LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

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-BF083019.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	5.034	498	501	510	rVB	31953	36621	1.46%	0.180%
2	5.439	566	570	574	rBV	1614817	1639189	65.49%	8.068%
3	6.457	738	743	755	rBV	1889179	1824234	72.88%	8.979%
4	6.592	762	766	769	rBV	2095274	1847584	73.82%	9.094%
5	6.822	801	805	813	rBV	562297	465558	18.60%	2.292%
6	6.981	828	832	835	rBV	1678742	1394145	55.70%	6.862%
7	7.381	895	900	903	rBV	1192722	1082327	43.24%	5.327%
8	8.104	1019	1023	1040	rBV	642450	626641	25.04%	3.084%
9	9.175	1201	1205	1216	rBV	2533825	2257556	90.20%	11.112%
10	9.569	1268	1272	1282	rBV	180898	170538	6.81%	0.839%
11	9.851	1317	1320	1330	rBV	816125	750006	29.97%	3.692%
12	10.639	1450	1454	1466	rBV	1441310	1300344	51.95%	6.401%
13	11.333	1568	1572	1579	rBV	839902	776375	31.02%	3.821%
14	11.863	1657	1662	1675	rBV	147384	185707	7.42%	0.914%
15	12.645	1790	1795	1806	rBV	182143	226673	9.06%	1.116%
16	12.915	1837	1841	1845	rBV	2569236	2502908	100.00%	12.320%
17	13.145	1872	1880	1885	rBV5	17341	31331	1.25%	0.154%
18	13.815	1990	1994	2011	rBV2	183477	409118	16.35%	2.014%
19	13.968	2015	2020	2023	rBV	807035	730323	29.18%	3.595%
20	14.127	2044	2047	2050	rBV	37858	34428	1.38%	0.169%
21	14.433	2088	2099	2102	rBV	107709	180689	7.22%	0.889%
22	14.462	2103	2104	2117	rVB5	30109	56850	2.27%	0.280%
23	14.733	2146	2150	2154	rVB	106410	104434	4.17%	0.514%
24	14.809	2159	2163	2166	rBV	44087	47828	1.91%	0.235%
25	15.062	2202	2206	2211	rVB	152937	165668	6.62%	0.815%
26	15.139	2211	2219	2224	rBV9	17837	46299	1.85%	0.228%
27	15.415	2260	2266	2275	rVB	535186	810536	32.38%	3.990%
28	15.627	2297	2302	2309	rBV6	27458	38537	1.54%	0.190%
29	15.856	2336	2341	2348	rVB	129435	190829	7.62%	0.939%
30	15.945	2348	2356	2358	rBV5	28247	66684	2.66%	0.328%
31	16.345	2418	2424	2433	rBV5	48701	91014	3.64%	0.448%
32	16.627	2467	2472	2478	rVB8	21281	40591	1.62%	0.200%
33	16.921	2516	2522	2527	rVB6	24508	48311	1.93%	0.238%
34	17.086	2542	2550	2561	rBV6	13388	49377	1.97%	0.243%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

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-BF083019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.180	2561	2566	2572	rVB8	16436	28167	1.13%	0.139%
36	17.445	2603	2611	2613	rBV7	13359	25936	1.04%	0.128%
37	18.409	2768	2775	2784	rVB7	12273	32774	1.31%	0.161%

