LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117326.D
Acq On : 3 Oct 2019 19:46
Operator : JU
Sample : K5155-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STOCKPILE

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-BF091319.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	5.440	566	570	591	rBV	1184883	1263109	74.45%	9.417%
2	6.451	738	742	760	rBV	1175609	1488194	87.71%	11.095%
3	6.581	760	764	779	rVB	1573023	1500646	88.45%	11.188%
4	6.804	799	802	813	rBV	330069	304972	17.98%	2.274%
5	6.963	825	829	843	rBV	1231449	1119830	66.00%	8.349%
6	7.369	894	898	929	rBV	727333	912611	53.79%	6.804%
7	8.087	1016	1020	1045	rBV	306230	393251	23.18%	2.932%
8	9.163	1198	1203	1217	rBV	1777275	1696643	100.00%	12.649%
9	9.551	1266	1269	1283	rBB	123713	144370	8.51%	1.076%
10	9.681	1287	1291	1305	rBV	252578	441132	26.00%	3.289%
11	9.839	1314	1318	1334	rVB	471905	463842	27.34%	3.458%
12	10.633	1448	1453	1469	rBV	841407	899959	53.04%	6.709%
13	11.328	1567	1571	1579	rBV	343752	386909	22.80%	2.885%
14	11.851	1656	1660	1671	rBV2	68538	90035	5.31%	0.671%
15	12.910	1835	1840	1848	rBV	1219053	1221561	72.00%	9.107%
16	13.127	1872	1877	1883	rBV	11756	17631	1.04%	0.131%
17	13.798	1985	1991	2003	rBV4	87365	188586	11.12%	1.406%
18	13.969	2016	2020	2030	rBV	204932	222989	13.14%	1.662%
19	14.116	2041	2045	2047	rBV	21932	19220	1.13%	0.143%
20	14.416	2091	2096	2099	rBV	33626	35050	2.07%	0.261%
21	14.445	2099	2101	2110	rVB7	9674	20721	1.22%	0.154%
22	14.716	2143	2147	2151	rBV	40863	40438	2.38%	0.301%
23	14.792	2156	2160	2163	rVB	60650	61272	3.61%	0.457%
24	15.045	2199	2203	2207	rVB	47675	52293	3.08%	0.390%
25	15.421	2261	2267	2275	rBV	175382	270013	15.91%	2.013%
26	15.827	2331	2336	2343	rVB2	37637	57552	3.39%	0.429%
27	15.921	2343	2352	2359	rBV2	12984	45144	2.66%	0.337%
28	16.315	2414	2419	2427	rVB3	22873	36636	2.16%	0.273%
29	16.880	2512	2515	2523	rVB7	9666	18675	1.10%	0.139%

Sum of corrected areas: 13413284

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
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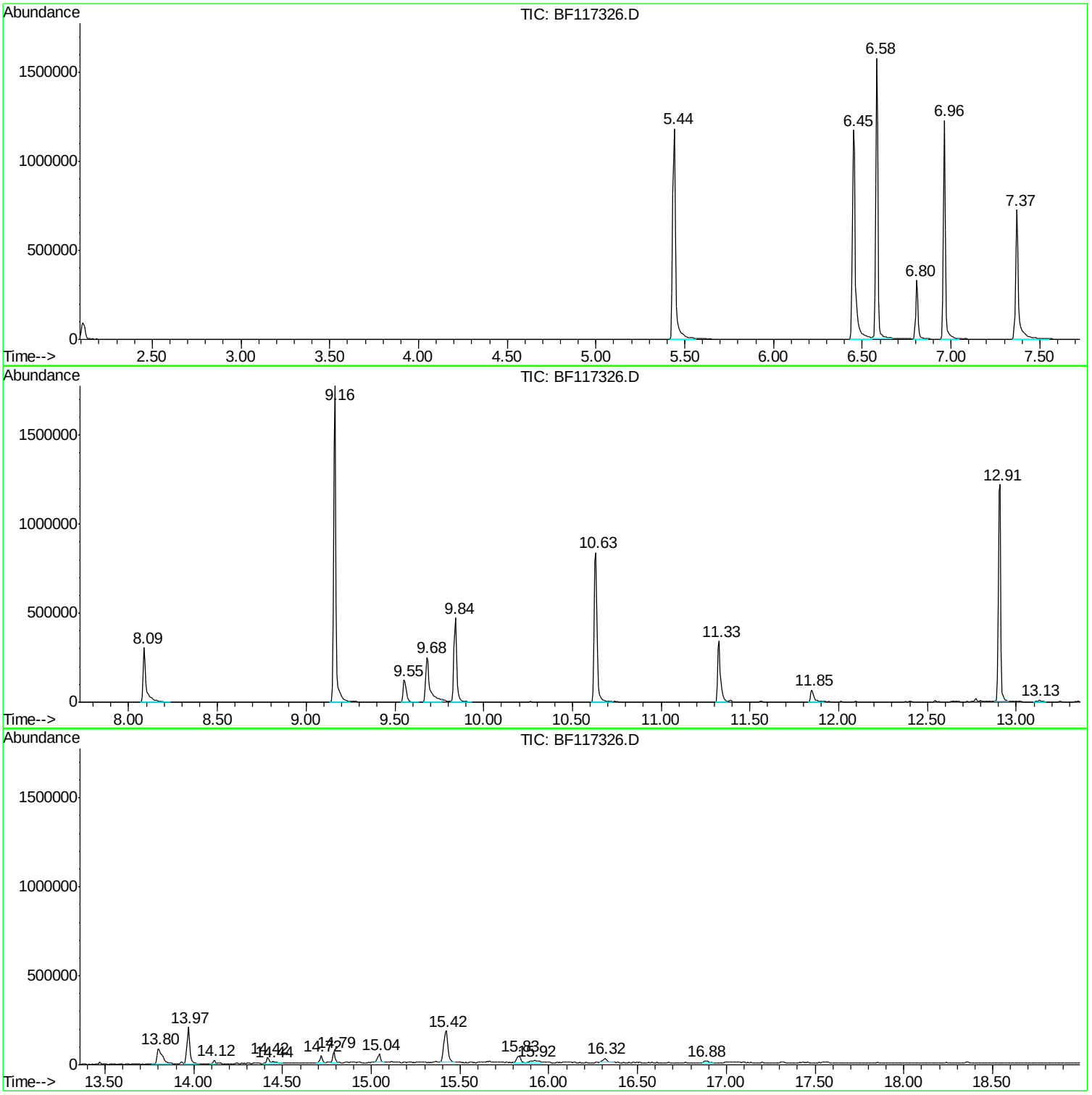
Operator : JU
Sample : K5155-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STOCKPILE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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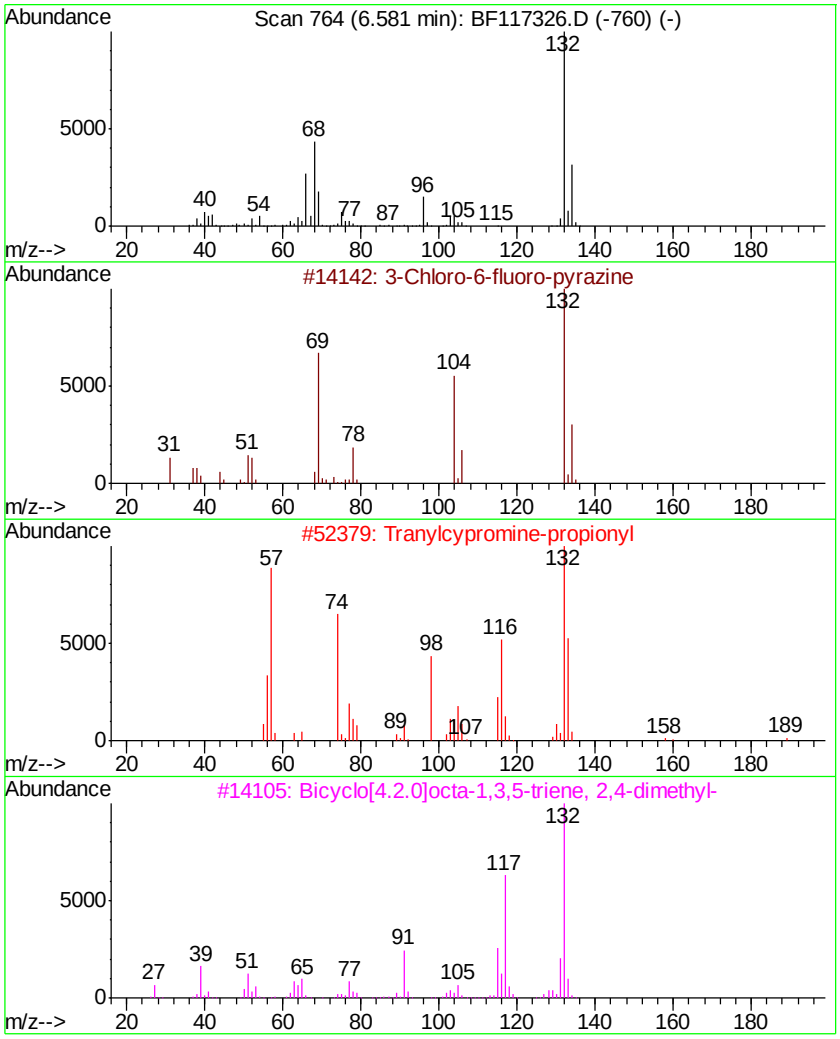
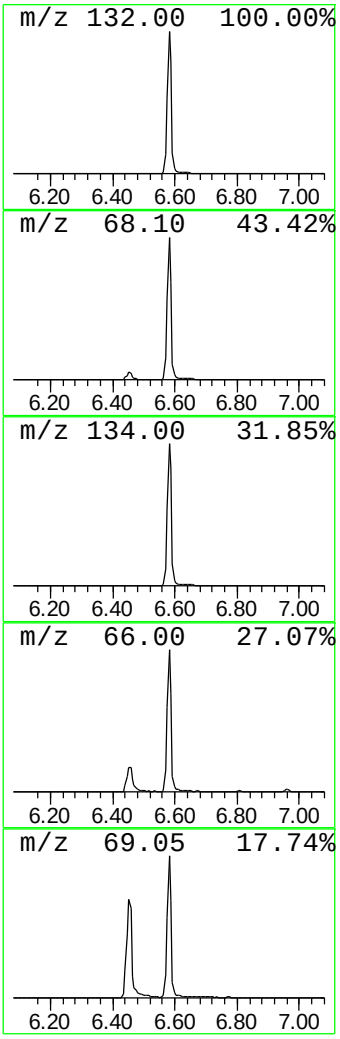
Peak Number 1 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	98.41 ng	1500650	1,4-Dichlorobenzene-d4	6.80

