LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
Data File : BF114494.D
Acq On : 22 May 2019 20:21
Operator : JU/SJ
Sample : K2962-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-3

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-BF051019.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	5.463	570	574	593	rBV	2887788	3261615	93.52%	9.346%
2	6.475	742	746	764	rBV	3233591	3487477	100.00%	9.993%
3	6.604	764	768	782	rVB	3759606	3361162	96.38%	9.631%
4	6.828	803	806	816	rBV	1217704	1009967	28.96%	2.894%
5	6.987	829	833	847	rBV	2617670	2531198	72.58%	7.253%
6	7.392	898	902	915	rBV	2064498	2131682	61.12%	6.108%
7	8.110	1020	1024	1045	rBV	1277192	1342223	38.49%	3.846%
8	9.186	1203	1207	1219	rBV	3515267	3424582	98.20%	9.813%
9	9.581	1270	1274	1287	rVB	431921	438196	12.56%	1.256%
10	9.863	1318	1322	1335	rBV	1508942	1434570	41.13%	4.111%
11	10.657	1453	1457	1473	rBV	2099043	2216430	63.55%	6.351%
12	11.351	1571	1575	1590	rBV	1539781	1526932	43.78%	4.375%
13	11.874	1661	1664	1676	rBV2	228963	291580	8.36%	0.836%
14	12.933	1840	1844	1847	rBV	3188812	2939088	84.28%	8.422%
15	13.857	1992	2001	2014	rBV4	127676	459284	13.17%	1.316%
16	13.957	2015	2018	2021	rVB	52567	51884	1.49%	0.149%
17	13.998	2021	2025	2032	rBV	1169269	1174500	33.68%	3.365%
18	14.139	2046	2049	2052	rVB2	53932	43963	1.26%	0.126%
19	14.445	2097	2101	2104	rBV	105409	108839	3.12%	0.312%
20	14.745	2148	2152	2156	rBV	154393	151341	4.34%	0.434%
21	14.821	2161	2165	2169	rVV	1009753	1015672	29.12%	2.910%
22	15.074	2204	2208	2213	rVB	196216	225803	6.47%	0.647%
23	15.462	2267	2274	2285	rBV2	899433	1506083	43.19%	4.316%
24	15.874	2339	2344	2350	rBV	213043	321774	9.23%	0.922%
25	16.368	2422	2428	2445	rVB2	151045	346690	9.94%	0.993%
26	16.945	2522	2526	2534	rVB3	47593	95848	2.75%	0.275%

