LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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	3.710	268	276	293	rBV	920558	1456552	100.00%	16.063%
2	4.934	481	484	494	rBV	9531	16150	1.11%	0.178%
3	5.357	552	556	585	rBV	562337	793405	54.47%	8.750%
4	6.387	727	731	747	rBV	649728	886961	60.89%	9.782%
5	6.504	747	751	768	rVB	951173	918220	63.04%	10.126%
6	6.728	786	789	800	rBV	224850	217261	14.92%	2.396%
7	6.881	812	815	833	rBV	709141	621266	42.65%	6.852%
8	7.292	882	885	909	rBV	423991	521196	35.78%	5.748%
9	8.010	1003	1007	1026	rBV	222274	276295	18.97%	3.047%
10	9.081	1185	1189	1208	rBV	854185	816293	56.04%	9.002%
11	9.481	1254	1257	1269	rBB	41118	49513	3.40%	0.546%
12	9.757	1301	1304	1317	rBV	299712	313636	21.53%	3.459%
13	10.557	1436	1440	1454	rBV	404141	464760	31.91%	5.126%
14	11.251	1554	1558	1567	rBV	232835	271170	18.62%	2.991%
15	11.774	1644	1647	1656	rBV	20550	26507	1.82%	0.292%
16	12.827	1822	1826	1833	rBV	691247	598189	41.07%	6.597%
17	13.739	1975	1981	1989	rBV5	19809	47533	3.26%	0.524%
18	13.892	2003	2007	2014	rBV	214999	231318	15.88%	2.551%
19	14.039	2029	2032	2035	rBV2	20908	25372	1.74%	0.280%
20	14.345	2080	2084	2087	rBV2	21019	21094	1.45%	0.233%
21	14.639	2127	2134	2137	rBV2	33448	37948	2.61%	0.419%
22	14.951	2184	2187	2195	rVB	38314	47382	3.25%	0.523%
23	15.333	2244	2252	2262	rVB	155451	255449	17.54%	2.817%
24	15.715	2312	2317	2323	rVB3	27853	40558	2.78%	0.447%
25	16.180	2391	2396	2402	rBV7	18114	33831	2.32%	0.373%
26	16.798	2495	2501	2510	rVB5	39840	79714	5.47%	0.879%

Sum of corrected areas: 9067573

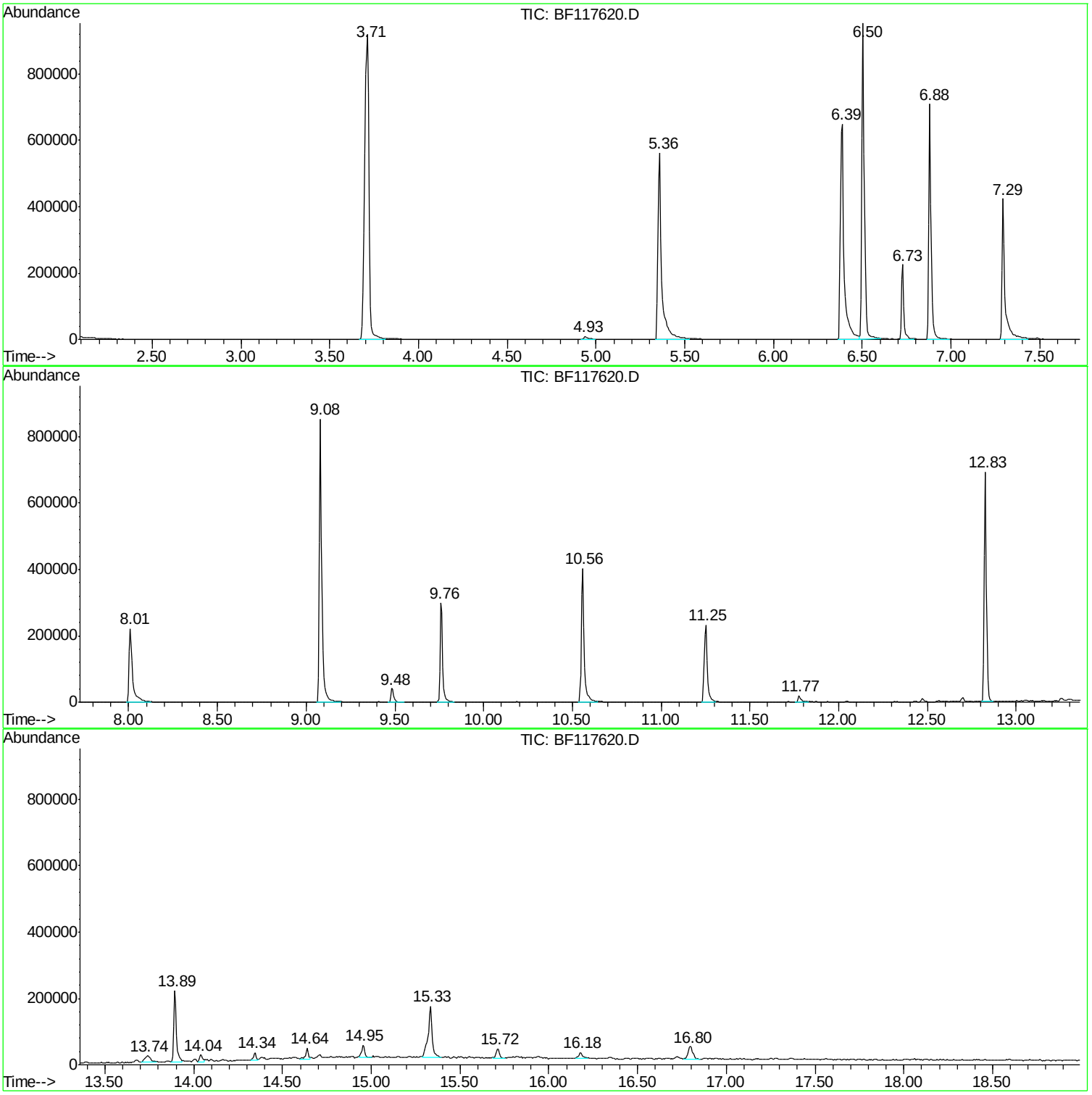
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
165-26-(0-1)