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Sample : K5155-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STOCKPILE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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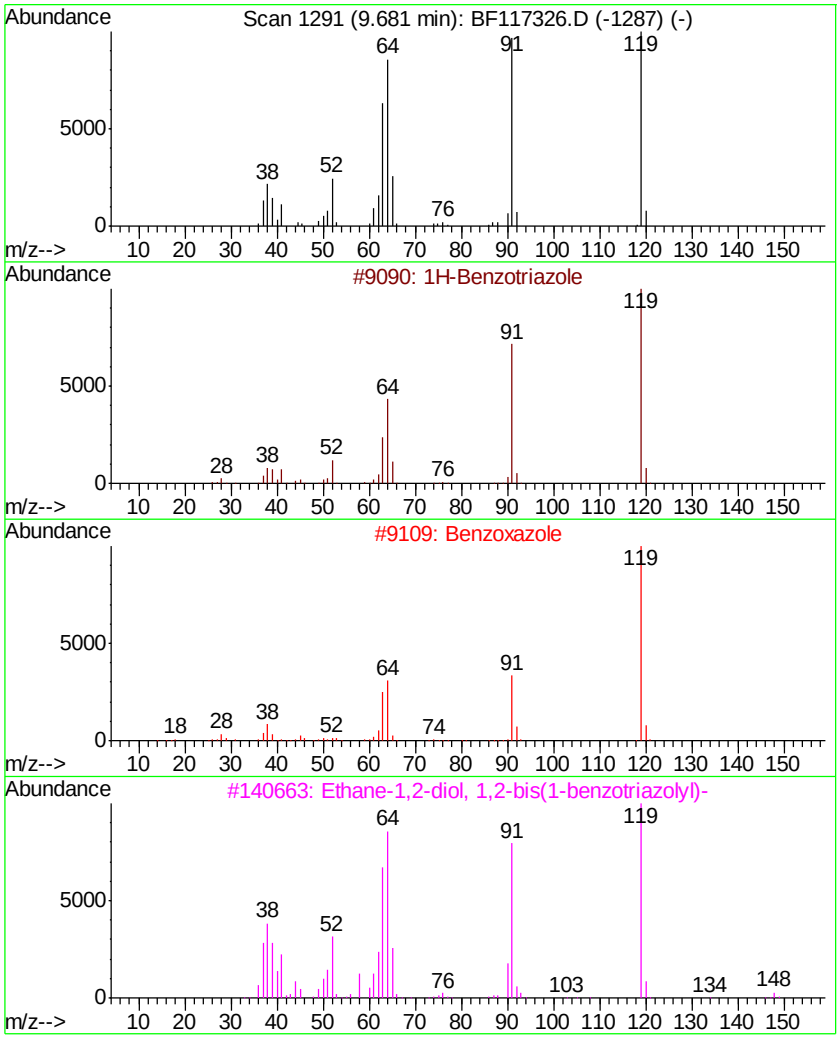
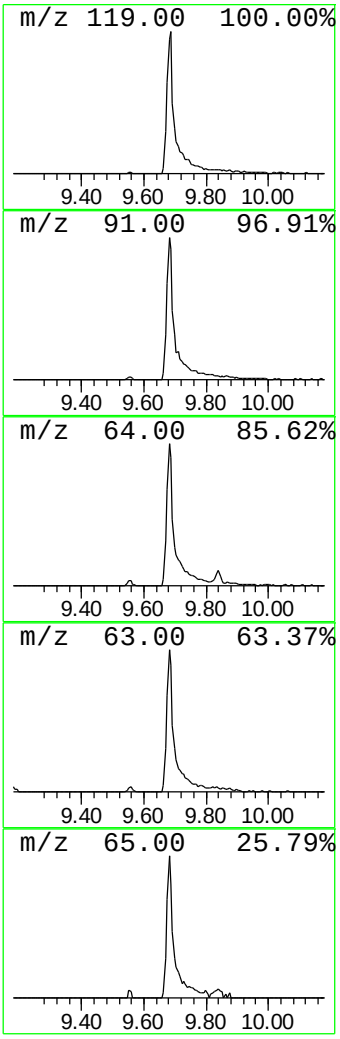
Peak Number 3 1H-Benzotriazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.68	19.02 ng	441132	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole	119	C6H5N3	000095-14-7	97
2	Benzoxazole	119	C7H5NO	000273-53-0	81
3	Ethane-1,2-diol, 1,2-bis(1-benzo...	296	C14H12N6O2	111507-88-1	78
4	2,1-Benzisoxazole	119	C7H5NO	000271-58-9	74
5	Benzonitrile, 2-hydroxy-	119	C7H5NO	000611-20-1	72





