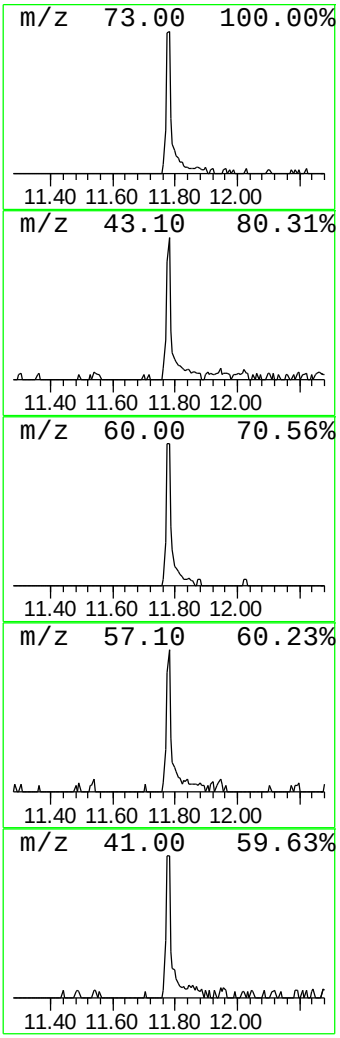
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	6.61 ng	129424	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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

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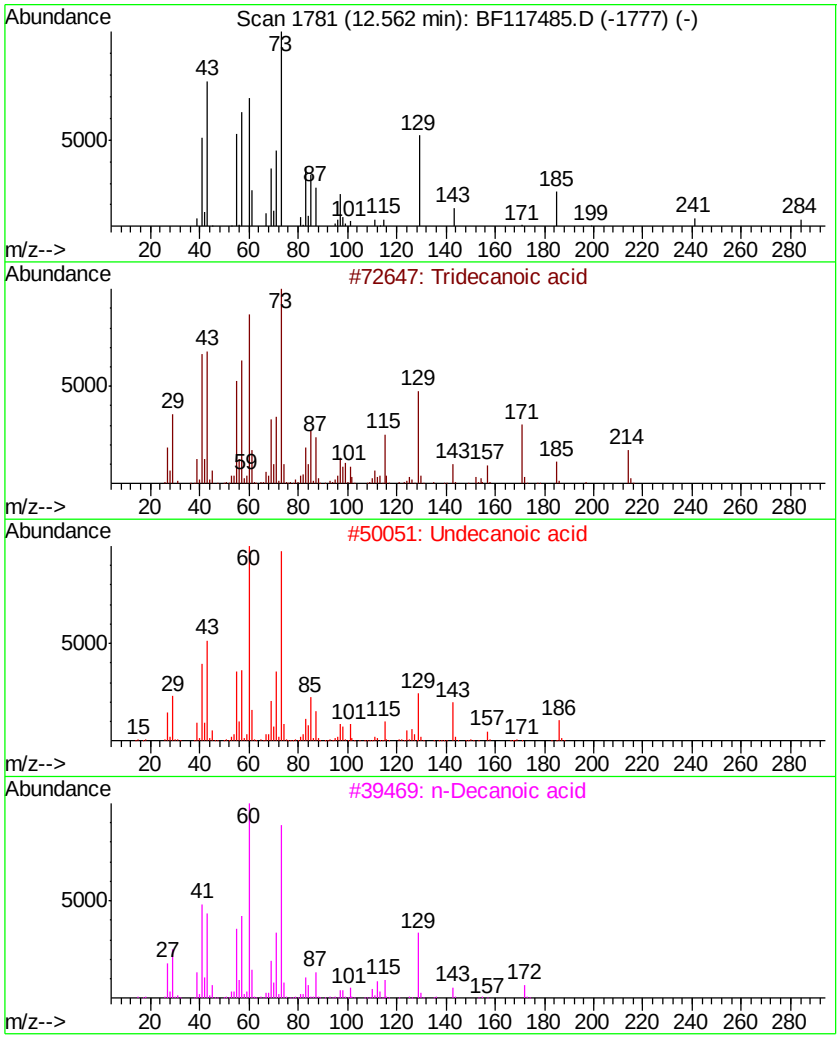
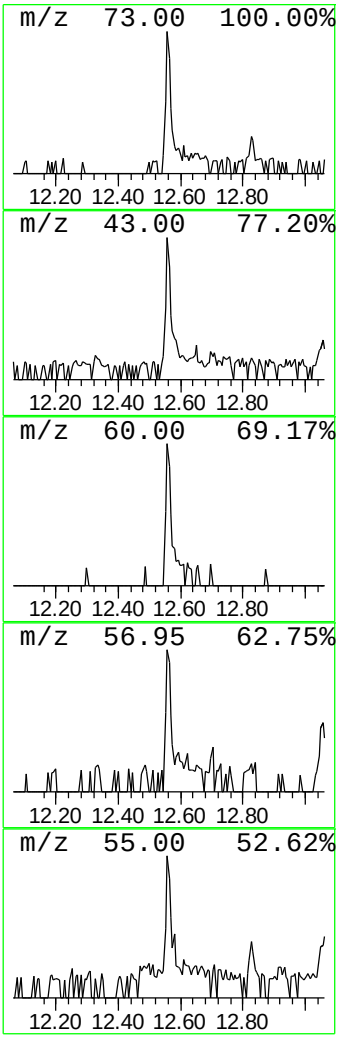
Peak Number 4 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	2.07 ng	40561	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	72
2	Undecanoic acid	186	C11H22O2	000112-37-8	59
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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