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\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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

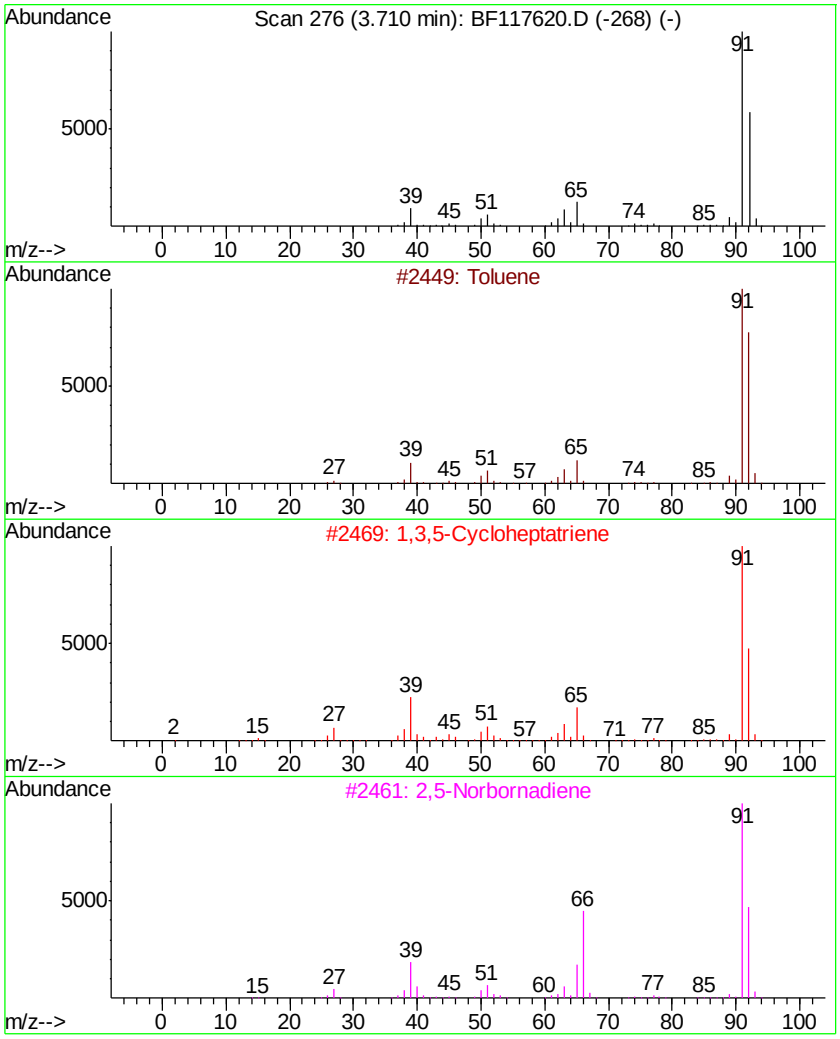
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

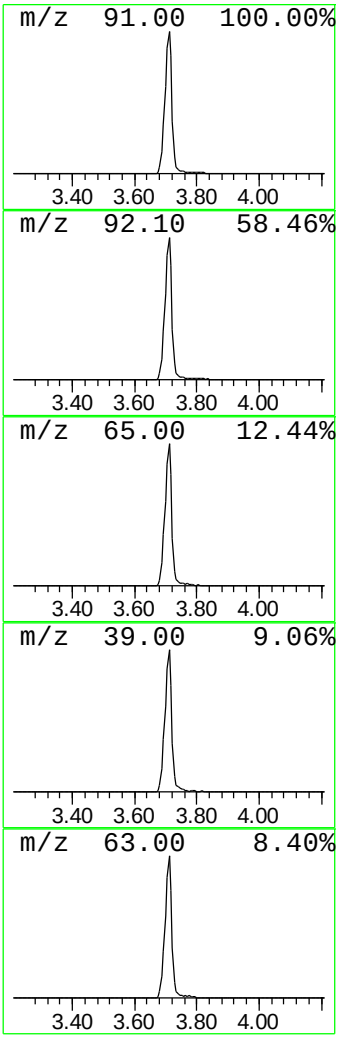
****

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.71	134.08 ng	1456550	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	95
2	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	87
3	2,5-Norbornadiene	92	C7H8	000121-46-0	72
4	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	64
5	Propanedinitrile, ethylidene-	92	C5H4N2	001508-07-2	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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