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ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STOCKPILE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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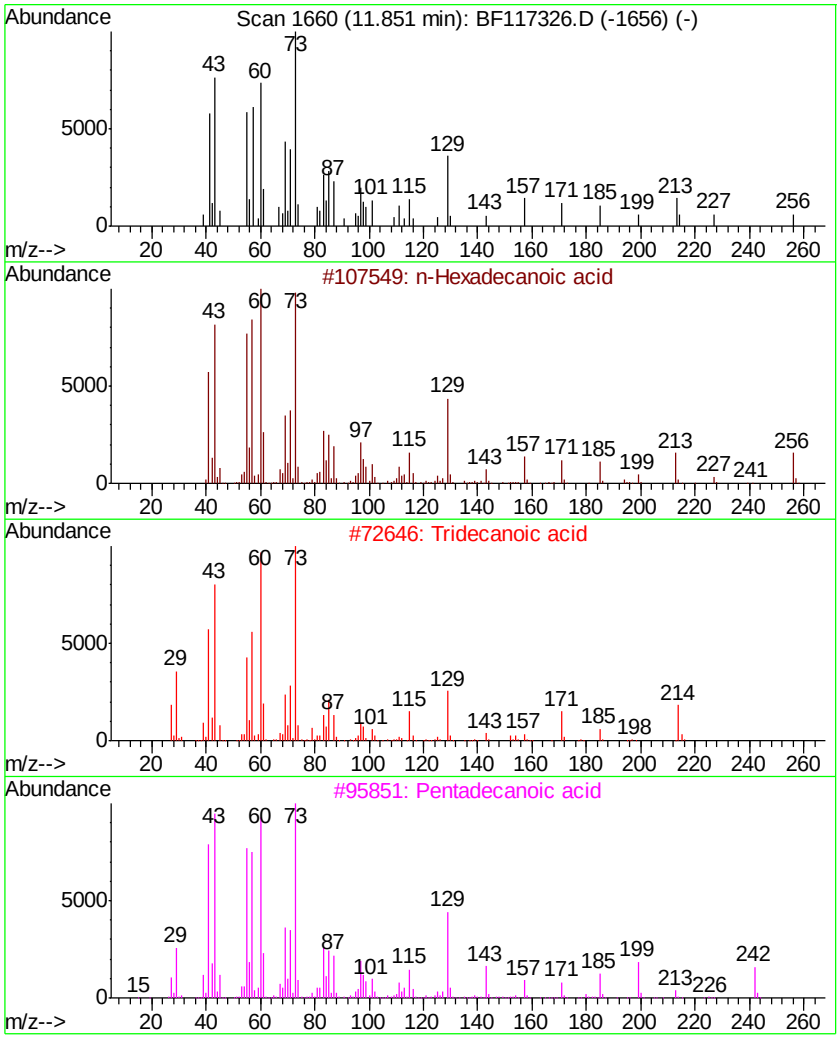
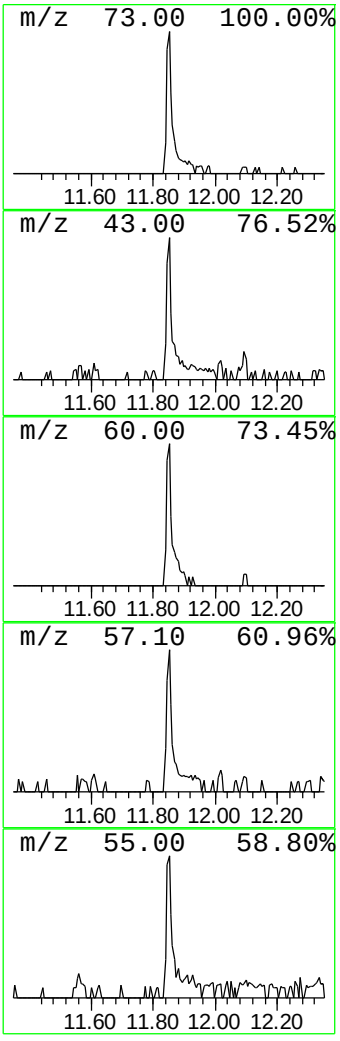
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	4.65 ng	90035	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59





