LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
Data File : BF118272.D
Acq On : 18 Dec 2019 21:26
Operator : JU
Sample : K6357-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-04

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-BF120619.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	2.110	3	4	10	rVB	206099	192774	6.25%	0.822%
2	5.063	502	506	522	rVB	287380	361096	11.70%	1.540%
3	5.475	572	576	594	rBV	2003593	1942156	62.95%	8.284%
4	6.492	744	749	766	rBV	2198680	2101137	68.10%	8.962%
5	6.628	768	772	775	rBV	2544256	2205519	71.48%	9.407%
6	6.857	808	811	820	rBV	698865	560210	18.16%	2.389%
7	7.016	834	838	841	rBV	2166027	1764115	57.18%	7.524%
8	7.422	903	907	920	rBV	1430881	1292686	41.90%	5.513%
9	8.145	1026	1030	1045	rBV	759925	724356	23.48%	3.089%
10	9.222	1209	1213	1229	rBV	2882528	2754978	89.29%	11.750%
11	9.622	1277	1281	1293	rBV	105709	112861	3.66%	0.481%
12	9.910	1326	1330	1343	rBV	918086	872996	28.29%	3.723%
13	10.698	1460	1464	1480	rBV	1714698	1827636	59.23%	7.795%
14	11.404	1580	1584	1593	rBV	874303	907466	29.41%	3.870%
15	11.922	1669	1672	1685	rBV	148612	175057	5.67%	0.747%
16	12.992	1850	1854	1857	rBV	3628783	3085438	100.00%	13.160%
17	13.886	2002	2006	2021	rBV	265414	395905	12.83%	1.689%
18	14.057	2031	2035	2043	rBV	737598	756744	24.53%	3.228%
19	14.204	2057	2060	2069	rBV2	31185	35629	1.15%	0.152%
20	14.510	2109	2112	2115	rBV	47385	47851	1.55%	0.204%
21	14.821	2161	2165	2169	rBV	64001	62306	2.02%	0.266%
22	14.898	2174	2178	2183	rVB	87650	88374	2.86%	0.377%
23	15.168	2219	2224	2228	rBV	70924	84300	2.73%	0.360%
24	15.545	2283	2288	2301	rBV	539421	784857	25.44%	3.348%
25	15.998	2360	2365	2371	rBV2	69739	108577	3.52%	0.463%
26	16.062	2371	2376	2383	rBV9	23684	59945	1.94%	0.256%
27	16.515	2447	2453	2462	rBV3	47686	89187	2.89%	0.380%
28	17.121	2551	2556	2563	rVB3	24555	51760	1.68%	0.221%