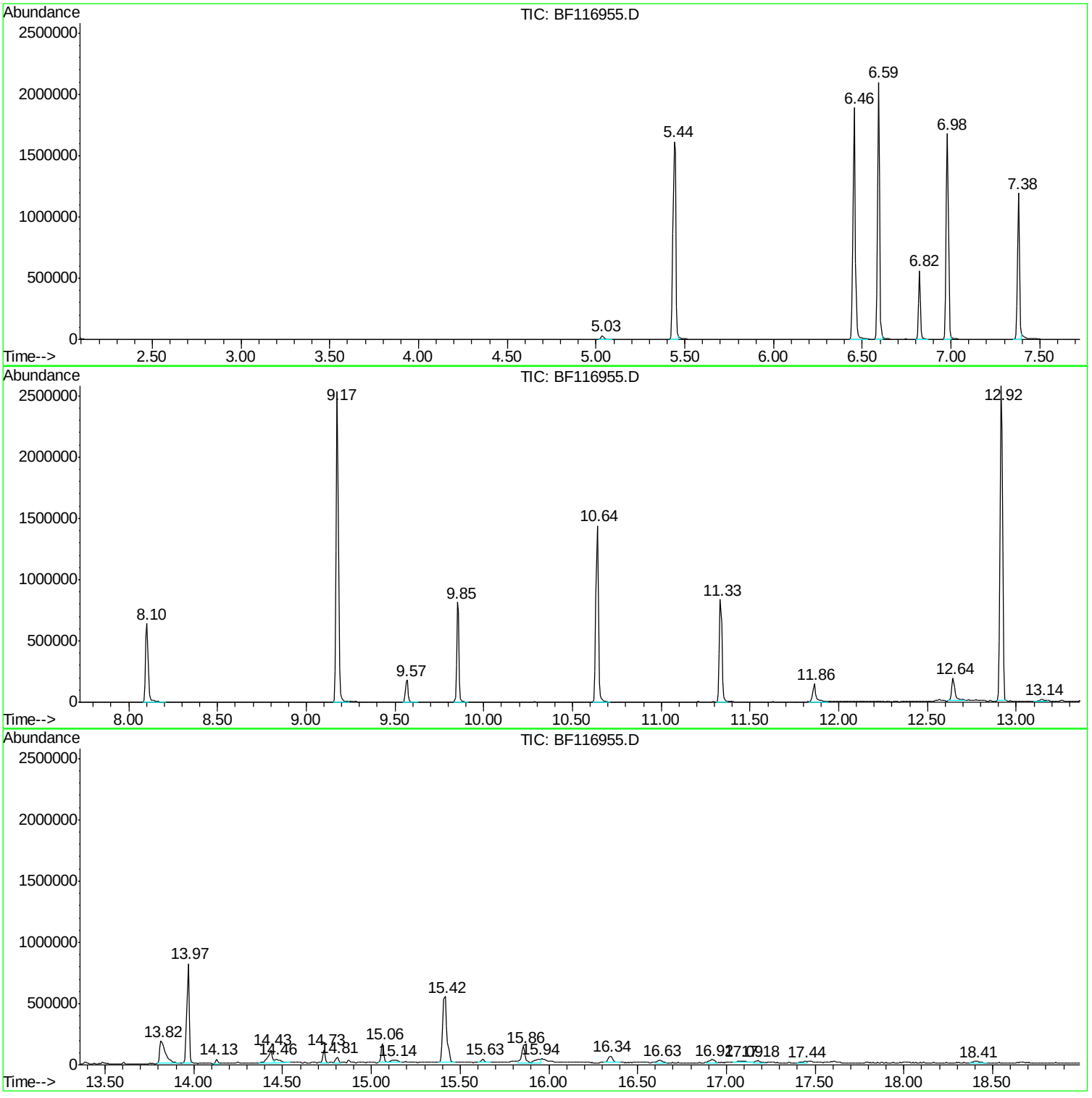
Sum of corrected areas: 20316130

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

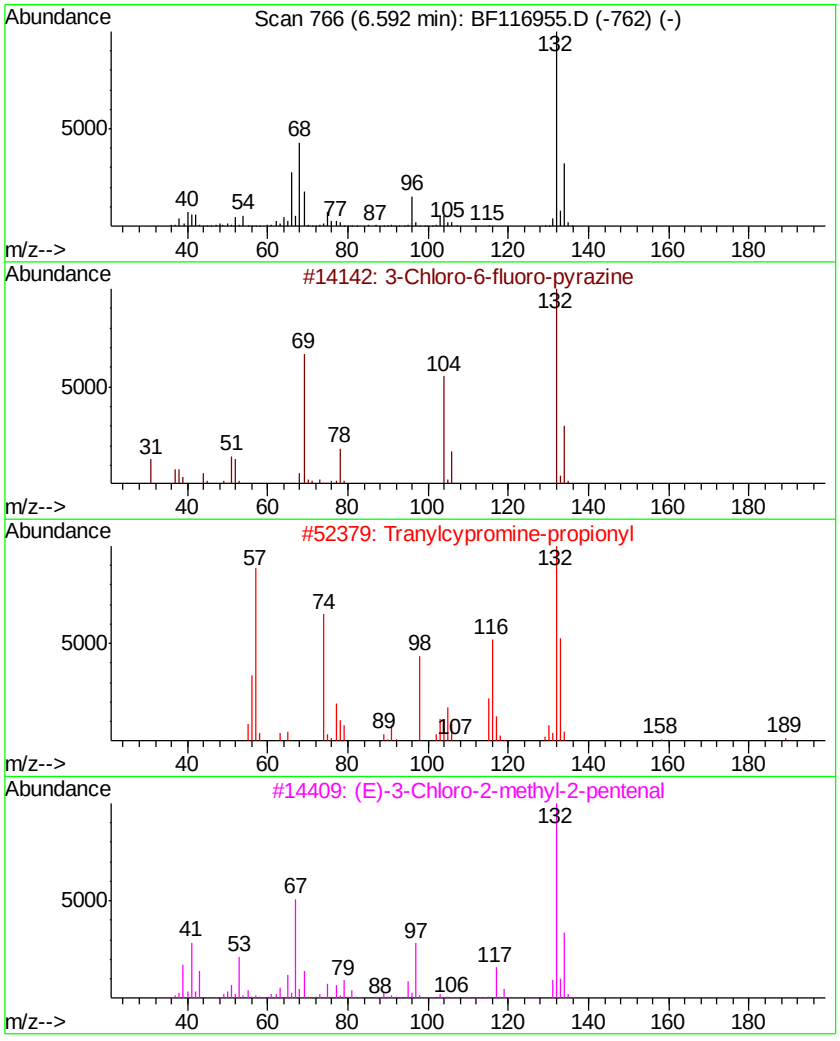
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

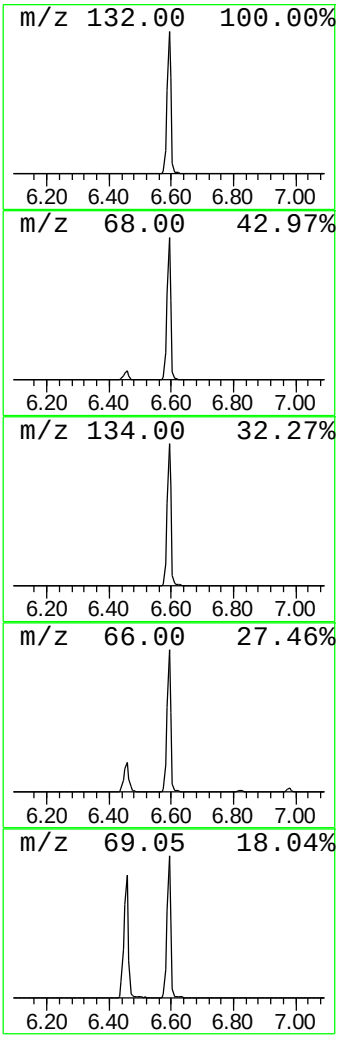
****

Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	79.37 ng	1847580	1,4-Dichlorobenzene-d4	6.82

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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	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\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