Sum of corrected areas: 34898383

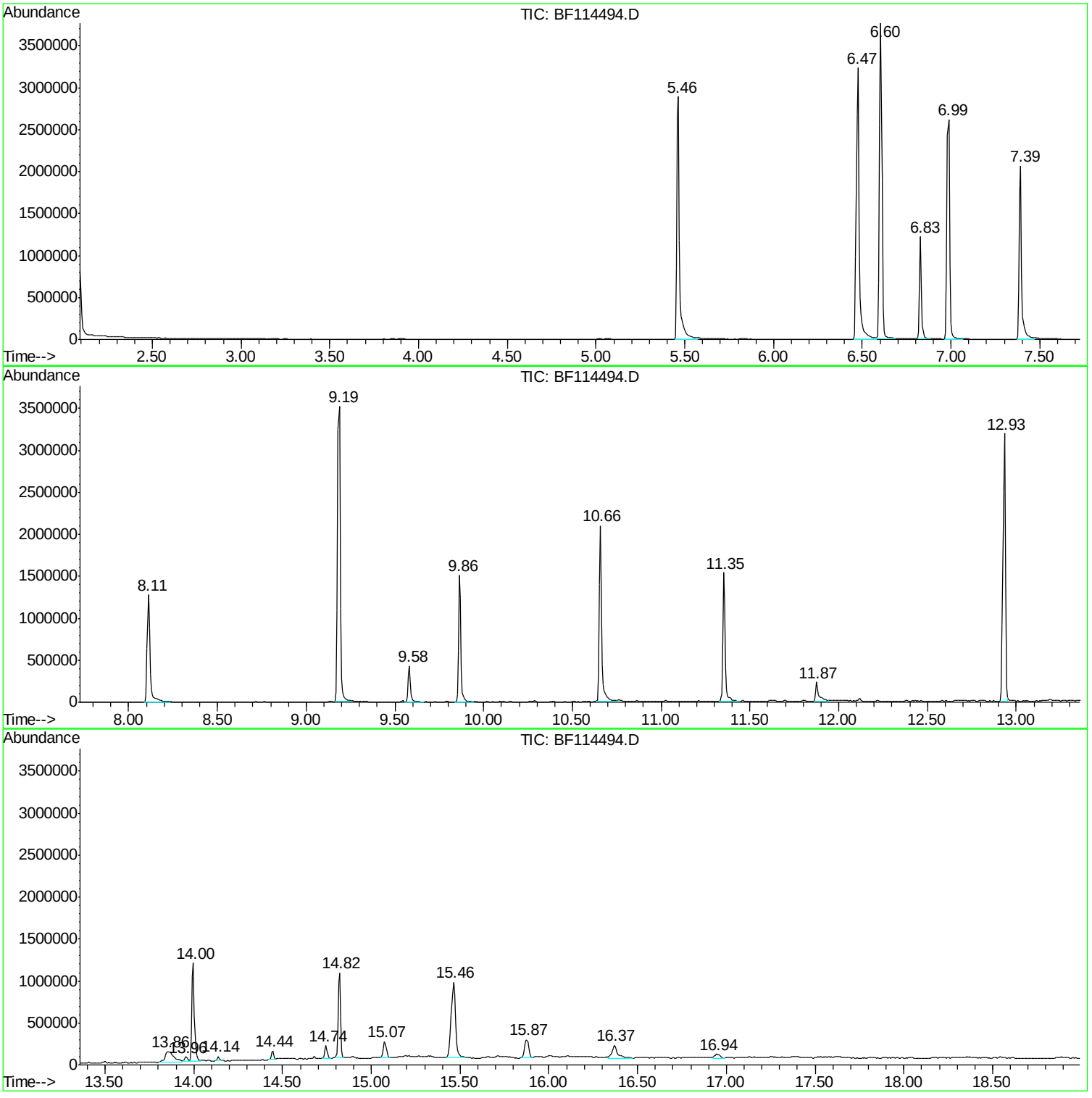
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
Data File : BF114494.D
Acq On : 22 May 2019 20:21
Operator : JU/SJ
Sample : K2962-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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\BF052219\
Data File : BF114494.D
Acq On : 22 May 2019 20:21
Operator : JU/SJ
Sample : K2962-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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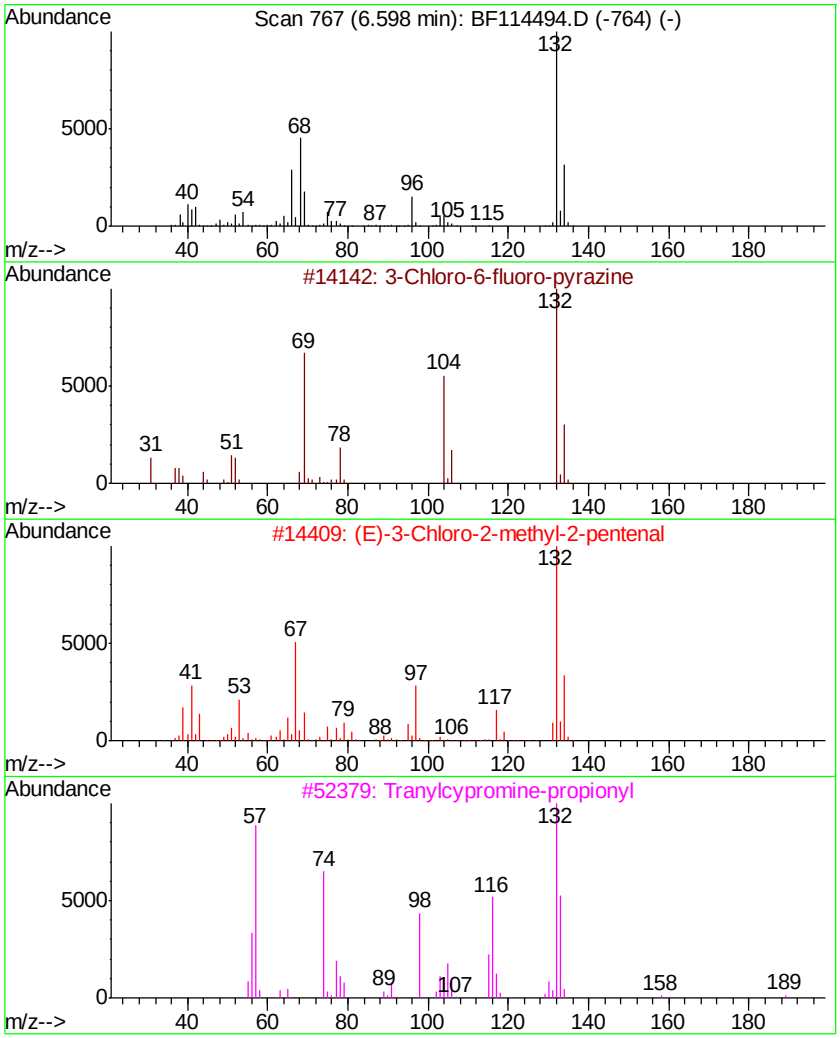
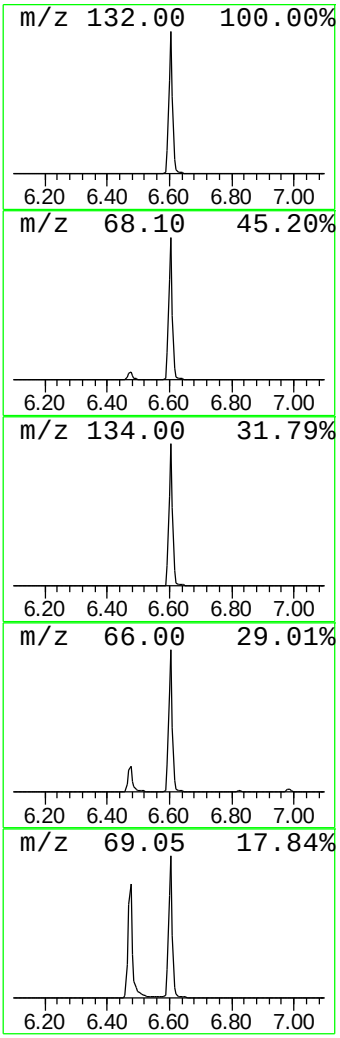
Peak Number 1 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	66.56 ng	3361160	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

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Data File : BF114494.D
Acq On : 22 May 2019 20:21
Operator : JU/SJ