Sum of corrected areas: 23445916

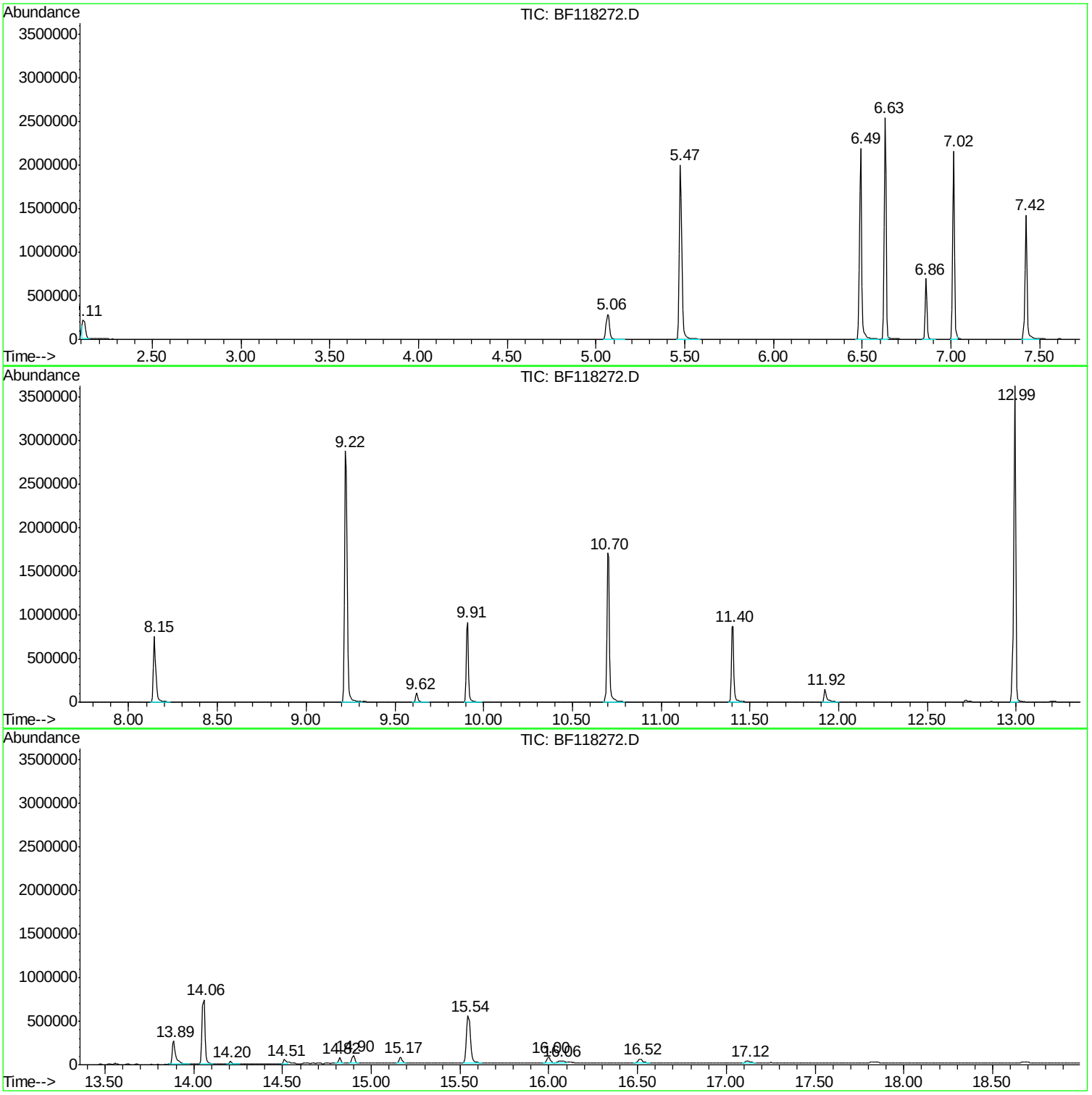
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
Data File : BF118272.D
Acq On : 18 Dec 2019 21:26
Operator : JU
Sample : K6357-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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\BF121819\
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Operator : JU
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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