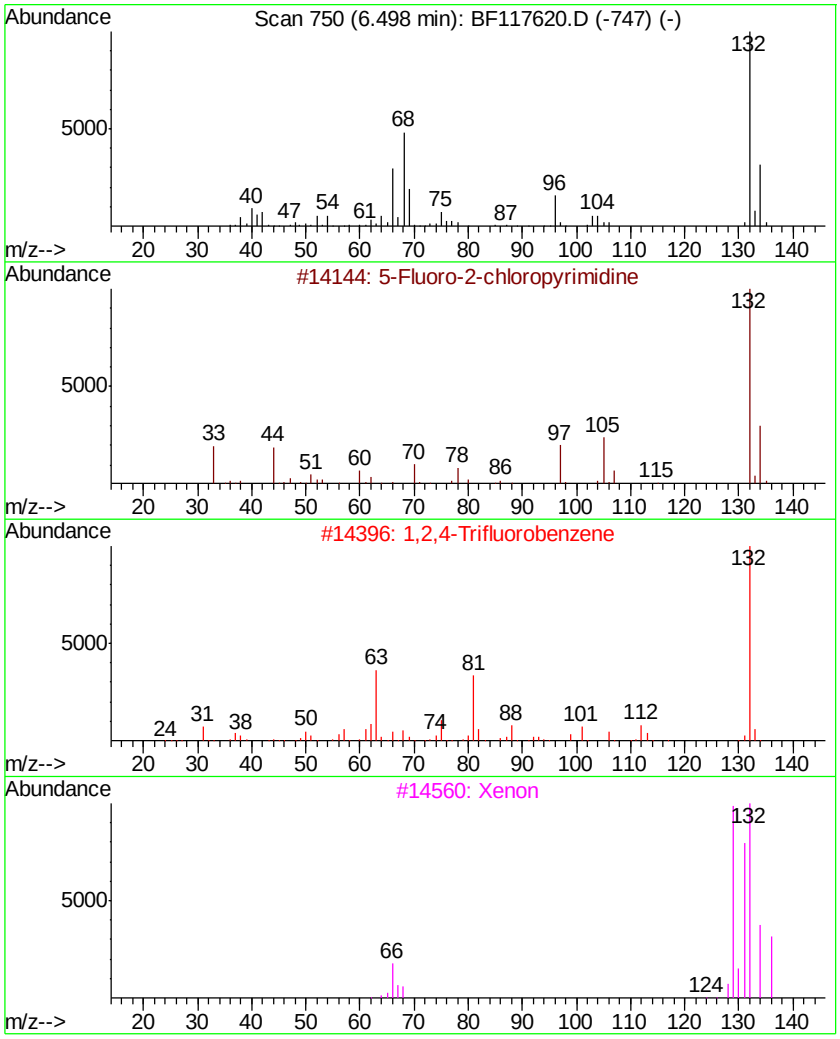
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