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Sample : K5155-01
Misc :
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Instrument : BNA_F
ClientSampleId : STOCKPILE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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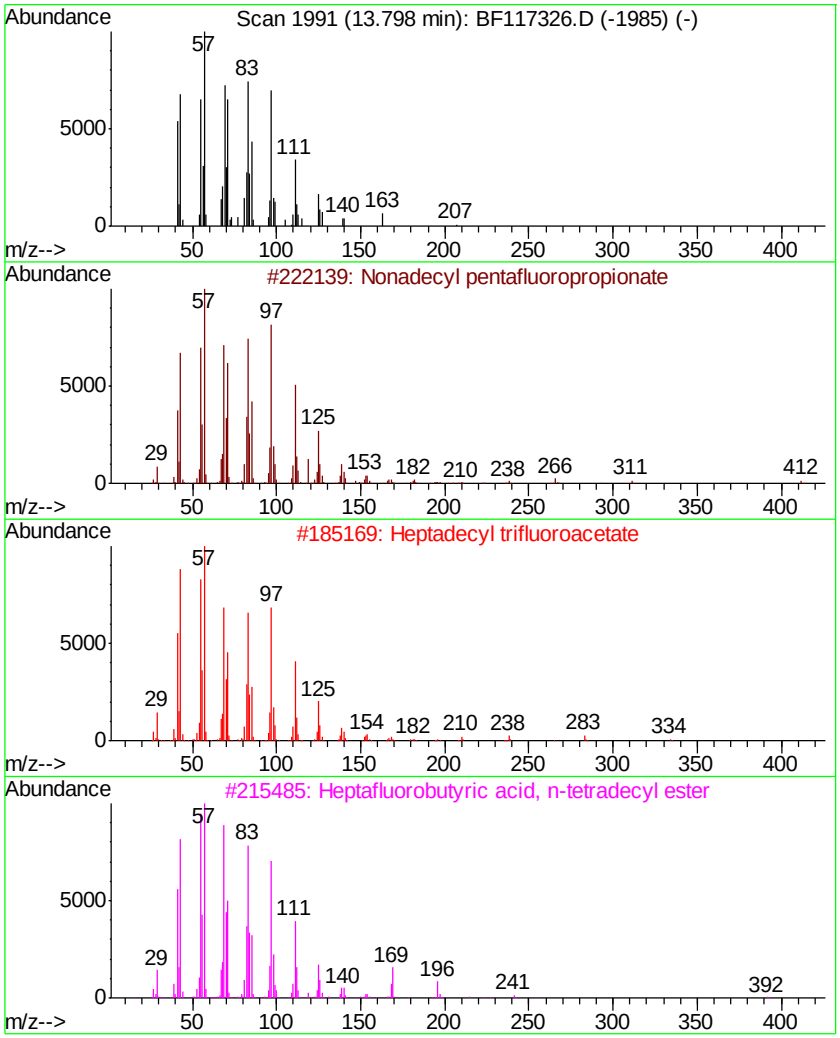
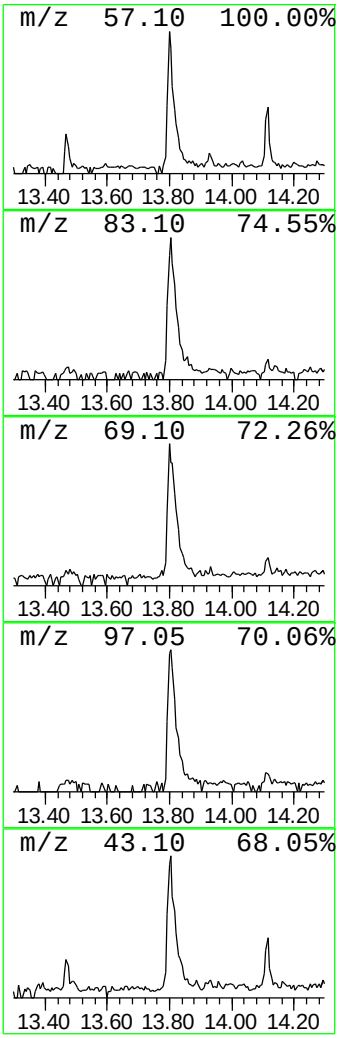
Peak Number 5 Nonadecyl pentafluoropropio... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	16.91 ng	188586	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	81
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	81
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	81





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Sample : K5155-01
Misc :
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Instrument : BNA_F
ClientSampleId : STOCKPILE

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TIC Integration Parameters: LSCINT.P

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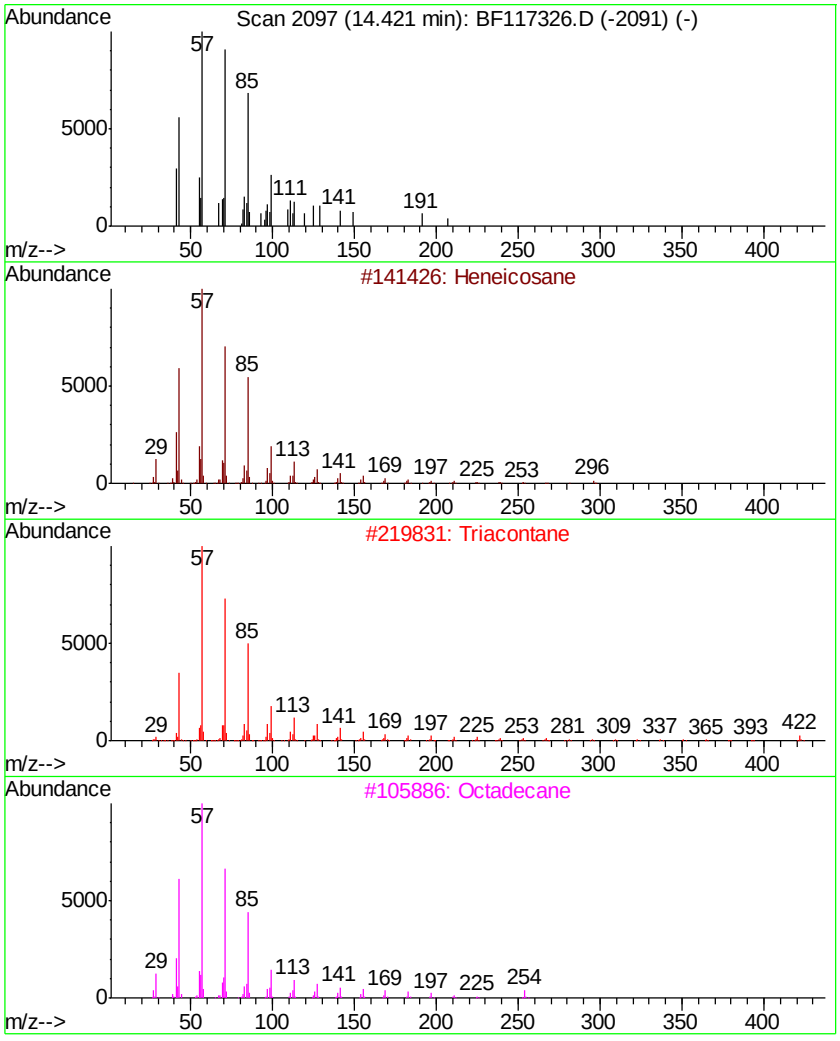
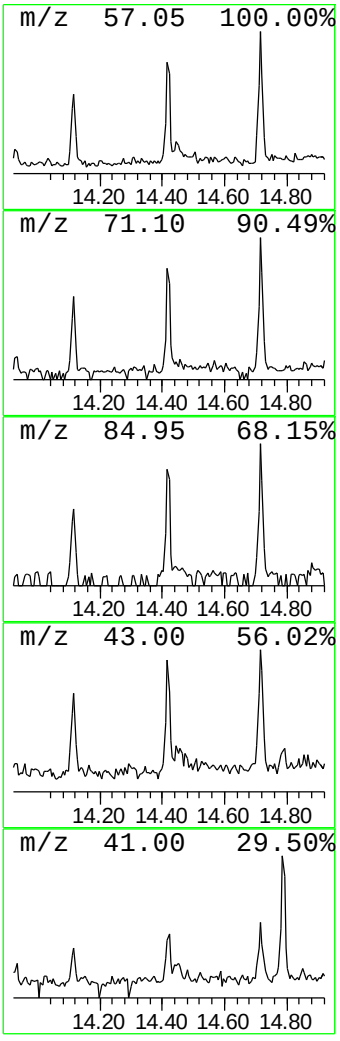
Peak Number 6 Triacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	3.14 ng	35050	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Triacontane	422	C30H62	000638-68-6	80
3	Octadecane	254	C18H38	000593-45-3	80
4	2-methyloctacosane	408	C29H60	1000376-72-8	80
5	Heptadecane	240	C17H36	000629-78-7	80