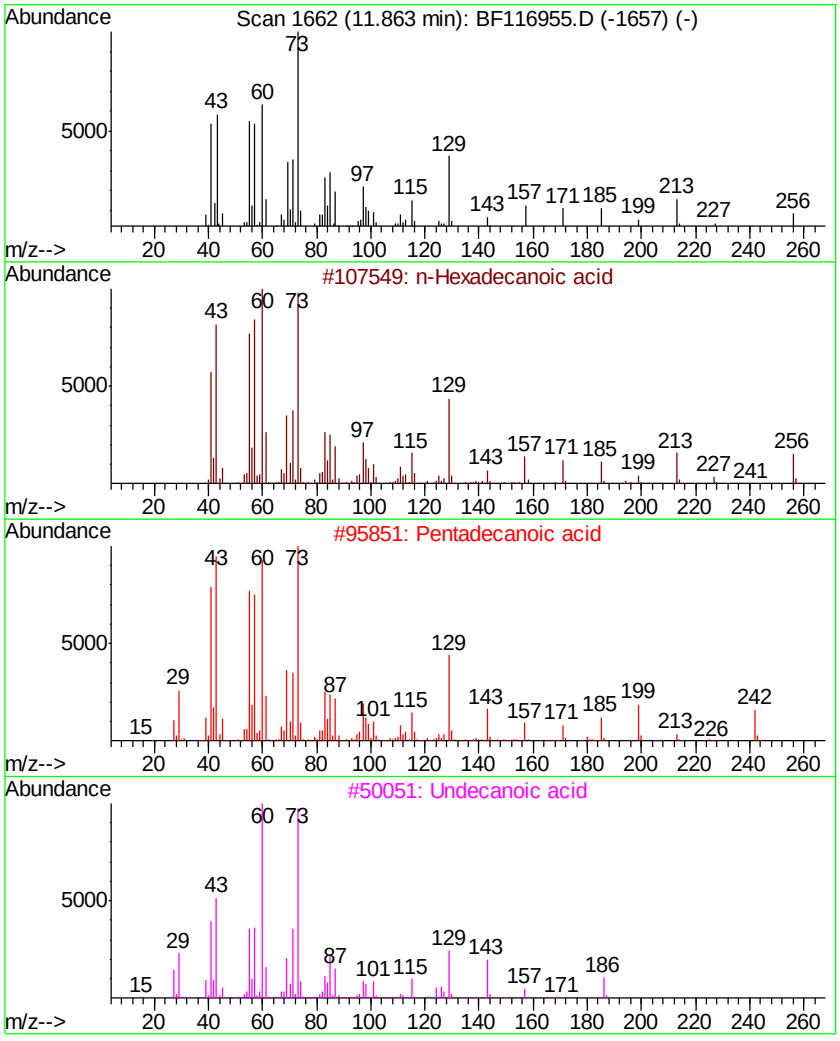
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

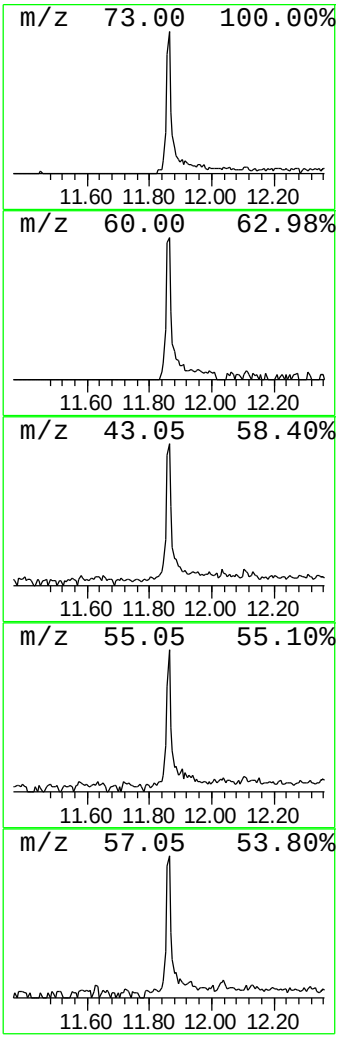
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	4.78 ng	185707	Phenanthrene-d10	11.33

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	80
3	Undecanoic acid	186	C11H22O2	000112-37-8	53
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	Tridecanoic acid	214	C13H26O2	000638-53-9	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

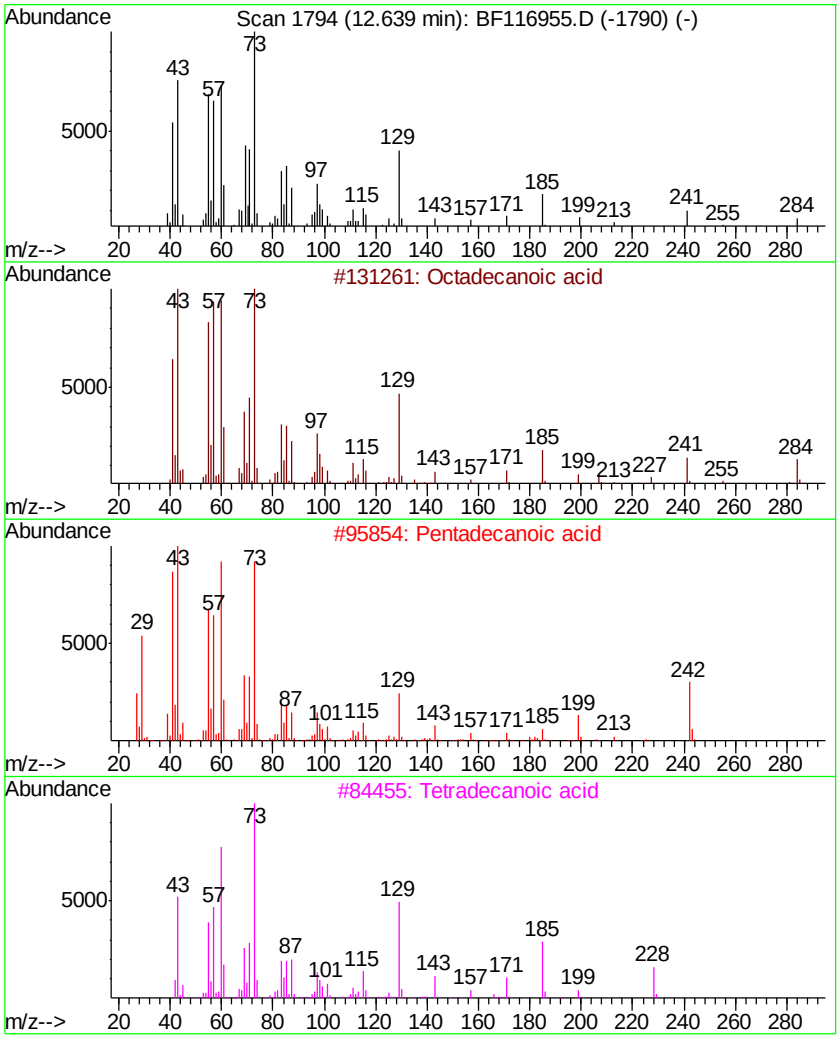
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