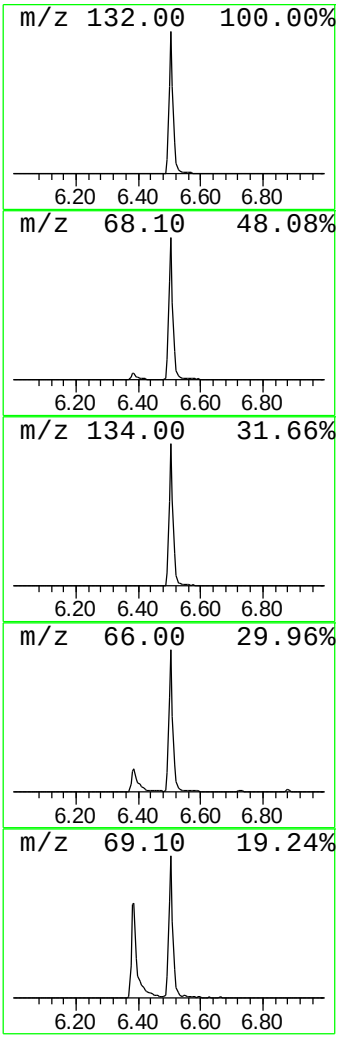
****

Peak Number 2 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	84.53 ng	918220	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
3	Xenon	132	Xe	007440-63-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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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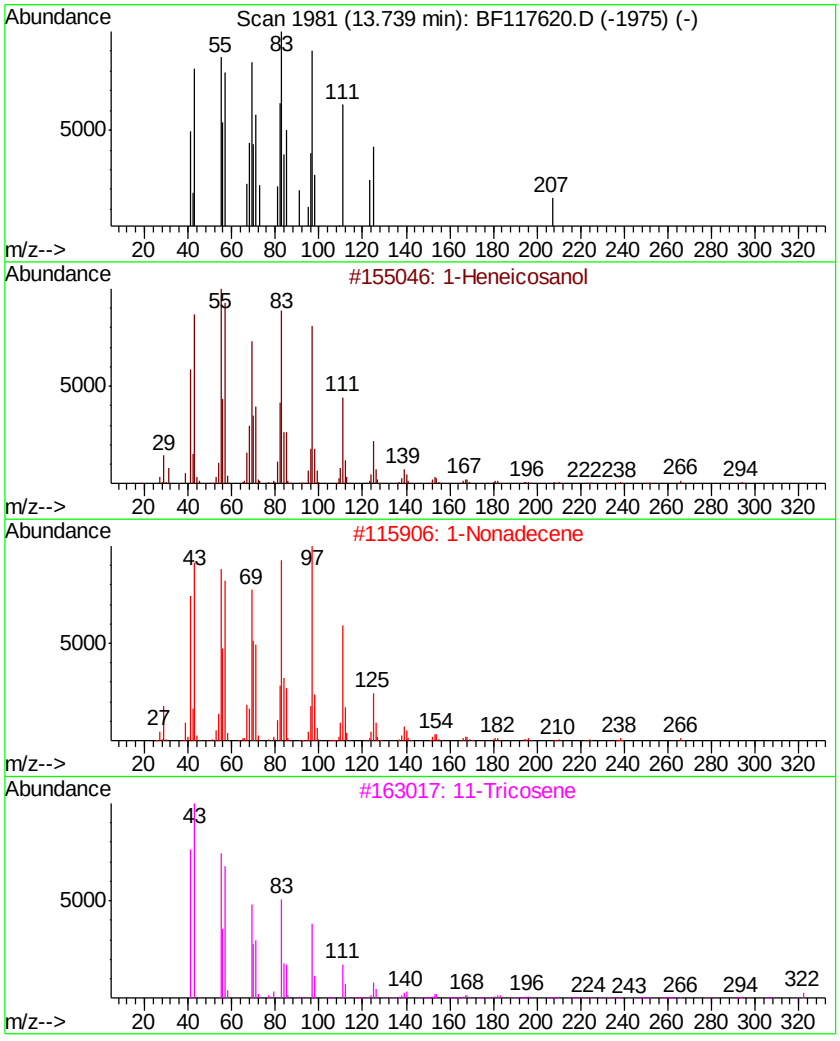
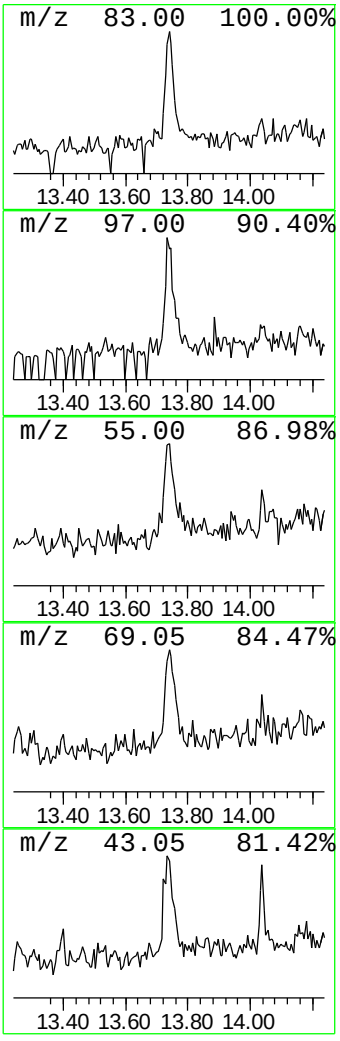
Peak Number 4 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	4.11 ng	47533	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	74
2	1-Nonadecene	266	C19H38	018435-45-5	74
3	11-Tricosene	322	C23H46	052078-56-5	74
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	72
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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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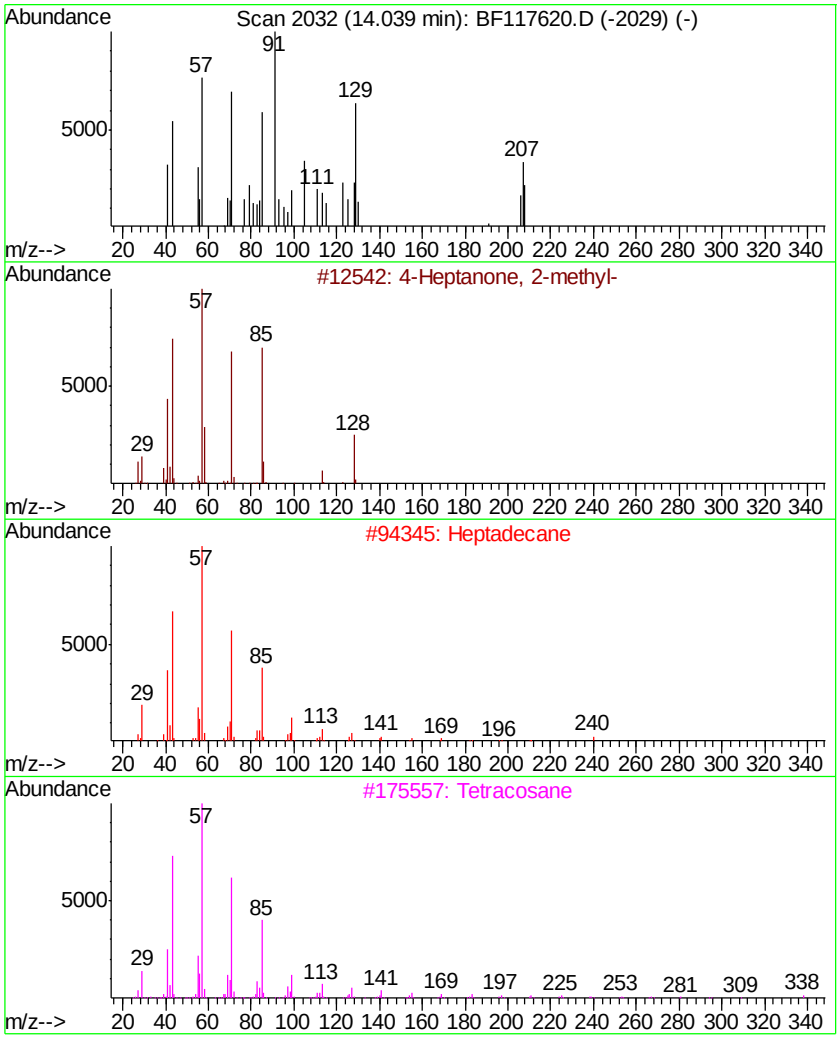
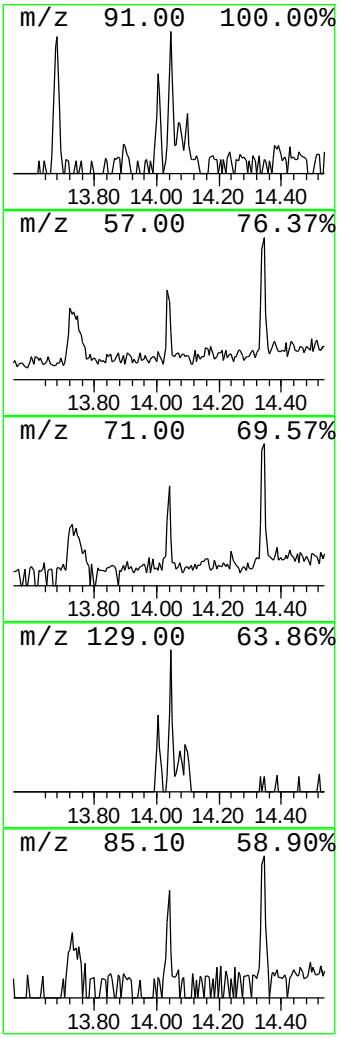
Peak Number 5 unknown14.04 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.19 ng	25372	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	30
2	Heptadecane	240	C17H36	000629-78-7	27
3	Tetracosane	338	C24H50	000646-31-1	27
4	10-Methylnonadecane	282	C20H42	056862-62-5	27
5	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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