Sample : K2962-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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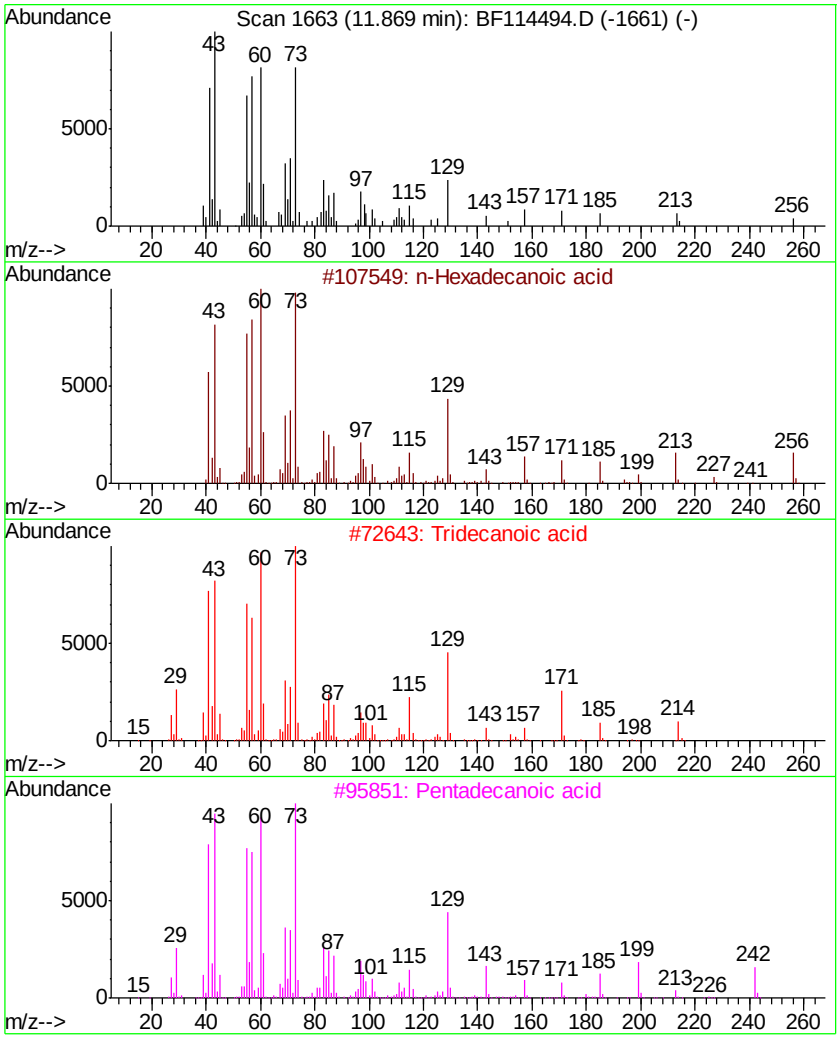
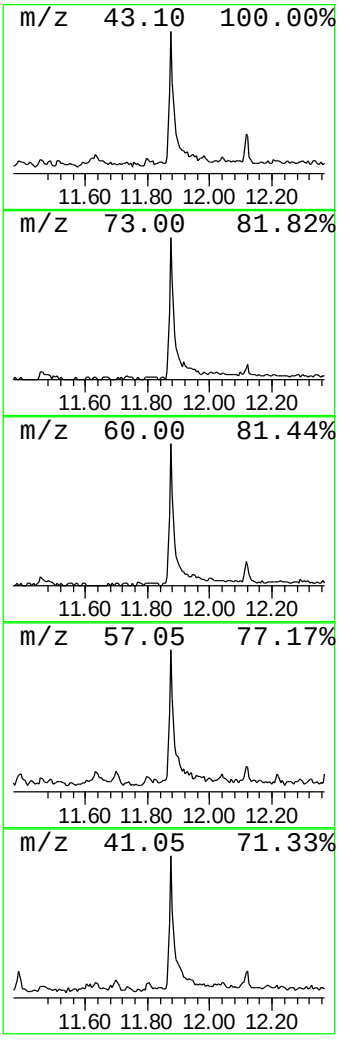
Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.82 ng	291580	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Undecanoic acid	186	C11H22O2	000112-37-8	62
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59





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Data File : BF114494.D
Acq On : 22 May 2019 20:21
Operator : JU/SJ
Sample : K2962-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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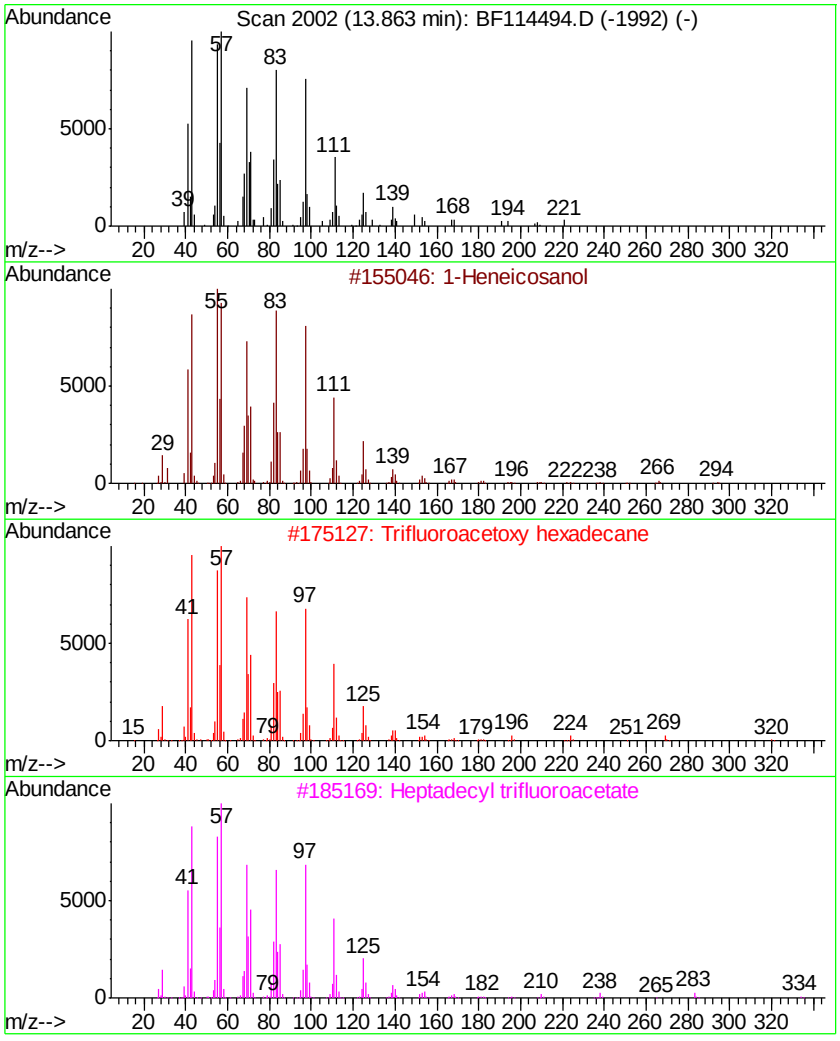
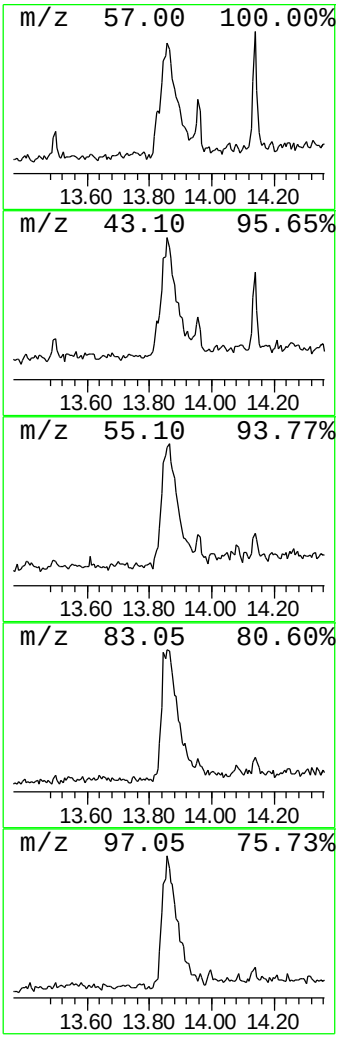
Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	7.82 ng	459284	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	1-Docosene	308	C22H44	001599-67-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