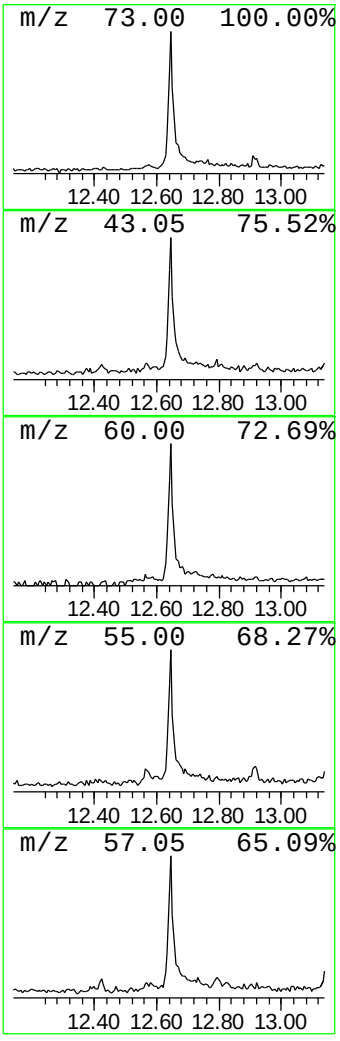
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	5.84 ng	226673	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	30





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

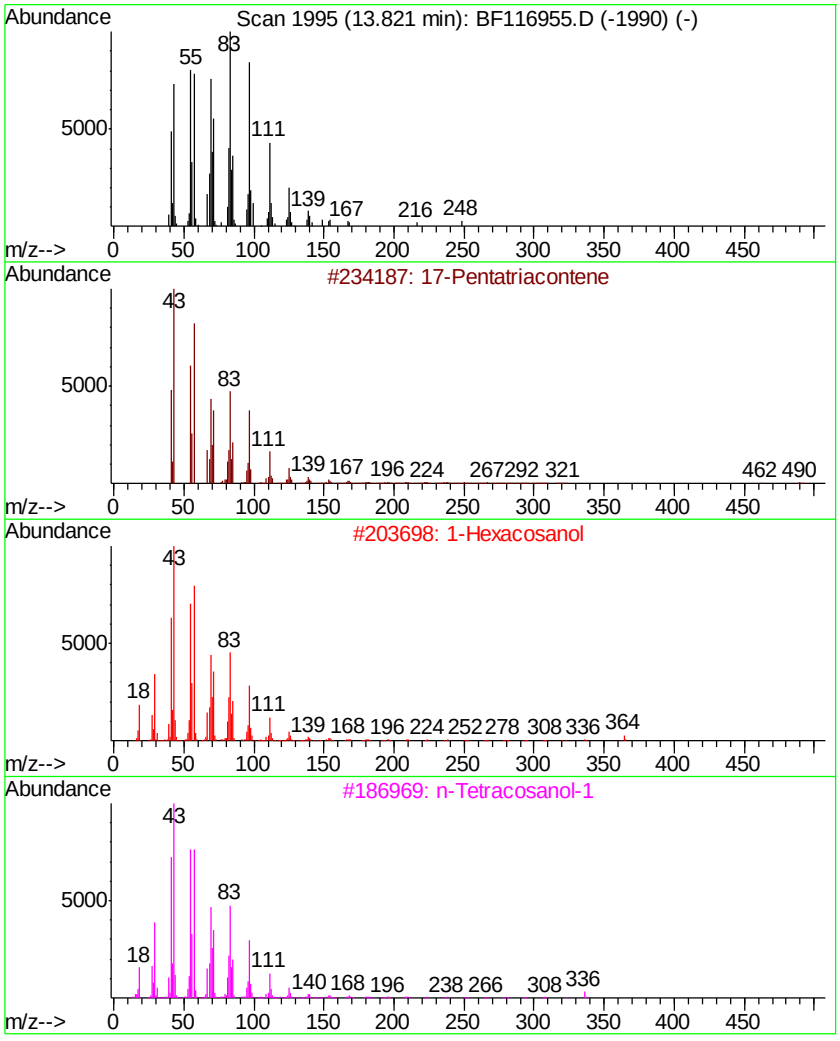
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