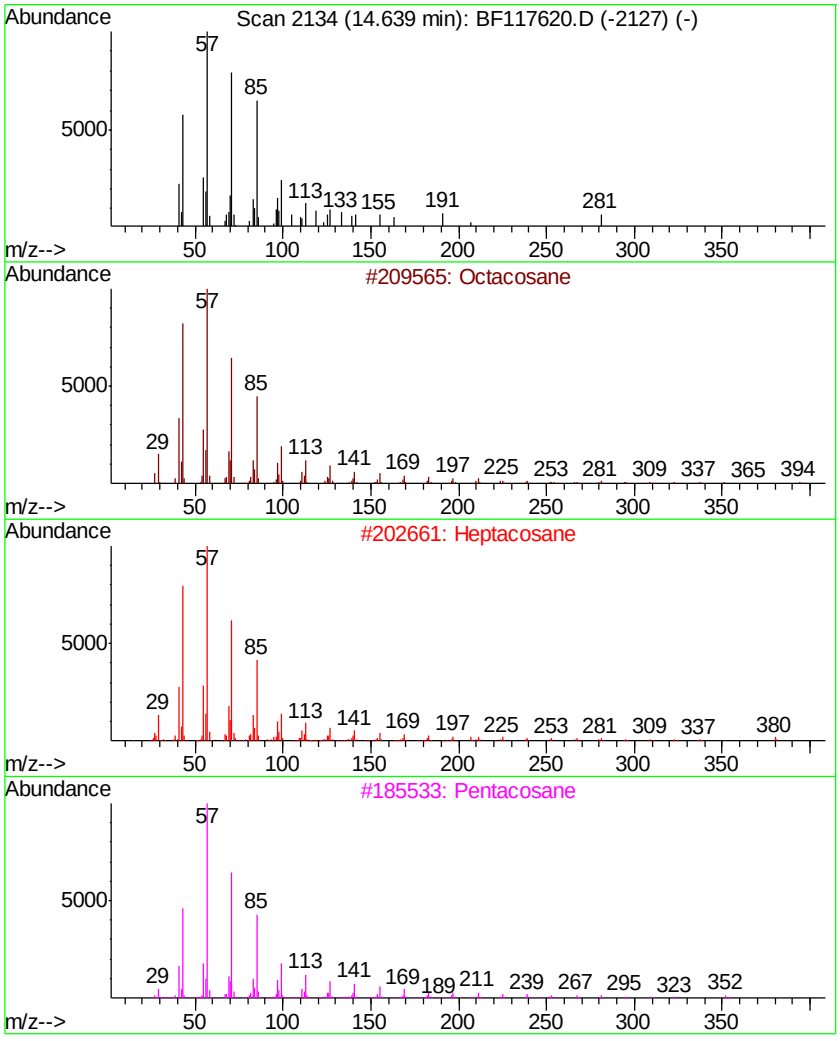
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

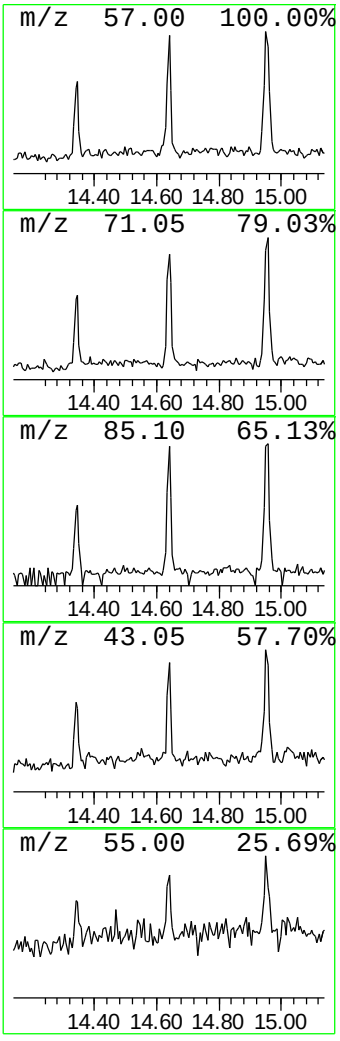
****

Peak Number 6 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.97 ng	37948	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Heptacosane	380	C27H56	000593-49-7	86
3	Pentacosane	352	C25H52	000629-99-2	86
4	Hentriacontane	437	C31H64	000630-04-6	86
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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