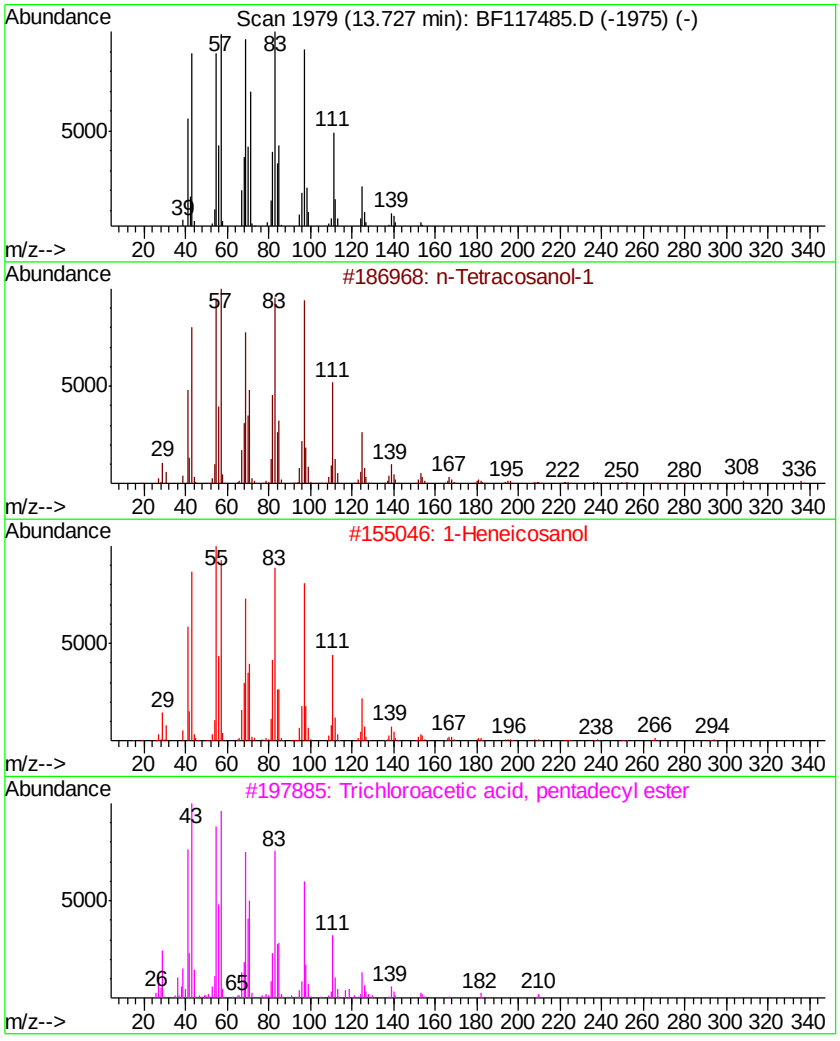
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