Data File : BF114494.D
Acq On : 22 May 2019 20:21
Operator : JU/SJ
Sample : K2962-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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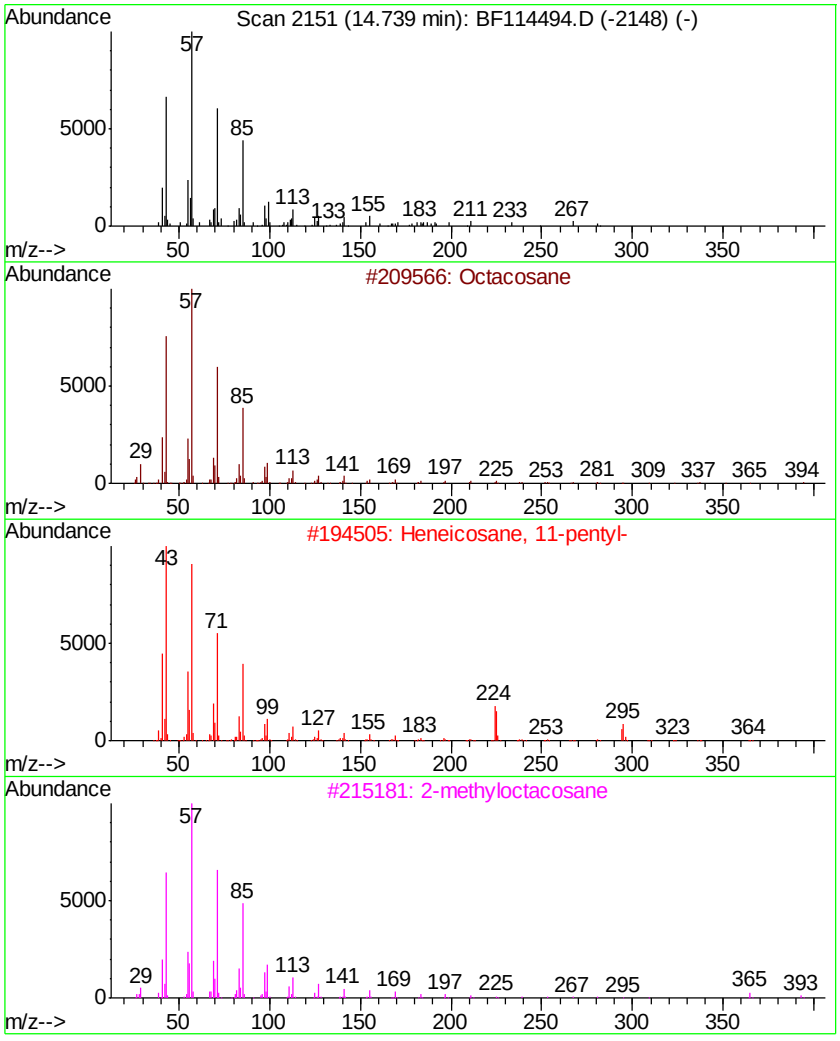
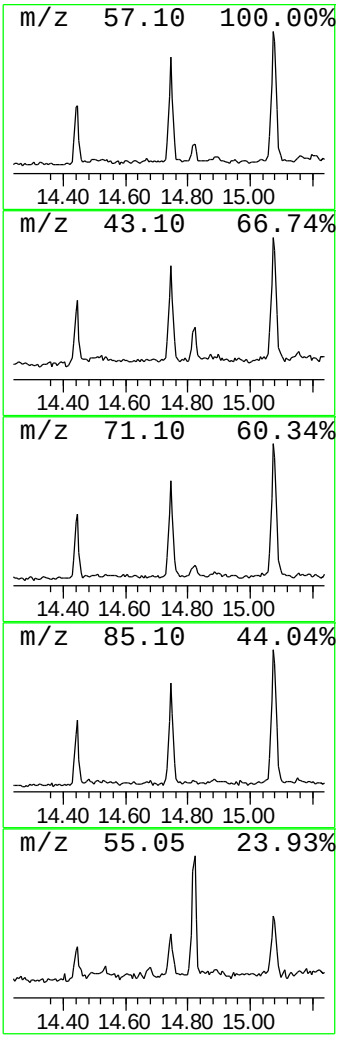
Peak Number 5 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.01 ng	151341	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	86
3	2-methyloctacosane	408	C29H60	1000376-72-8	81
4	Docosane	310	C22H46	000629-97-0	80
5	Tetratetracontane	619	C44H90	007098-22-8	76





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
Data File : BF114494.D
Acq On : 22 May 2019 20:21
Operator : JU/SJ
Sample : K2962-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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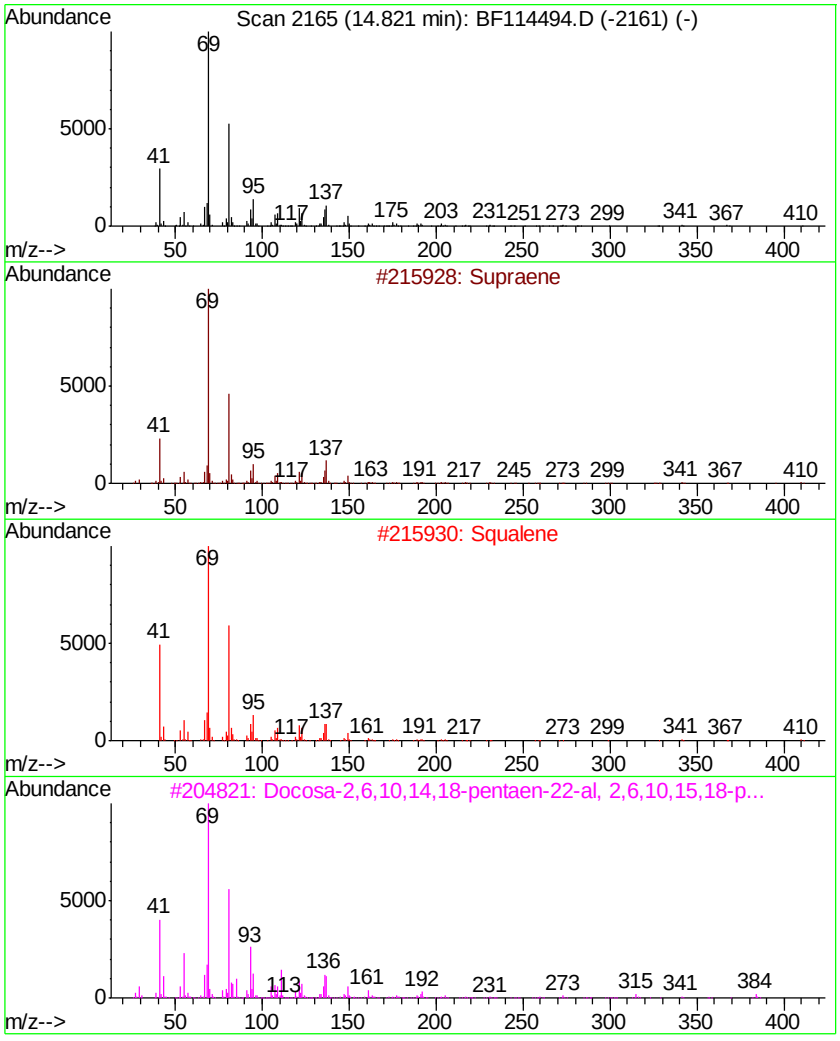