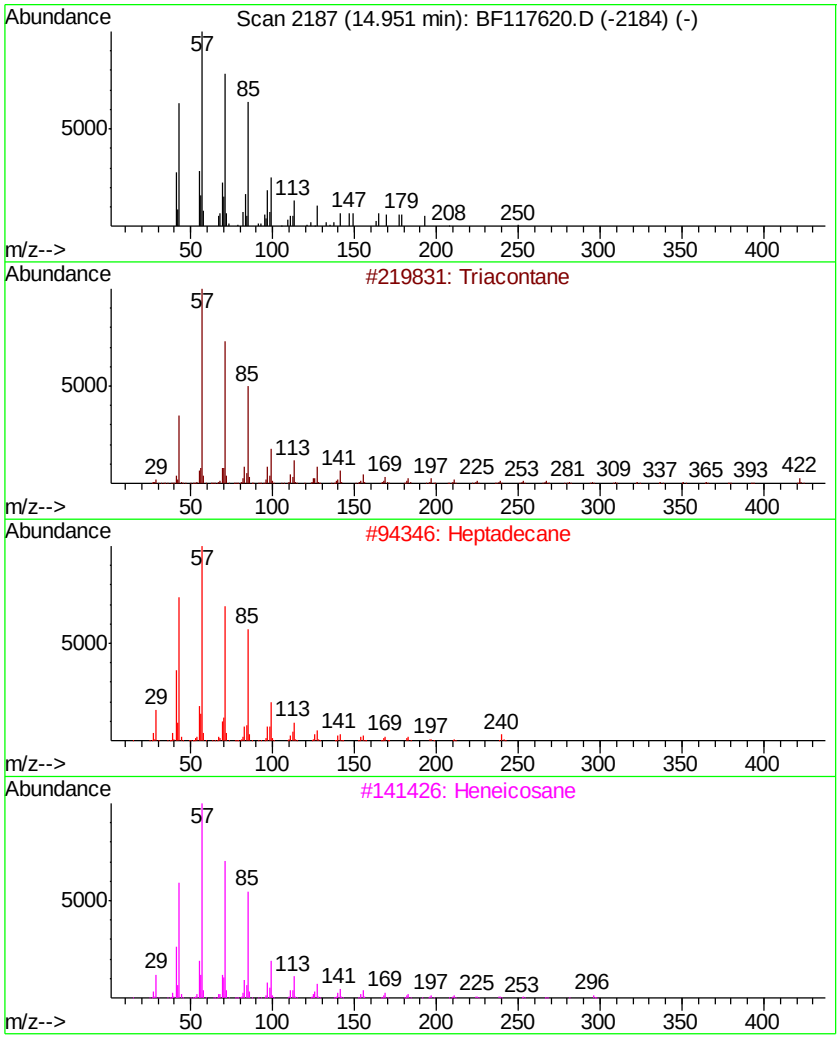
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

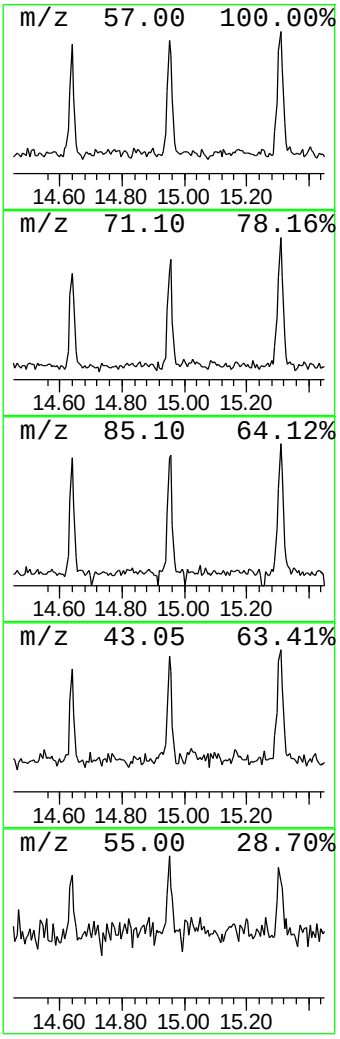
****

Peak Number 7 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.71 ng	47382	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	86
2	Heptadecane	240	C17H36	000629-78-7	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Tetradecane, 2-methyl-	212	C15H32	001560-95-8	86
5	Hexacosane	366	C26H54	000630-01-3	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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

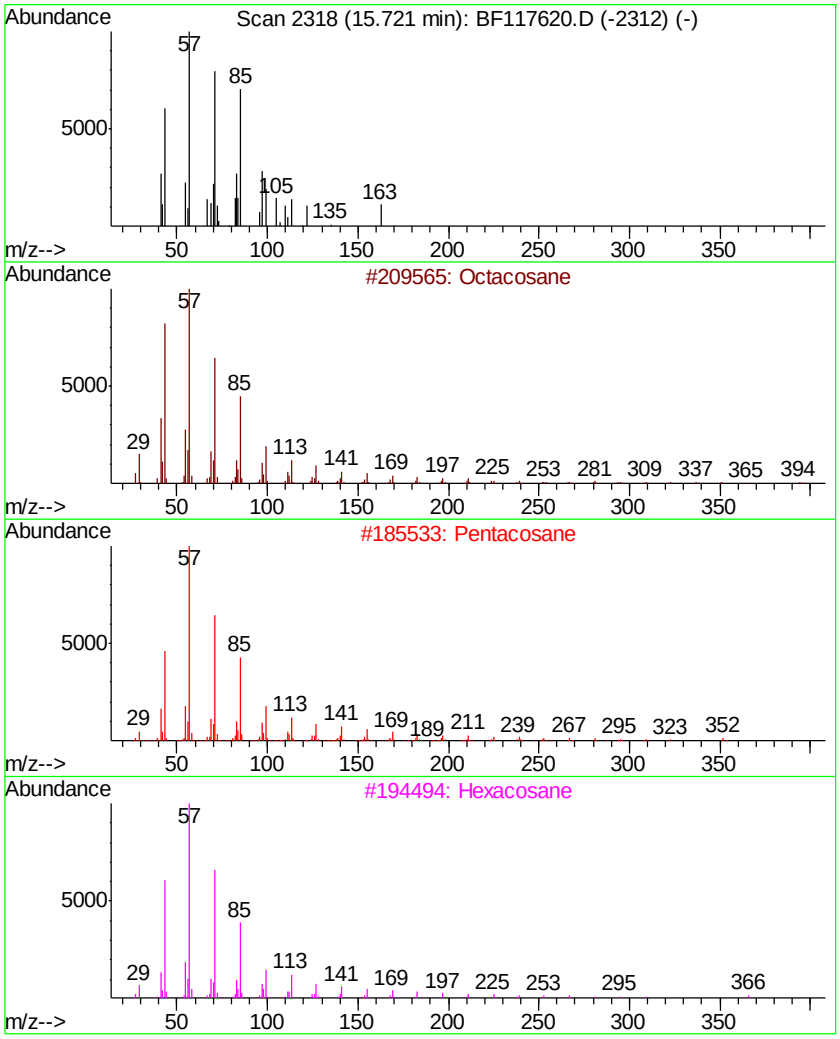
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