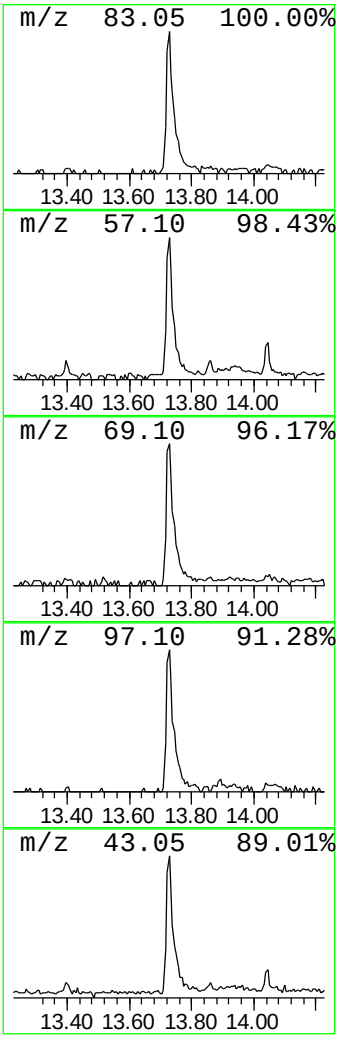
****

Peak Number 5 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	11.96 ng	236201	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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

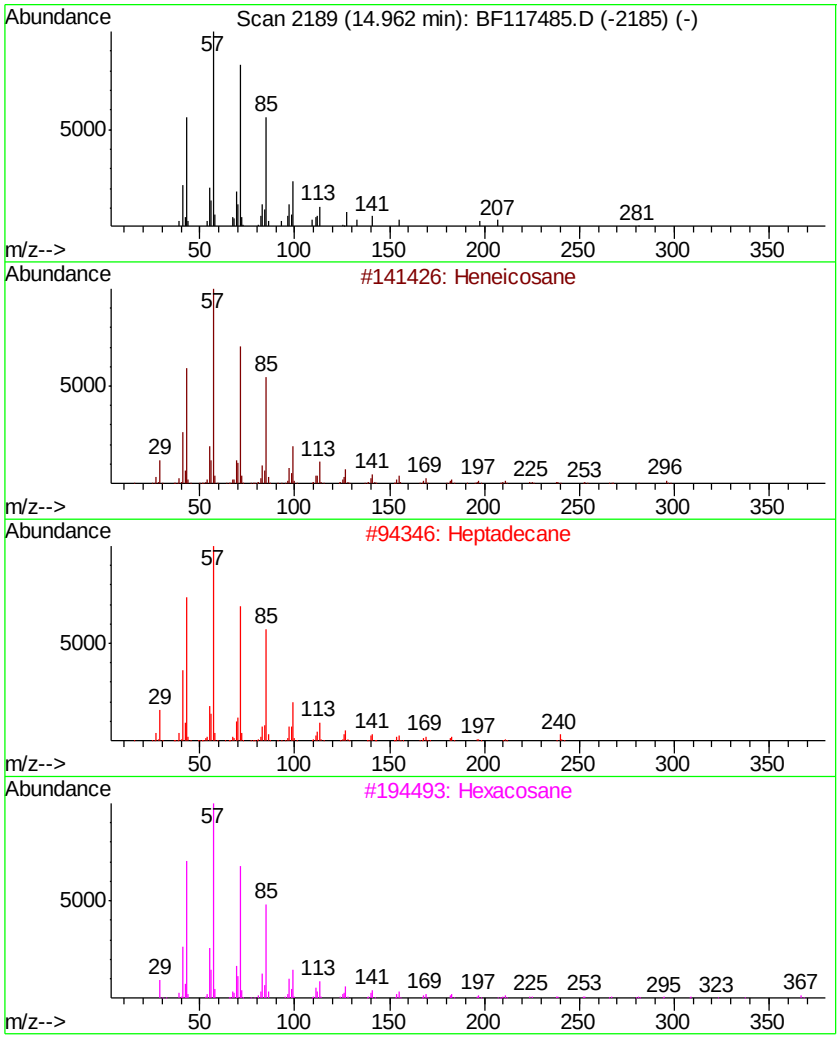
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