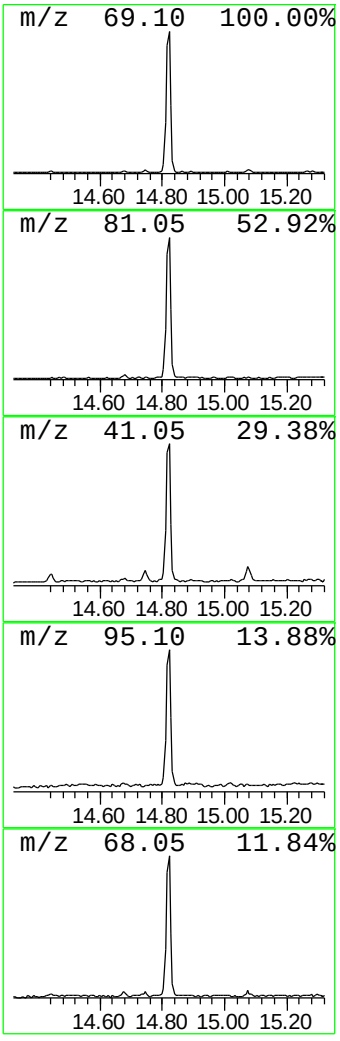
Peak Number 6 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	13.49 ng	1015670	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
Data File : BF114494.D
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Operator : JU/SJ
Sample : K2962-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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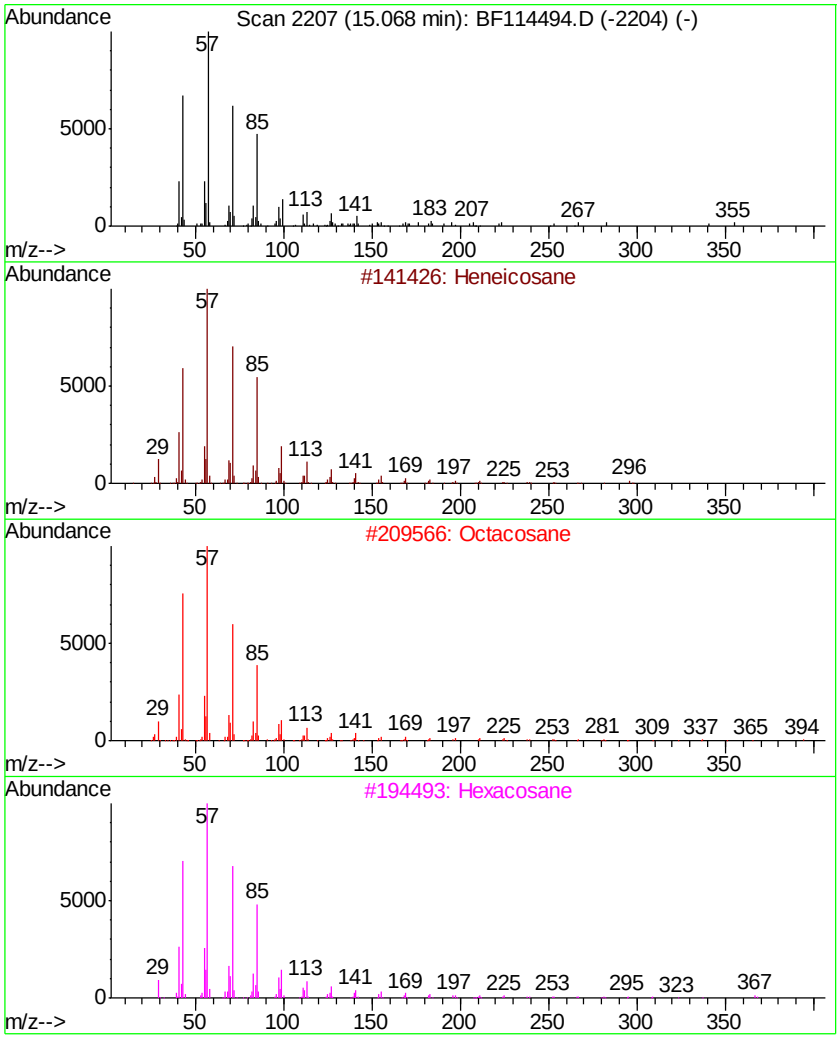
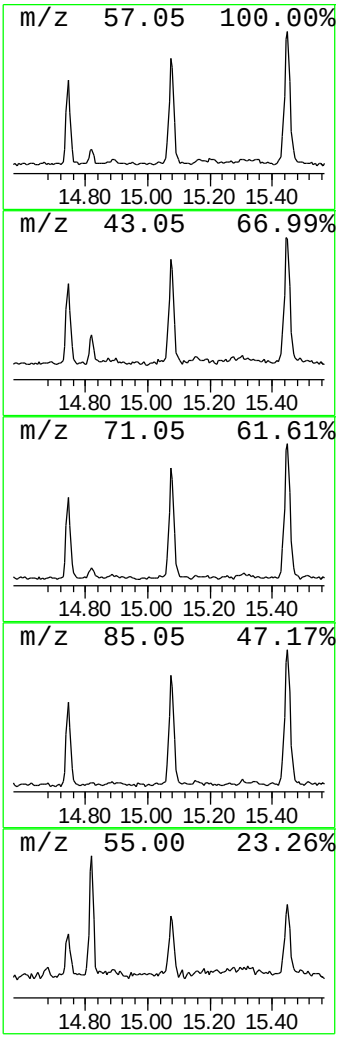
Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	3.00 ng	225803	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91





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Sample : K2962-06
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Instrument : BNA_F
ClientSampleId : DB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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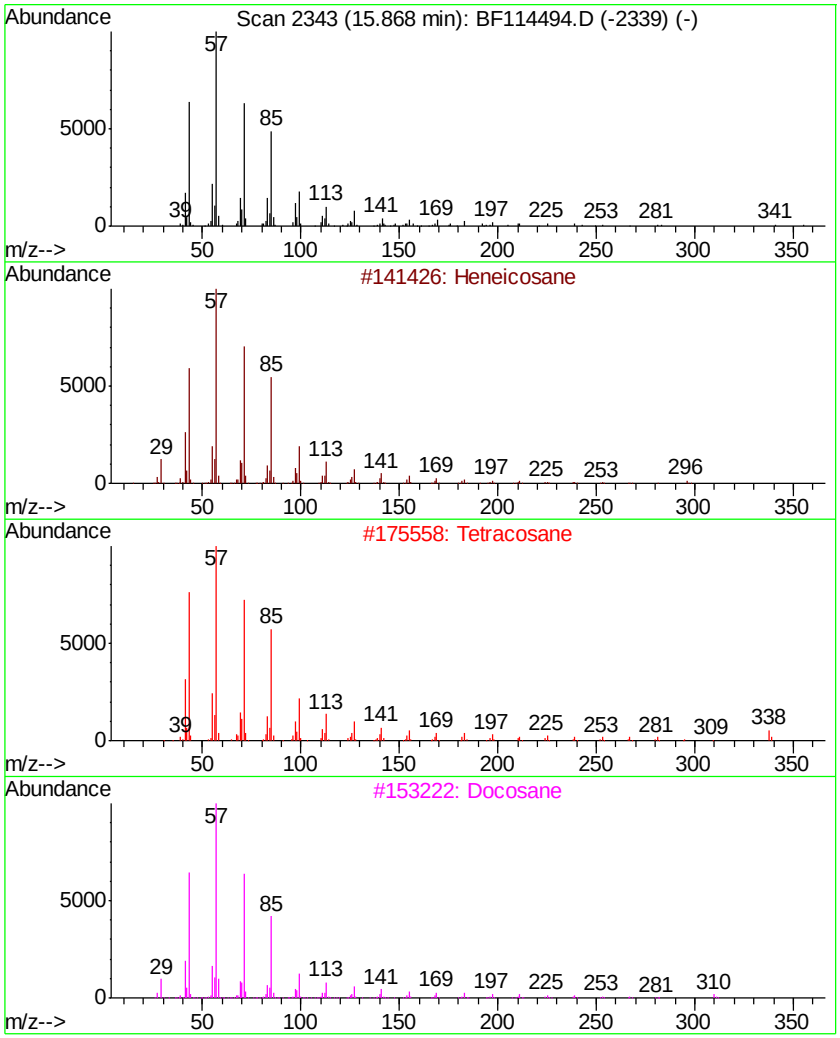