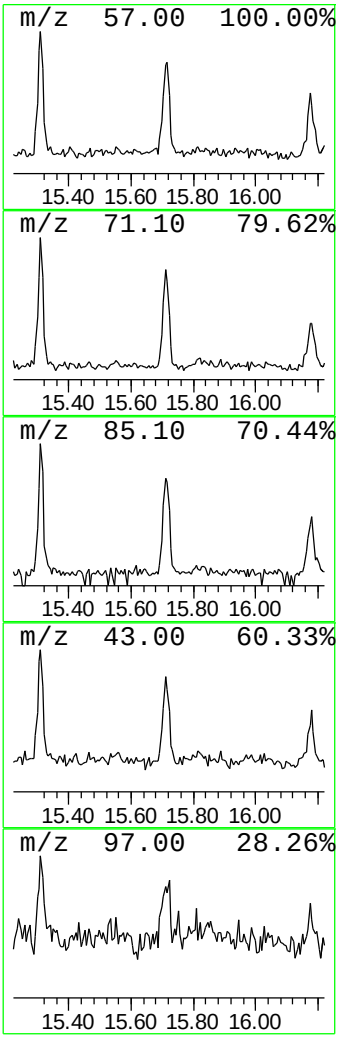
****

Peak Number 8 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.18 ng	40558	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Triacontane	422	C30H62	000638-68-6	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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

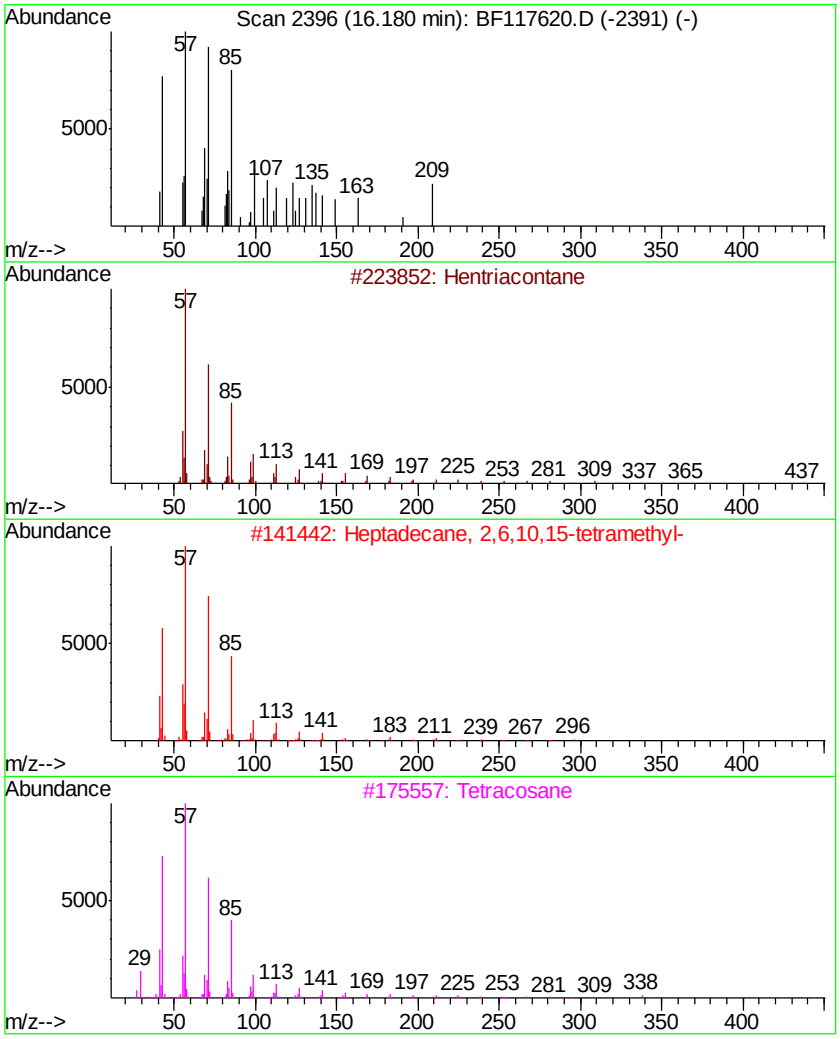
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

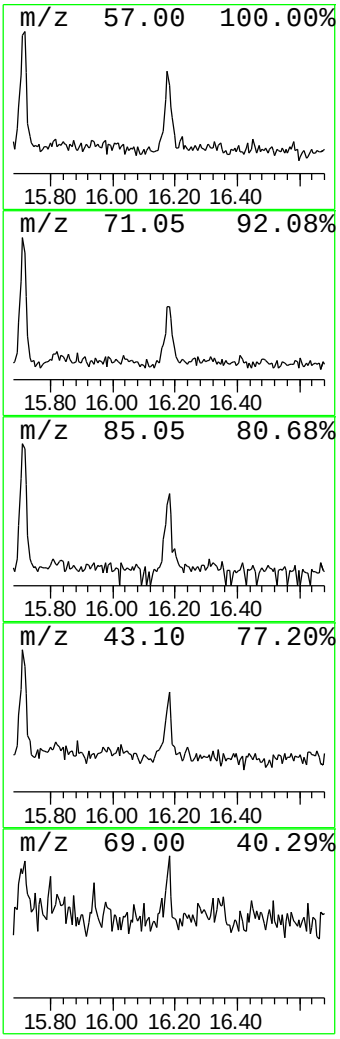
****

Peak Number 9 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.65 ng	33831	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	50
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	50
3	Tetracosane	338	C24H50	000646-31-1	50
4	Dotriacontane	451	C32H66	000544-85-4	50
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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