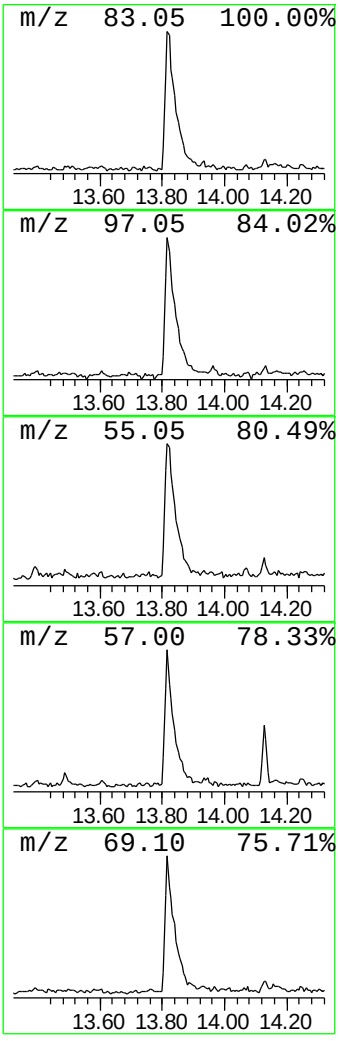
****

Peak Number 5 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	11.20 ng	409118	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	1-Hexacosanol	382	C26H54O	000506-52-5	83
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	83
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	76
5	1-Heptacosanol	396	C27H56O	002004-39-9	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

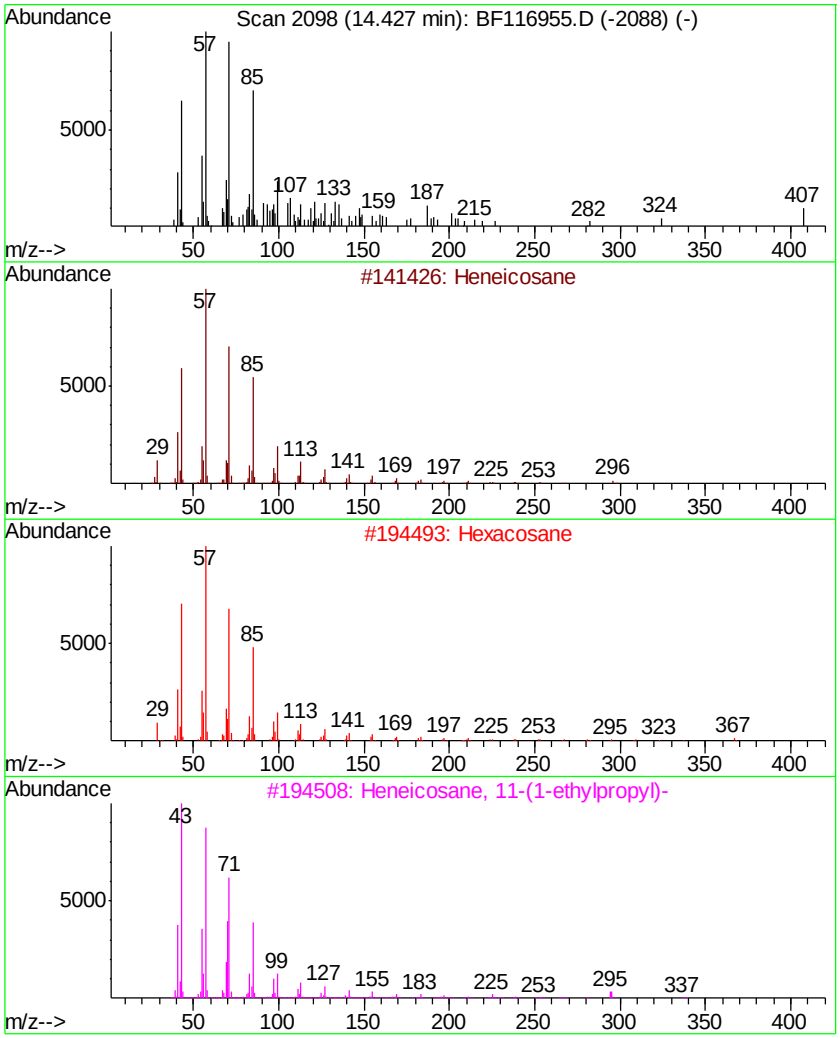
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

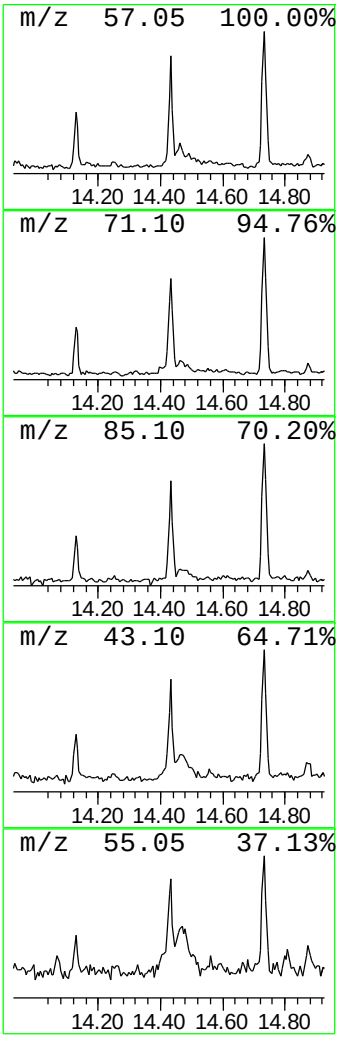
****

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	4.95 ng	180689	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Hentriacontane	437	C31H64	000630-04-6	87
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