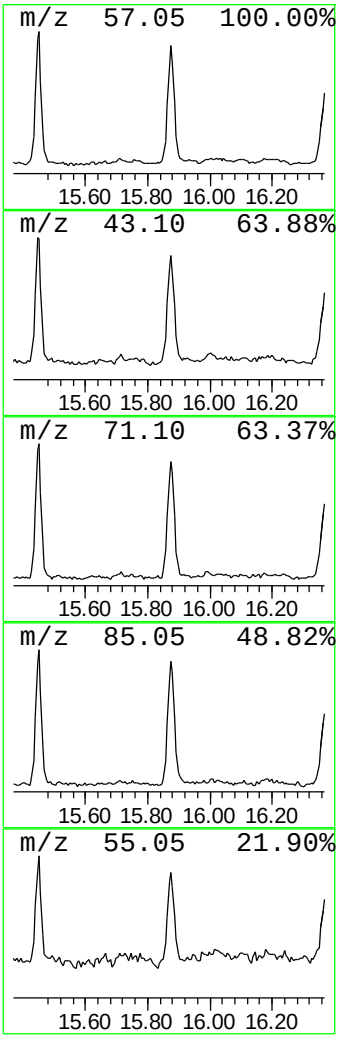
Peak Number 8 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	4.27 ng	321774	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Docosane	310	C22H46	000629-97-0	87
4	Heptadecane	240	C17H36	000629-78-7	87
5	Hentriacontane	437	C31H64	000630-04-6	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052219\
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Misc :
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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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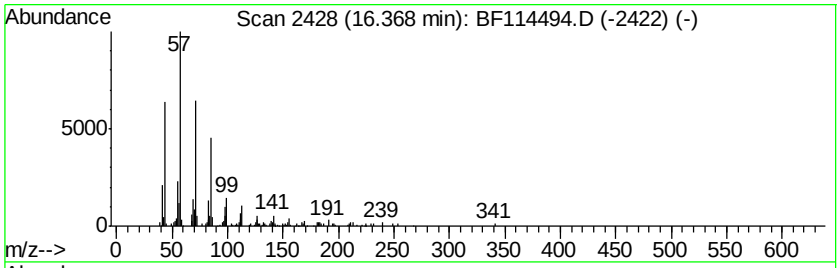
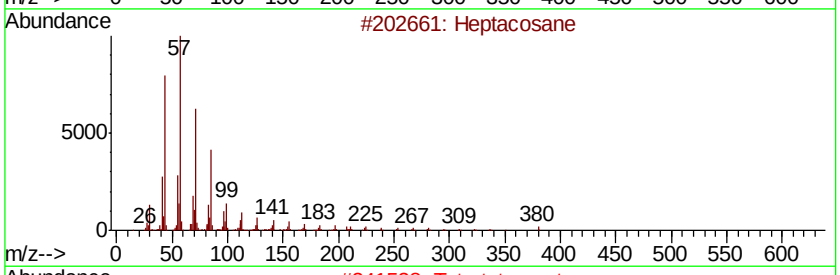
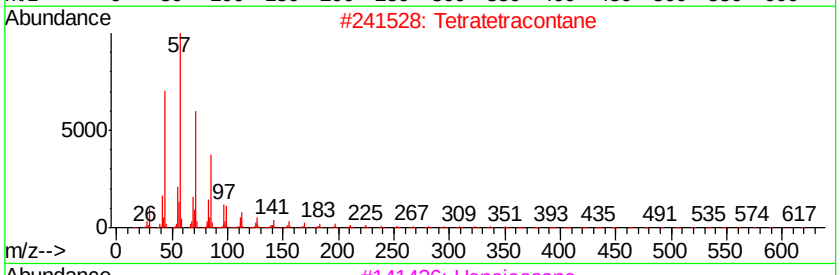
Peak Number 9 Heptacosane Concentration Rank 5

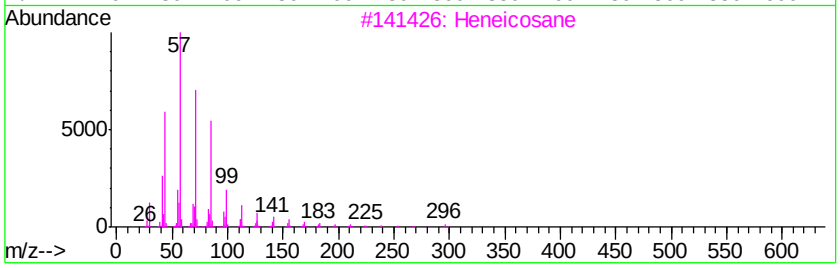