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
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TIC Library : C:\DATABASE\NIST11.L
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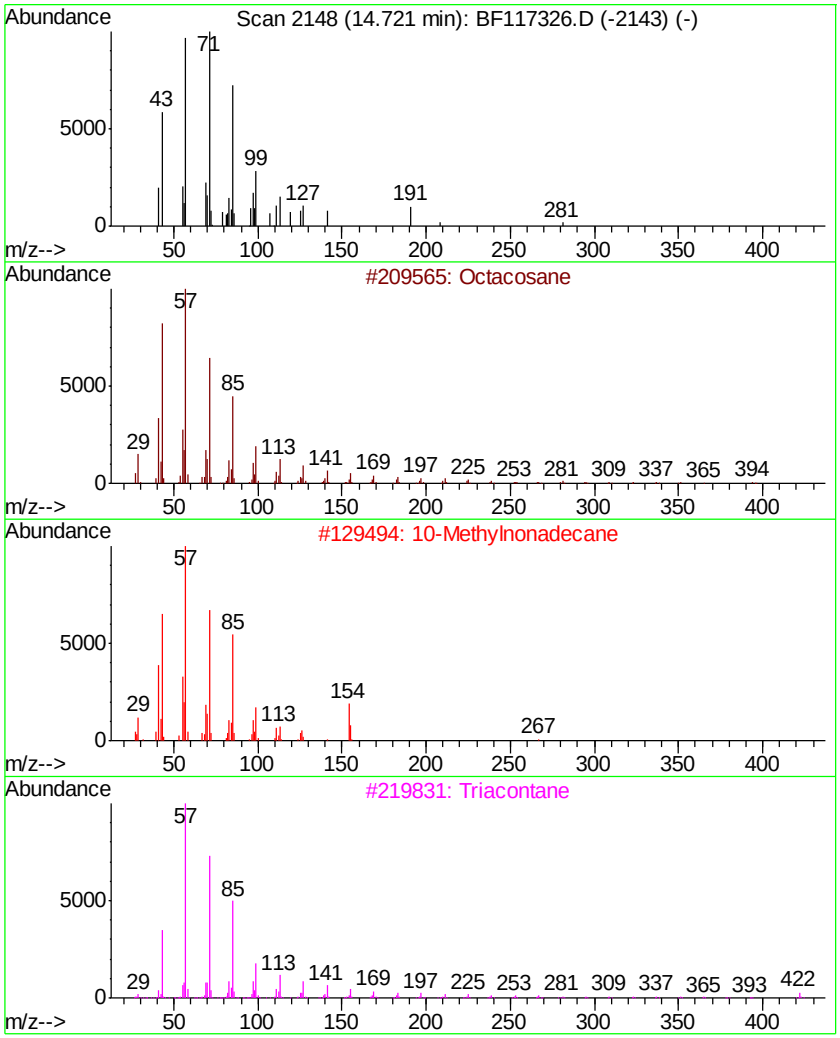
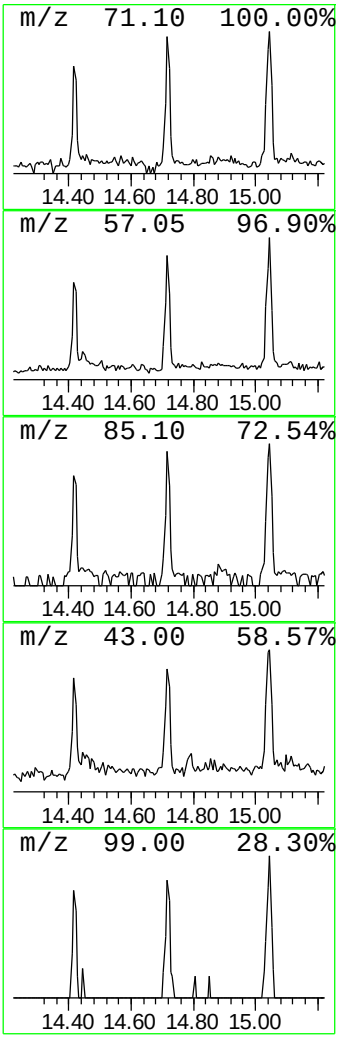
Peak Number 7 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.00 ng	40438	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	86
2	10-Methylnonadecane	282	C20H42	056862-62-5	86
3	Triacontane	422	C30H62	000638-68-6	86
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
5	Heneicosane	296	C21H44	000629-94-7	86