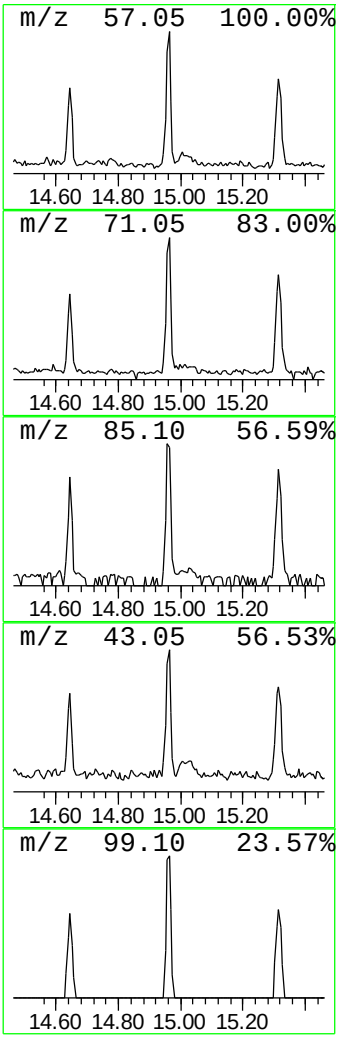
****

Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.45 ng	63753	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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

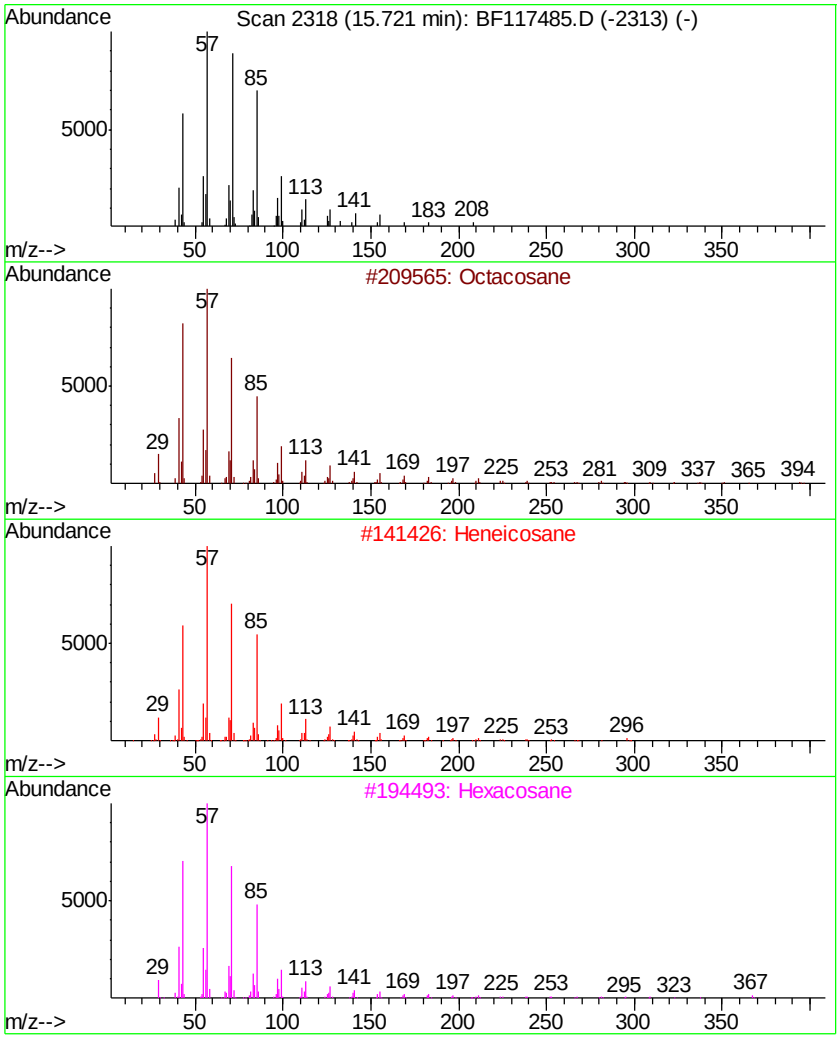
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