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	4.60 ng	346690	Perylene-d12	15.46

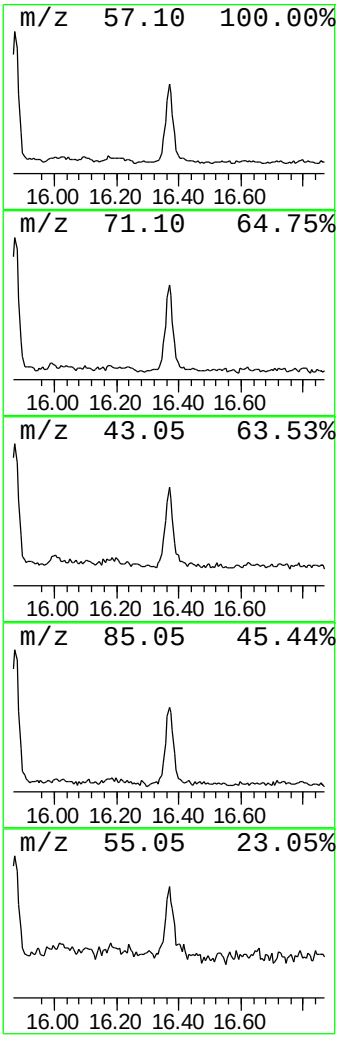
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Octacosane	394	C28H58	000630-02-4	90











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052219\
Data File : BF114494.D
Acq On : 22 May 2019 20:21
Operator : JU/SJ
Sample : K2962-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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
unknown6.60	6.60	66.6	ng	3361160	1	6.83	1009970	20.0
n-Hexadecanoic acid	11.87	3.8	ng	291580	4	11.35	1526930	20.0
1-Heneicosanol	13.86	7.8	ng	459284	5	14.00	1174500	20.0
Octacosane	14.74	2.0	ng	151341	6	15.46	1506080	20.0
Supraene	14.82	13.5	ng	1015670	6	15.46	1506080	20.0
Heneicosane	15.07	3.0	ng	225803	6	15.46	1506080	20.0
Tetracosane	15.87	4.3	ng	321774	6	15.46	1506080	20.0
Heptacosane	16.37	4.6	ng	346690	6	15.46	1506080	20.0