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TIC Library : C:\DATABASE\NIST11.L
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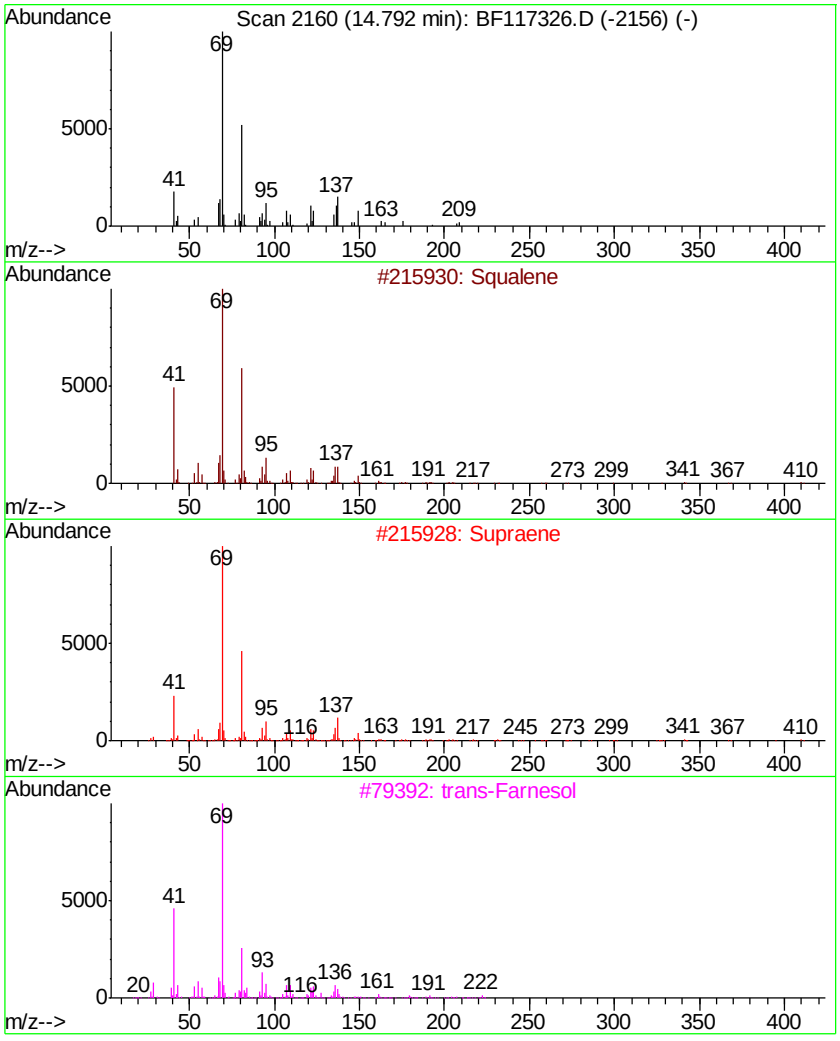
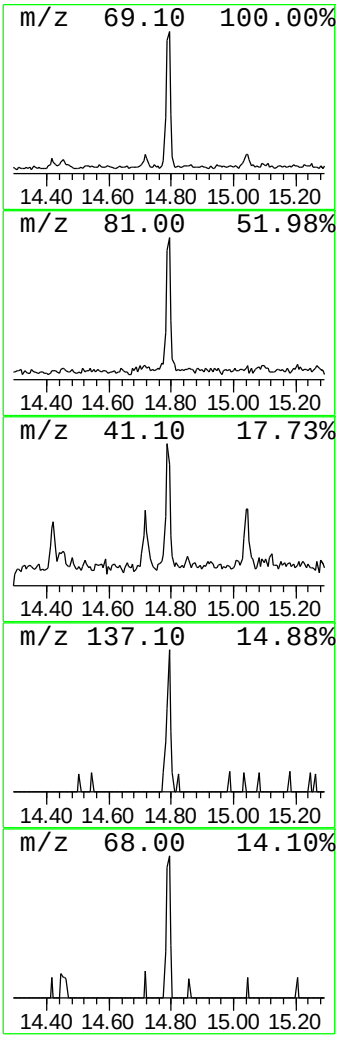
Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	4.54 ng	61272	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	trans-Farnesol	222	C15H26O	000106-28-5	64
4	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	64
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





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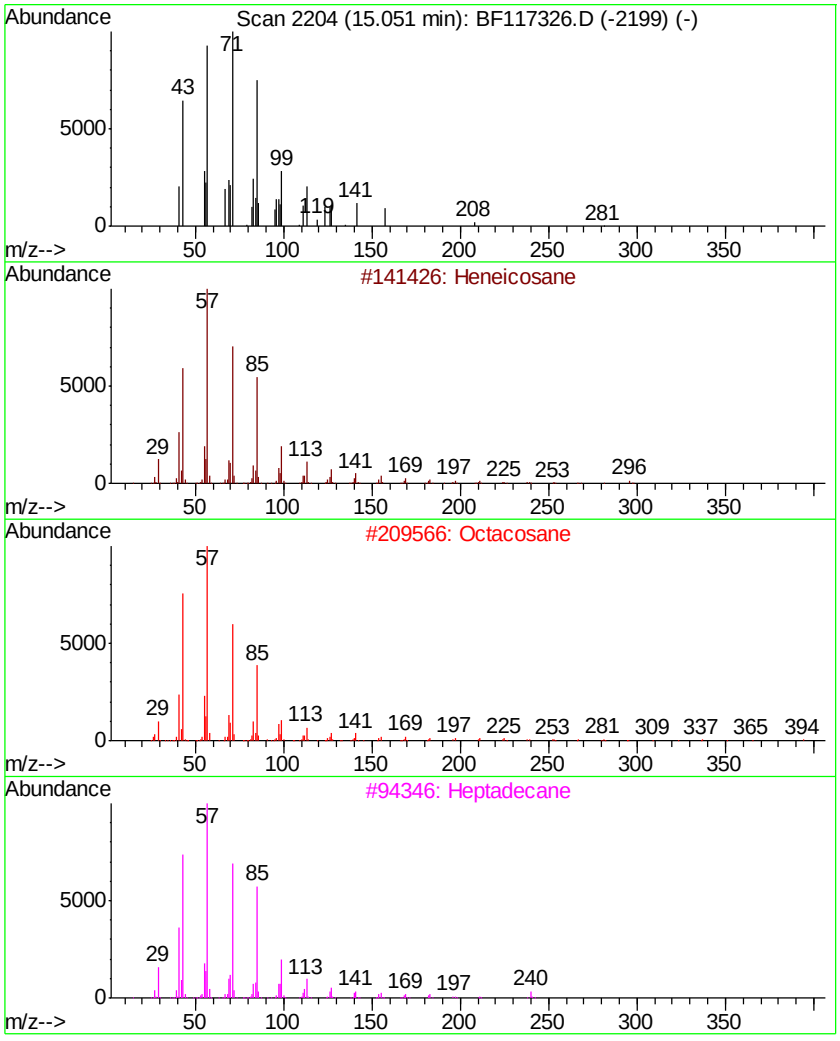
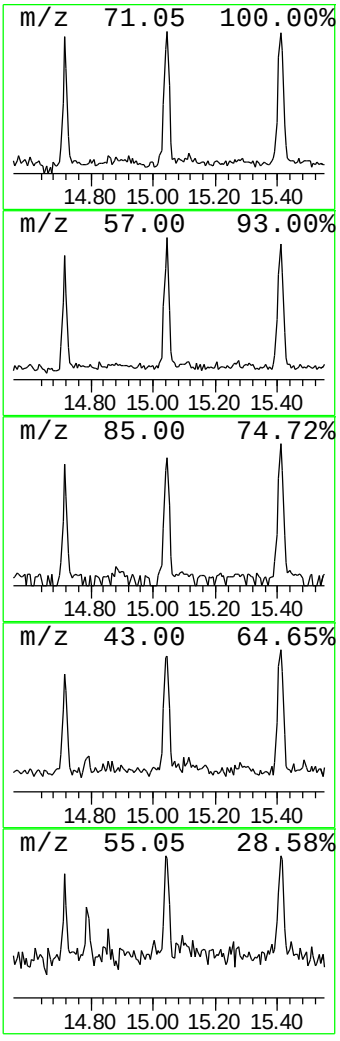
Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	3.87 ng	52293	Perylene-d12	15.42

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	Heptadecane	240	C17H36	000629-78-7	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Pentacosane	352	C25H52	000629-99-2	90