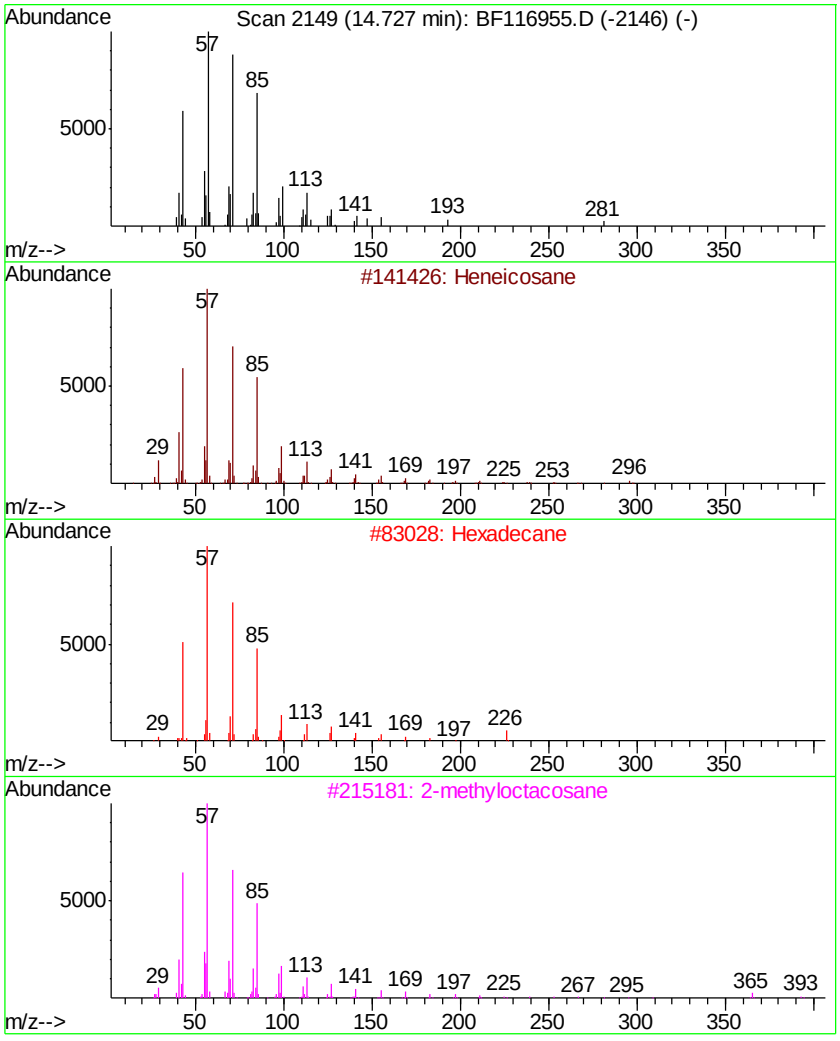
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

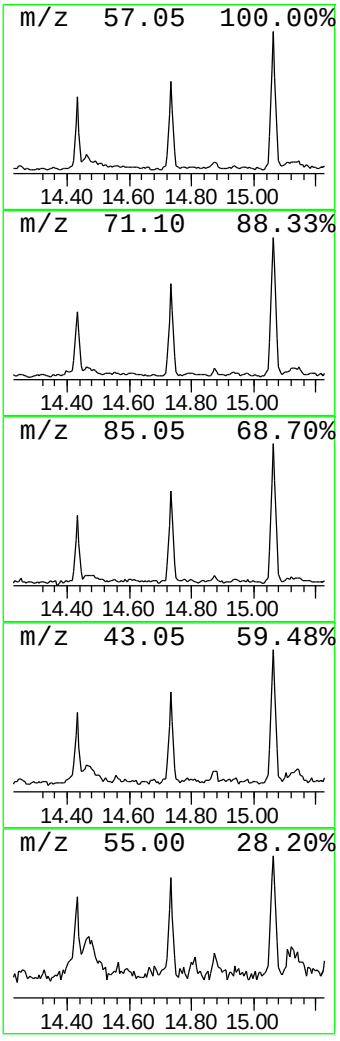
****

Peak Number 7 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.58 ng	104434	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexadecane	226	C16H34	000544-76-3	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Octadecane	254	C18H38	000593-45-3	86
5	Hentriacontane	437	C31H64	000630-04-6	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

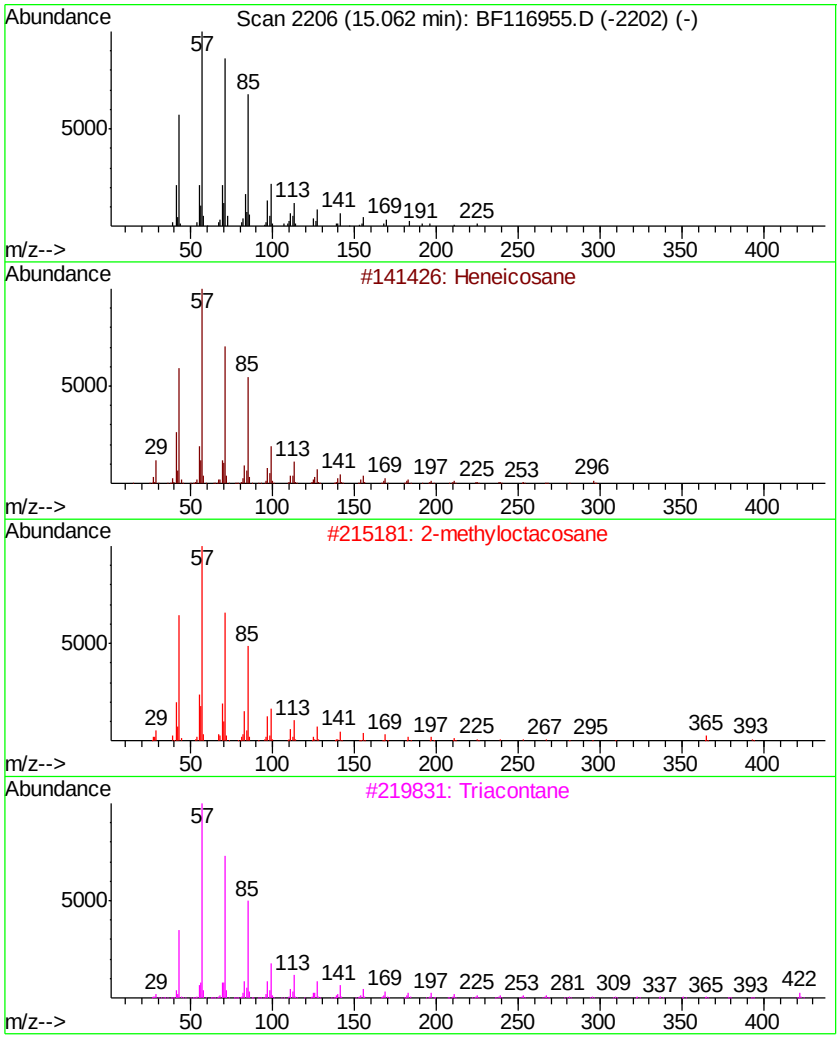
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