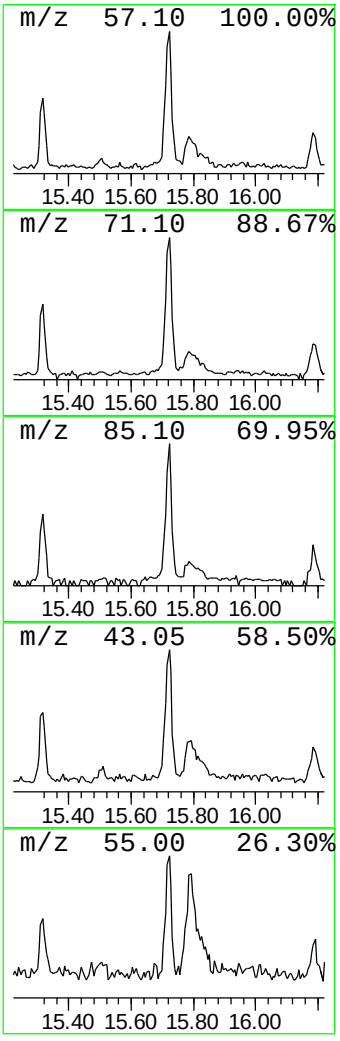
****

Peak Number 7 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	5.68 ng	105060	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Triacontane	422	C30H62	000638-68-6	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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

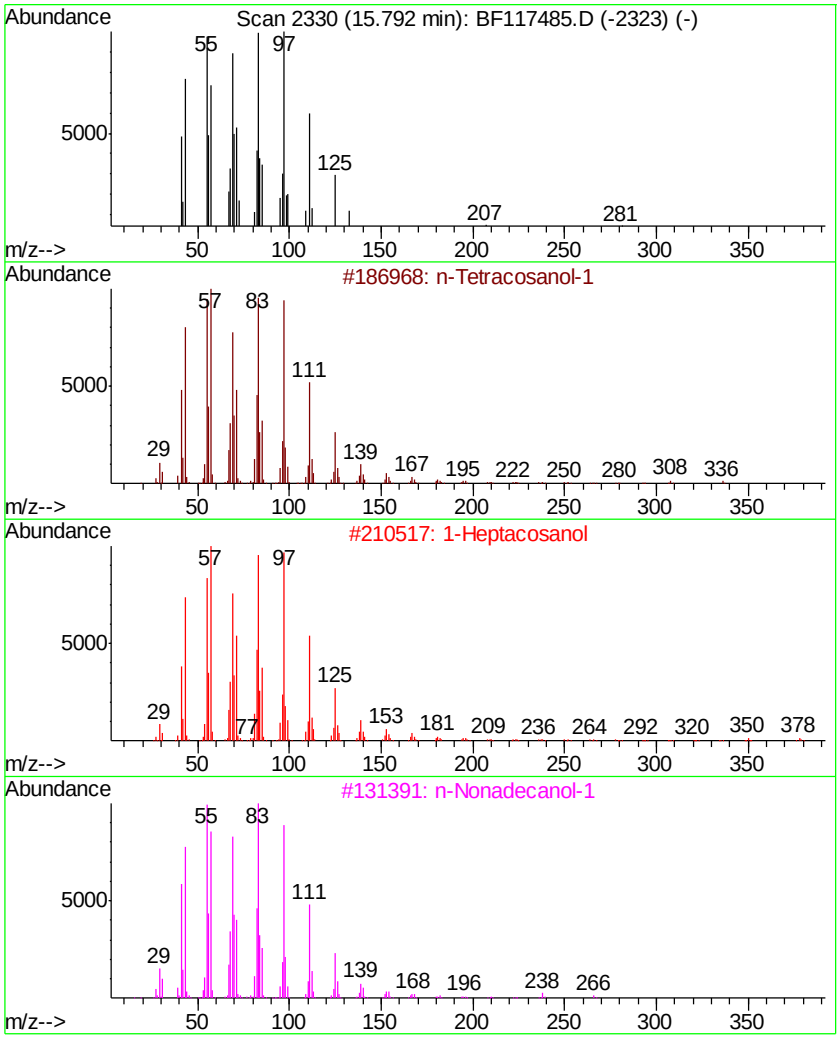
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