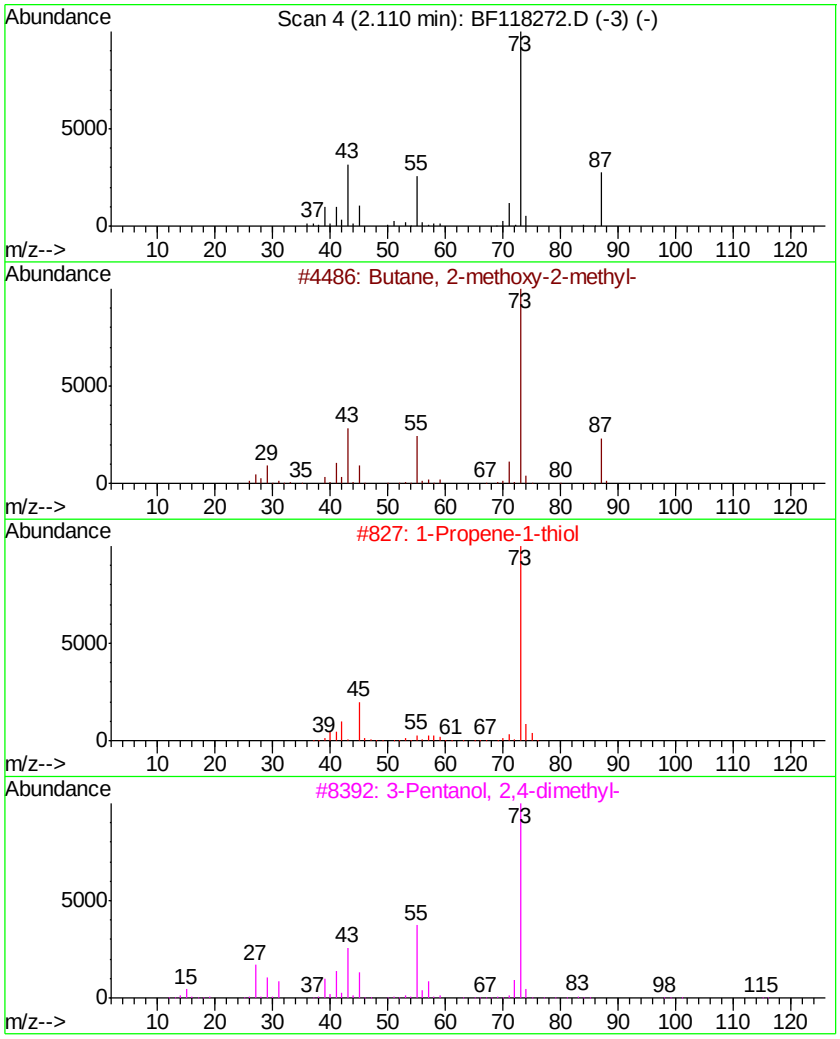
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

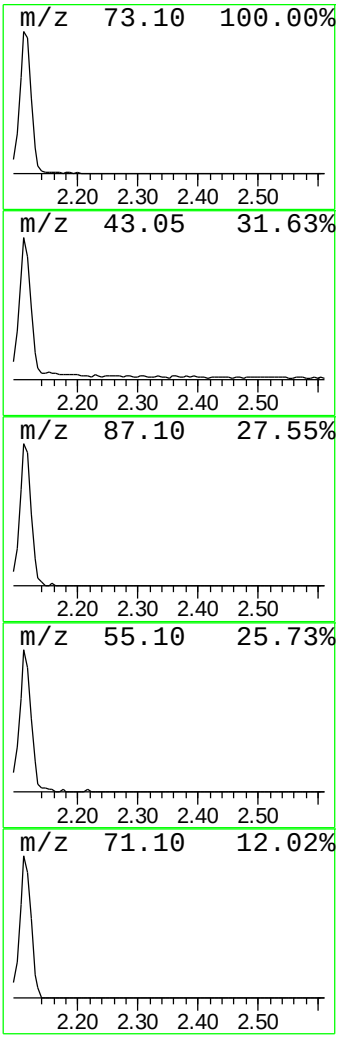
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.11	6.88 ng	192774	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	1-Propene-1-thiol	74	C3H6S	000925-89-3	9
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
Data File : BF118272.D
Acq On : 18 Dec 2019 21:26
Operator : JU
Sample : K6357-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-04