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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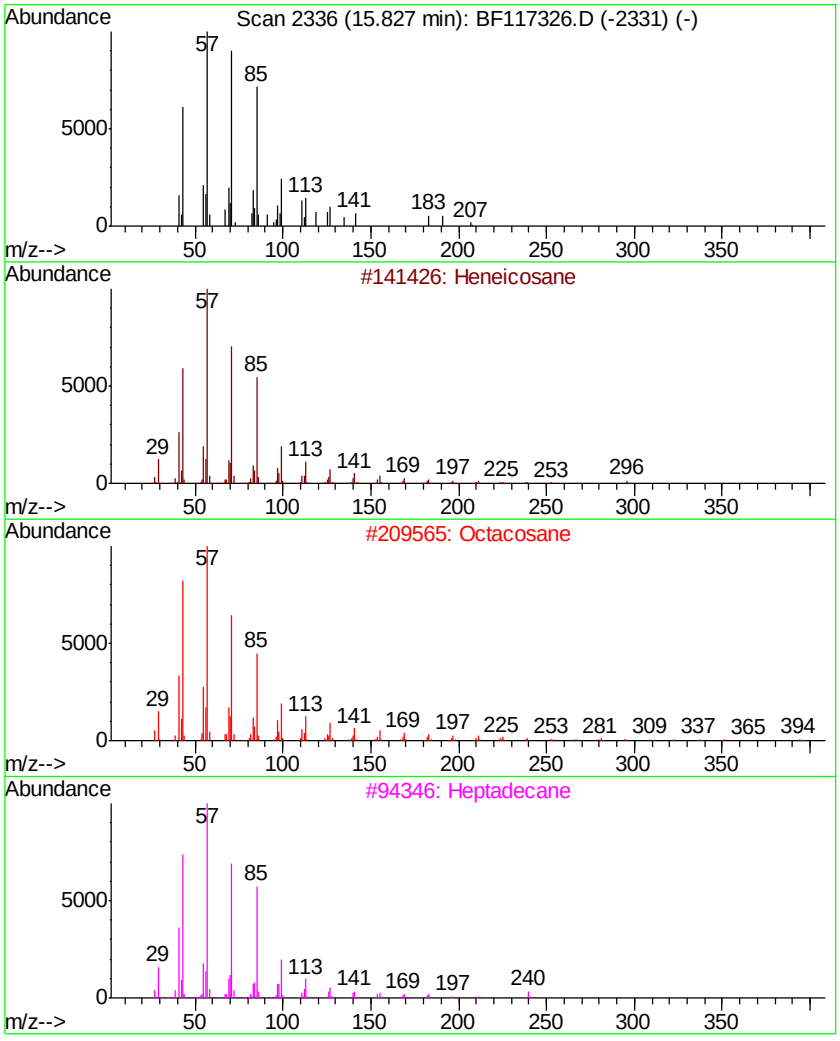
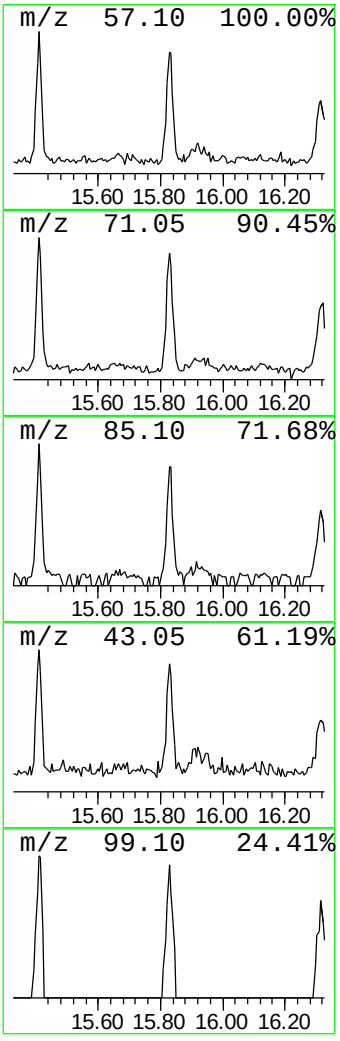
Peak Number 10 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	4.26 ng	57552	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptadecane	240	C17H36	000629-78-7	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86





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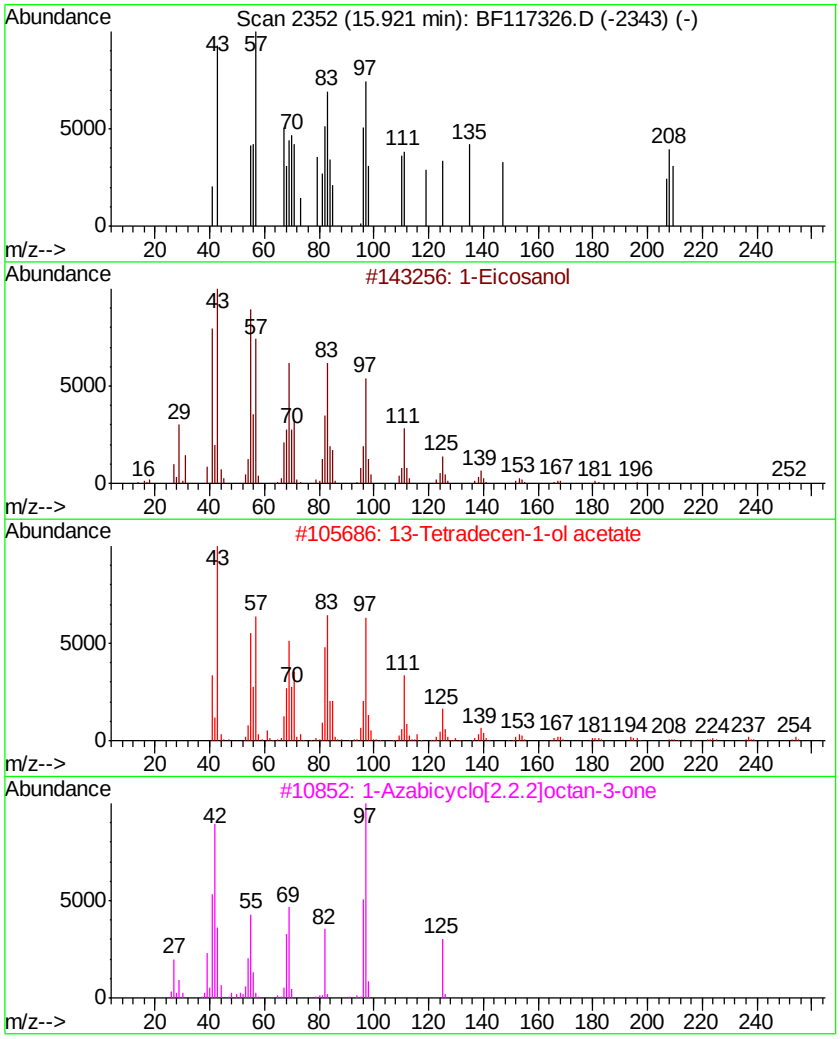
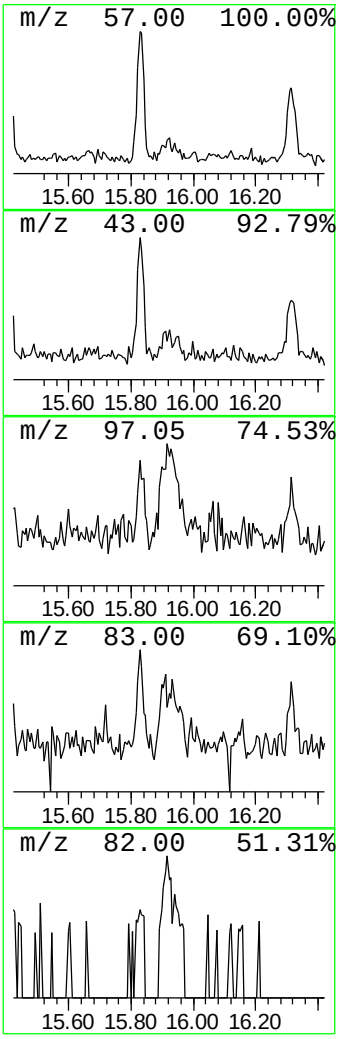
****