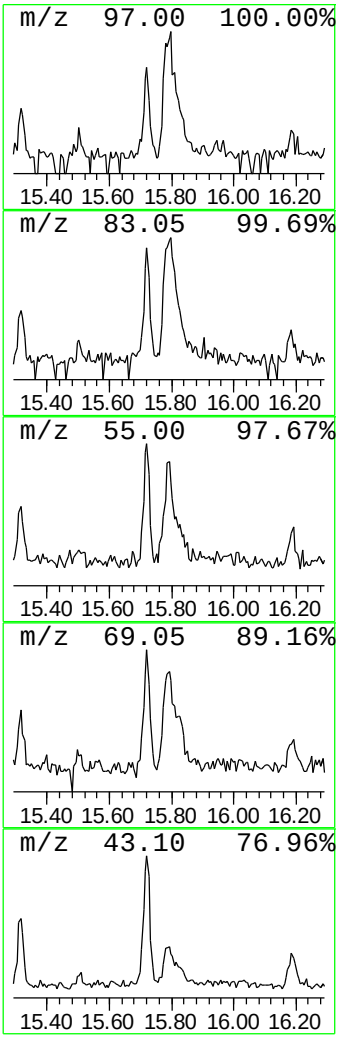
****

Peak Number 8 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	4.19 ng	77595	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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