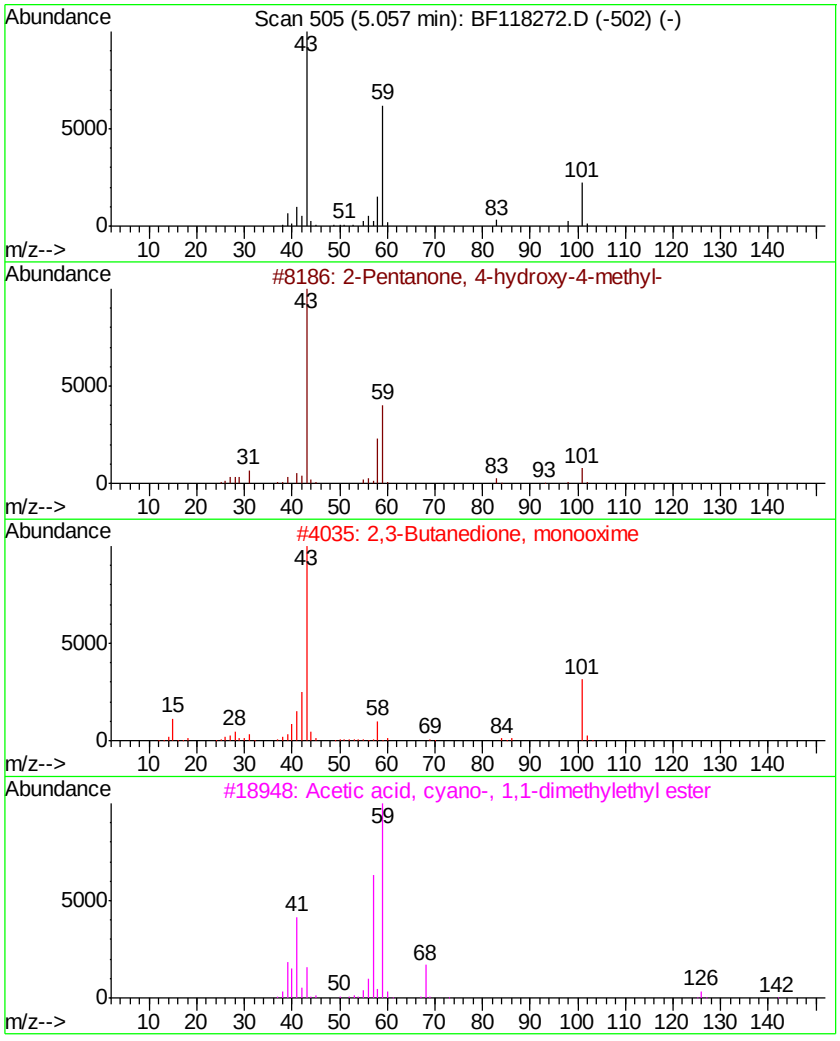
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

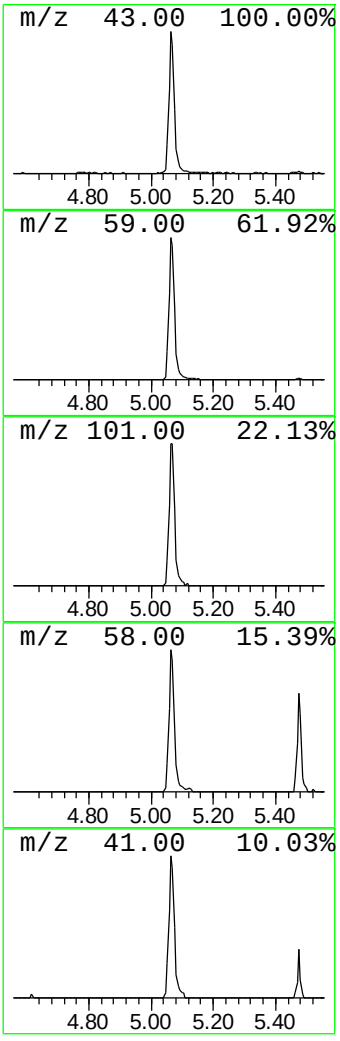
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	12.89 ng	361096	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
Data File : BF118272.D
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Operator : JU
Sample : K6357-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