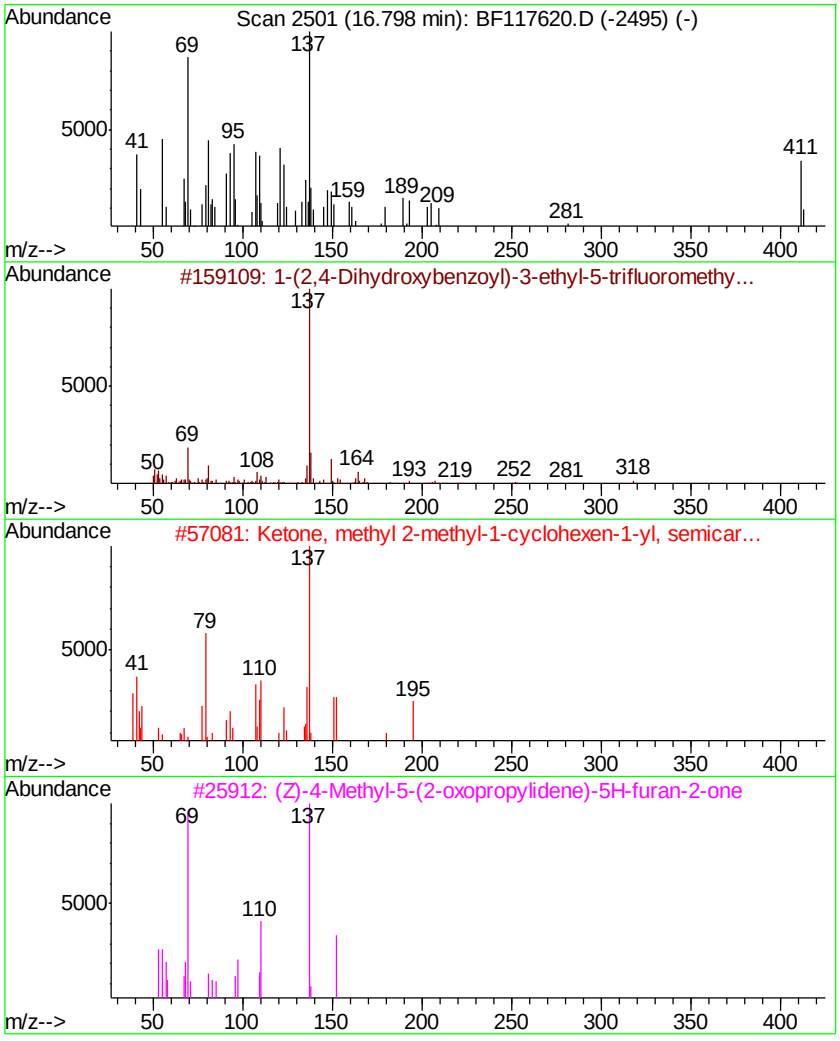
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

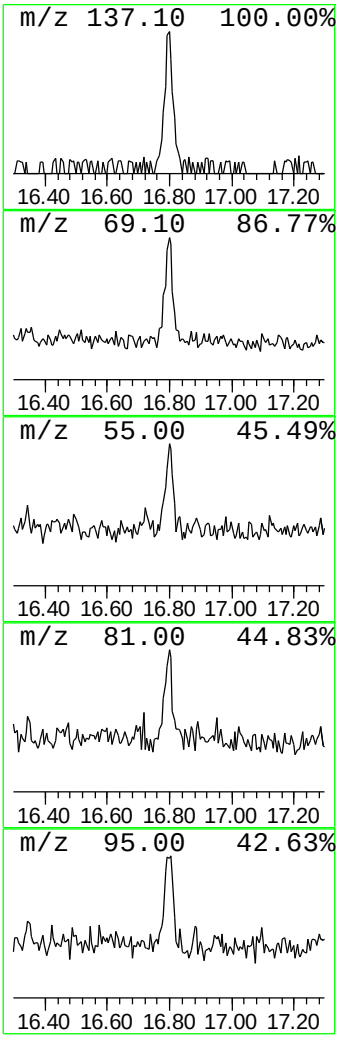
****

Peak Number 10 unknown16.80 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	6.24 ng	79714	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2,4-Dihydroxybenzoyl)-3-ethyl...	318	C13H13F3N2O4	331835-05-3	37
2	Ketone, methyl 2-methyl-1-cycloh...	195	C10H17N3O	016983-67-8	32
3	(Z)-4-Methyl-5-(2-oxopropylidene...	152	C8H8O3	026474-45-3	32
4	3,7,11-Trimethyl-3-hydroxy-6,10-...	282	C17H30O3	1000144-12-7	27
5	Neopentylidenecyclohexane	152	C11H20	039546-80-0	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
Data File : BF117620.D
Acq On : 30 Oct 2019 13:19
Operator : JU
Sample : K5539-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 165-26-(0-1)

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
1,3,5-Cycloheptat...	3.71	134.1	ng	1456550	1	6.73	217261	20.0
unknown6.50	6.50	84.5	ng	918220	1	6.73	217261	20.0
1-Heneicosanol	13.74	4.1	ng	47533	5	13.89	231318	20.0
unknown14.04	14.04	2.2	ng	25372	5	13.89	231318	20.0
Octacosane	14.64	3.0	ng	37948	6	15.33	255449	20.0
Triacontane	14.95	3.7	ng	47382	6	15.33	255449	20.0
Pentacosane	15.72	3.2	ng	40558	6	15.33	255449	20.0
Hentriacontane	16.18	2.6	ng	33831	6	15.33	255449	20.0
unknown16.80	16.80	6.2	ng	79714	6	15.33	255449	20.0