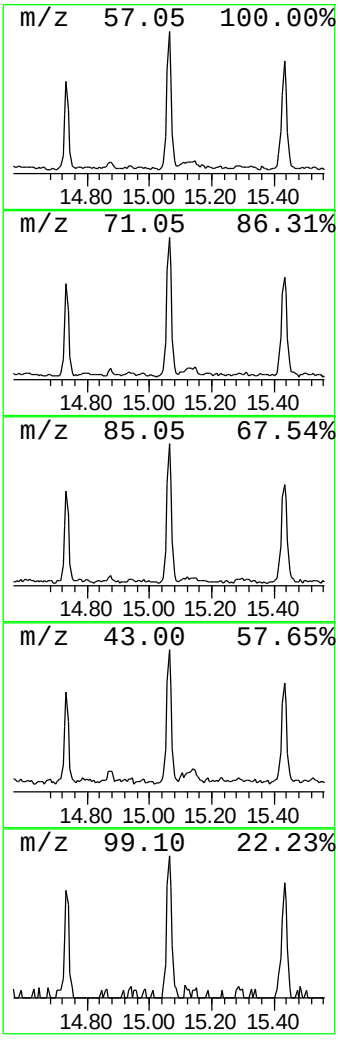
****

Peak Number 8 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	4.09 ng	165668	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
5	Hexacosane	366	C26H54	000630-01-3	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

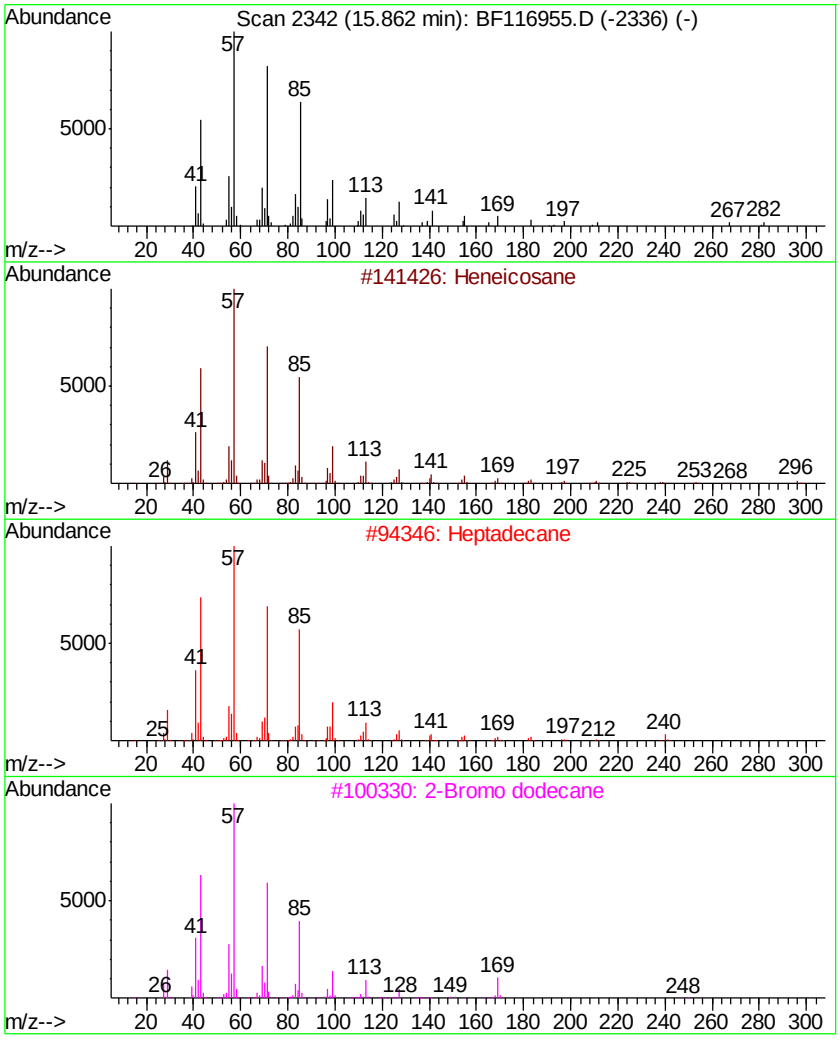
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

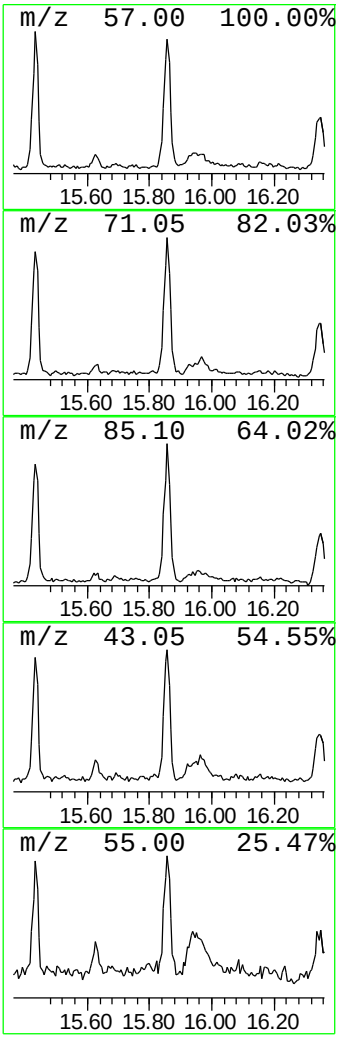
****

Peak Number 9 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	4.71 ng	190829	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	90
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86
5	Hexacosane	366	C26H54	000630-01-3	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