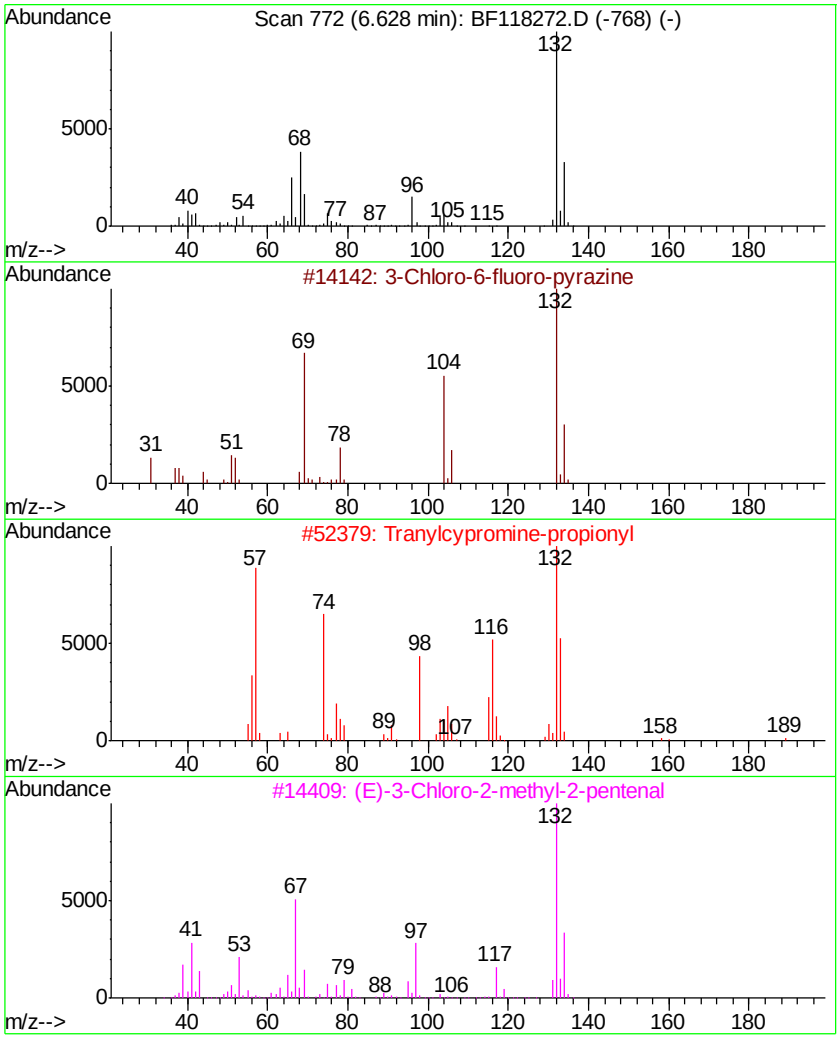
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

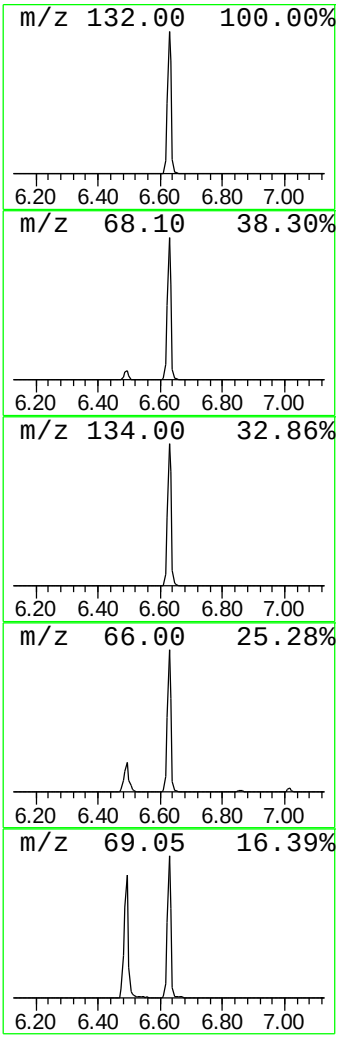
****

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	78.74 ng	2205520	1,4-Dichlorobenzene-d4	6.86

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	12
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





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
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Operator : JU
Sample : K6357-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