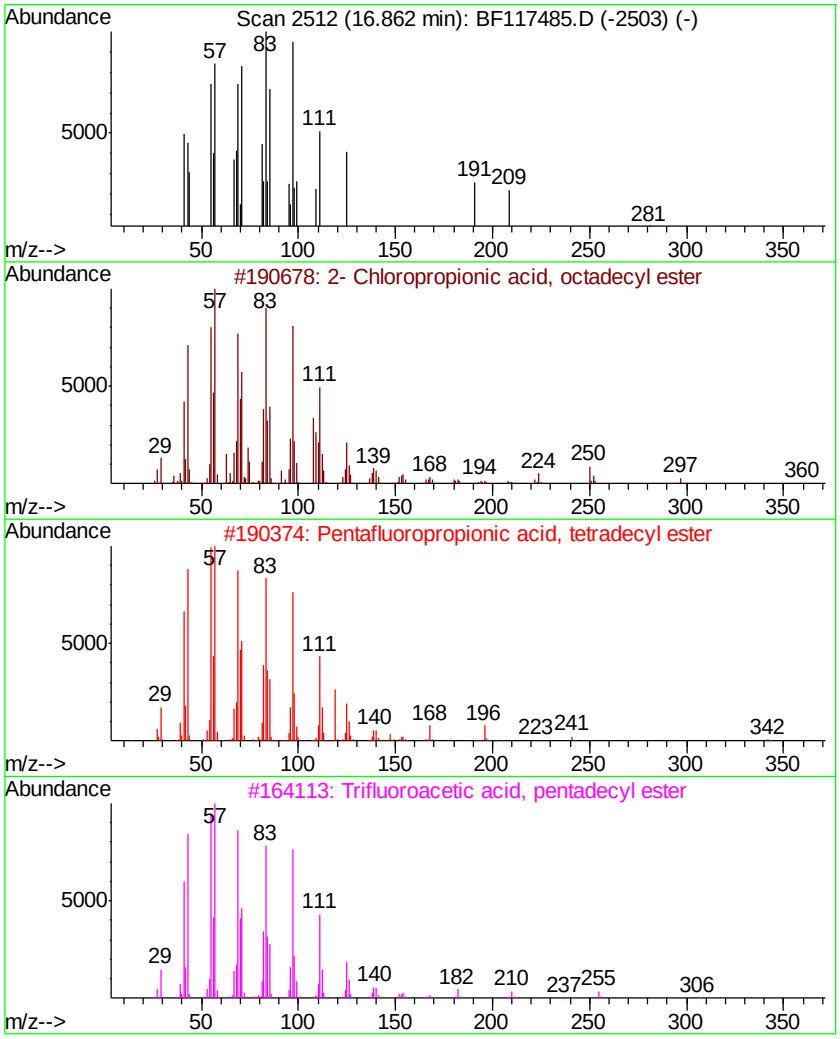
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

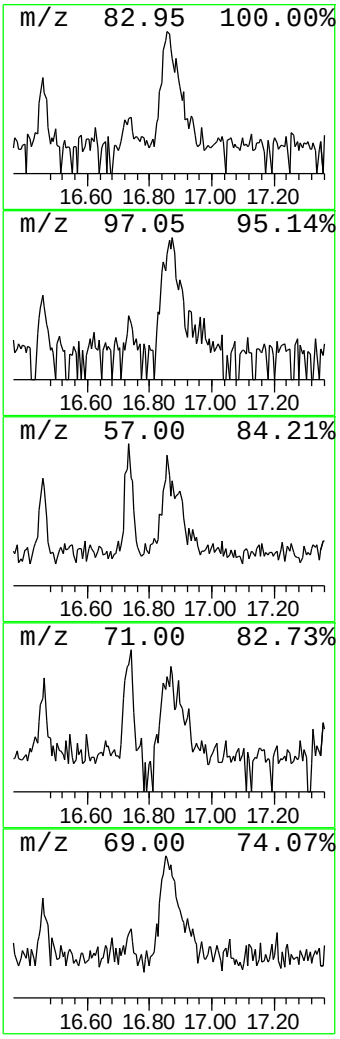
****

Peak Number 9 2- Chloropropionic acid, oc... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.86	2.66 ng	49255	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	72
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	58
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	58
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	58
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102319\
Data File : BF117485.D
Acq On : 23 Oct 2019 16:18
Operator : JU
Sample : K5494-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-6FT

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	74.5	ng	971099	1	6.73	260605	20.0
n-Hexadecanoic acid	11.78	6.6	ng	129424	4	11.24	391647	20.0
Tridecanoic acid	12.56	2.1	ng	40561	4	11.24	391647	20.0
n-Tetracosanol-1	13.73	12.0	ng	236201	5	13.89	394911	20.0
Heneicosane	14.96	3.5	ng	63753	6	15.32	370024	20.0
Octacosane	15.72	5.7	ng	105060	6	15.32	370024	20.0
1-Heptacosanol	15.79	4.2	ng	77595	6	15.32	370024	20.0
2- Chloropropioni...	16.86	2.7	ng	49255	6	15.32	370024	20.0