Peak Number 11 unknown15.92 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	3.34 ng	45144	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	35
2	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	35
3	1-Azabicyclo[2.2.2]octan-3-one	125	C7H11NO	003731-38-2	30
4	1-Octadecene	252	C18H36	000112-88-9	30
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117326.D
Acq On : 3 Oct 2019 19:46
Operator : JU
Sample : K5155-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STOCKPILE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

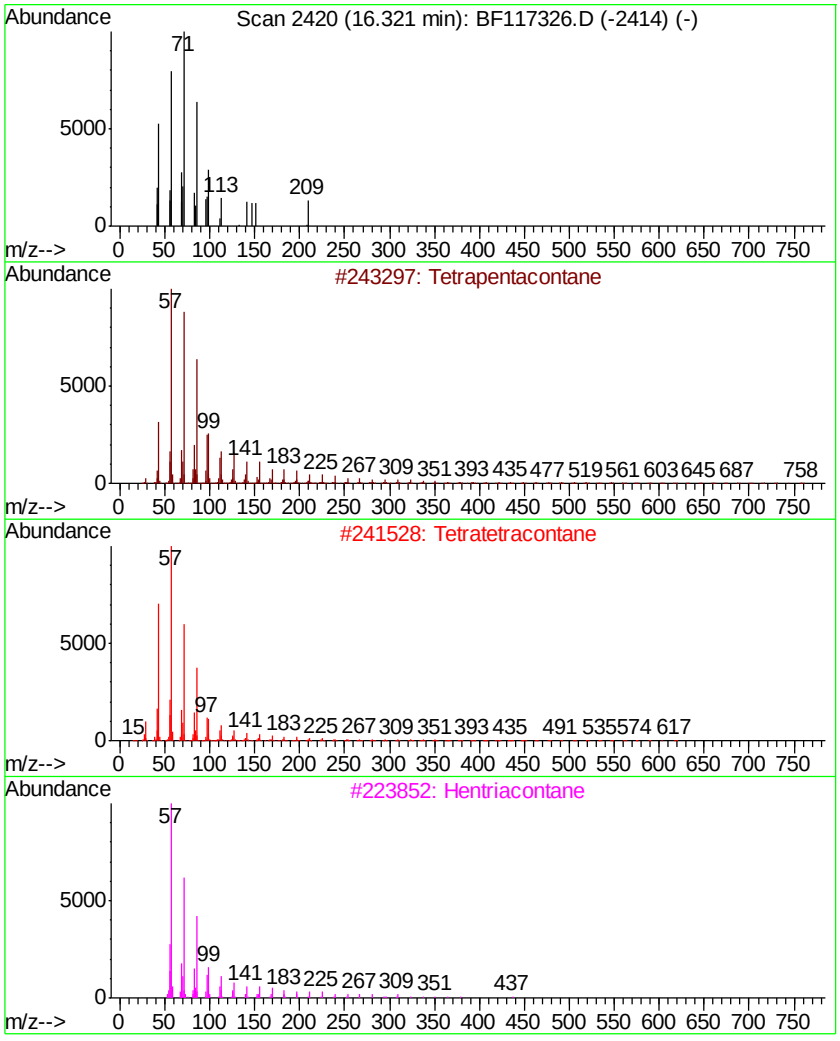
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

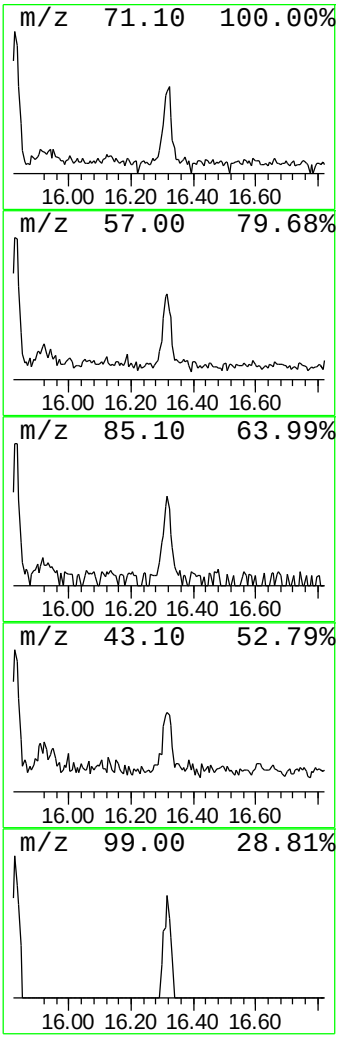
****

Peak Number 12 Tetrapentacontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	2.71 ng	36636	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrapentacontane	759	C54H110	005856-66-6	64
2	Tetratetracontane	619	C44H90	007098-22-8	59
3	Hentriacontane	437	C31H64	000630-04-6	59
4	2-methyltetracosane	352	C25H52	1000376-72-6	59
5	Hexatriacontane	507	C36H74	000630-06-8	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100319\
Data File : BF117326.D
Acq On : 3 Oct 2019 19:46
Operator : JU
Sample : K5155-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STOCKPILE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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
unknown6.58	6.58	98.4	ng	1500650	1	6.80	304972	20.0
1H-Benzotriazole	9.68	19.0	ng	441132	3	9.84	463842	20.0
n-Hexadecanoic acid	11.85	4.7	ng	90035	4	11.33	386909	20.0
Nonadecyl pentafl...	13.80	16.9	ng	188586	5	13.97	222989	20.0
Triacontane	14.42	3.1	ng	35050	5	13.97	222989	20.0
Octacosane	14.72	3.0	ng	40438	6	15.42	270013	20.0
Squalene	14.79	4.5	ng	61272	6	15.42	270013	20.0
Heneicosane	15.05	3.9	ng	52293	6	15.42	270013	20.0
Heptadecane	15.83	4.3	ng	57552	6	15.42	270013	20.0
unknown15.92	15.92	3.3	ng	45144	6	15.42	270013	20.0
Tetrapentacontane	16.32	2.7	ng	36636	6	15.42	270013	20.0