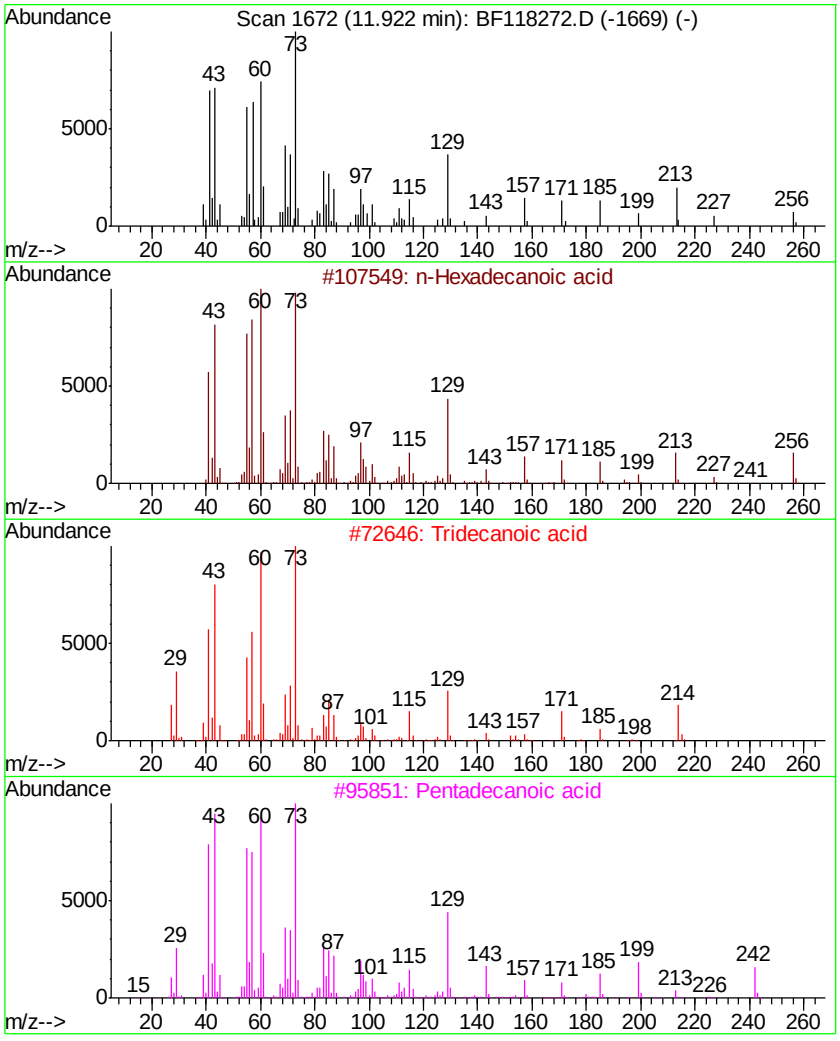
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

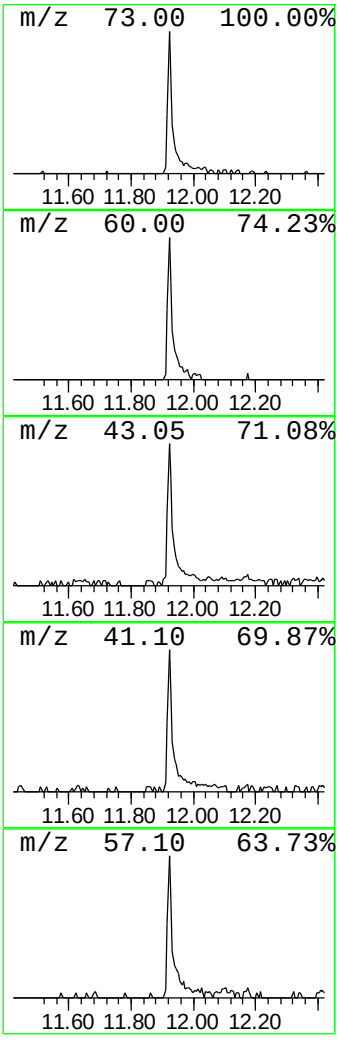
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.86 ng	175057	Phenanthrene-d10	11.40

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	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
Data File : BF118272.D
Acq On : 18 Dec 2019 21:26
Operator : JU
Sample : K6357-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