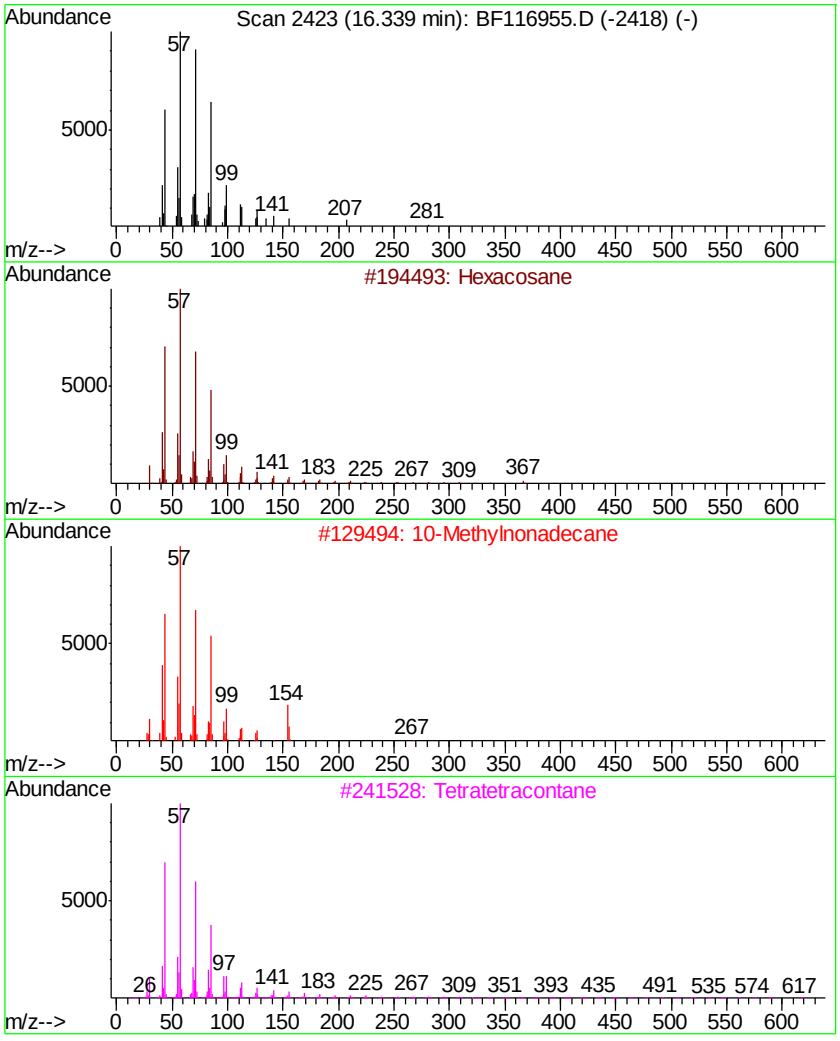
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

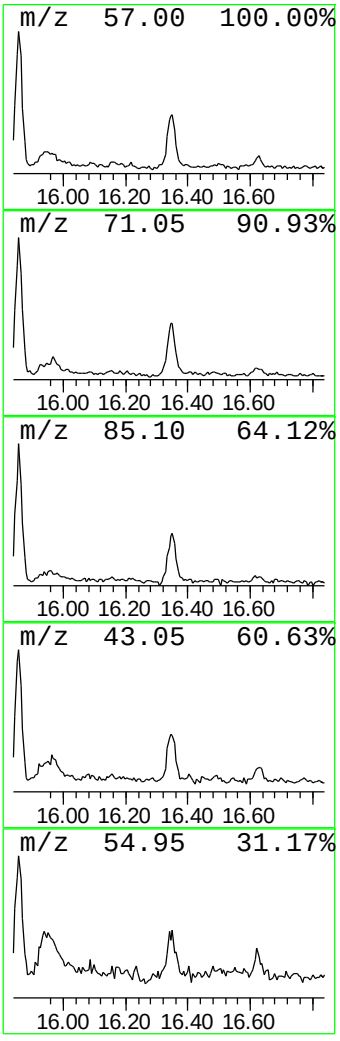
****

Peak Number 10 10-Methylnonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.34	2.25 ng	91014	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	10-Methylnonadecane	282	C20H42	056862-62-5	90
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Hexatriacontane	507	C36H74	000630-06-8	86
5	Octacosane	394	C28H58	000630-02-4	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091119\
Data File : BF116955.D
Acq On : 11 Sep 2019 19:21
Operator : HP/JU
Sample : K4786-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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
unknown6.59	6.59	79.4	ng	1847580	1	6.82	465558	20.0
n-Hexadecanoic acid	11.86	4.8	ng	185707	4	11.33	776375	20.0
Octadecanoic acid	12.64	5.8	ng	226673	4	11.33	776375	20.0
17-Pentatriacontene	13.82	11.2	ng	409118	5	13.97	730323	20.0
Heneicosane	14.43	5.0	ng	180689	5	13.97	730323	20.0
Hexadecane	14.73	2.6	ng	104434	6	15.42	810536	20.0
2-methyloctacosane	15.06	4.1	ng	165668	6	15.42	810536	20.0
Heptadecane	15.86	4.7	ng	190829	6	15.42	810536	20.0
10-Methylnonadecane	16.34	2.3	ng	91014	6	15.42	810536	20.0