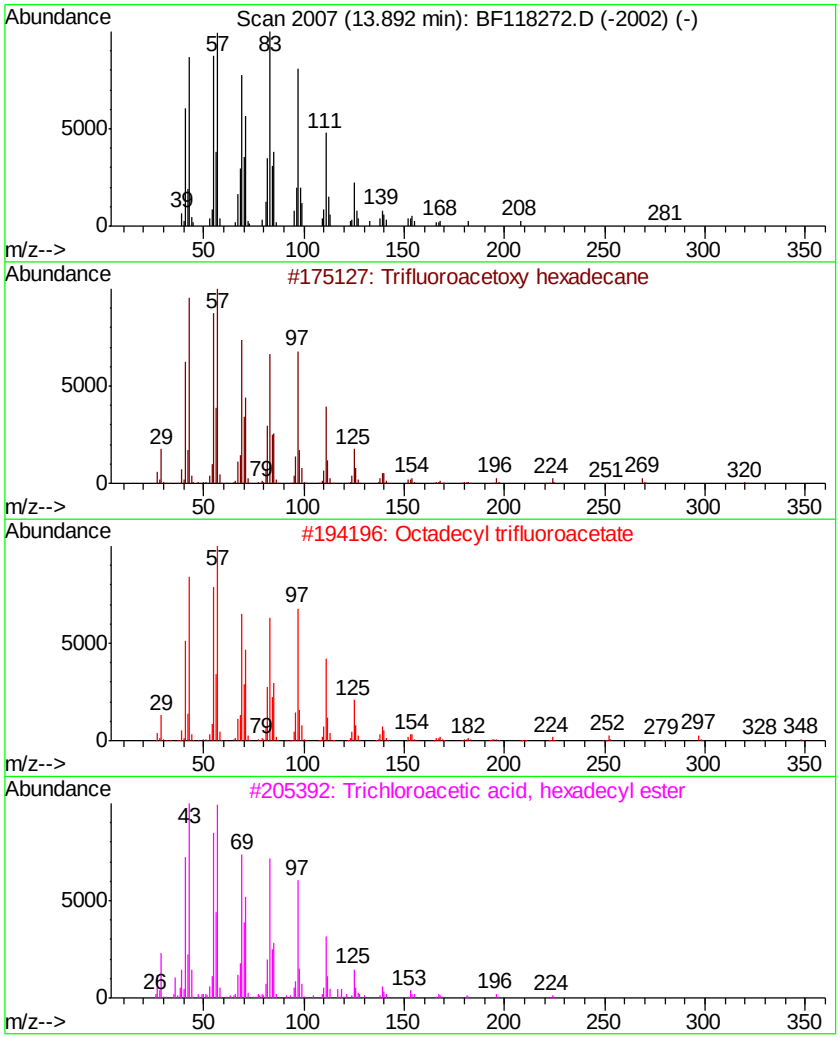
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

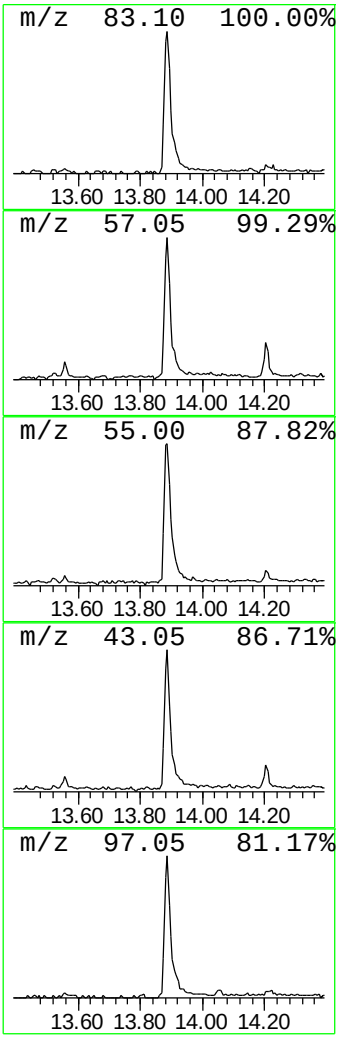
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	10.46 ng	395905	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
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Sample : K6357-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

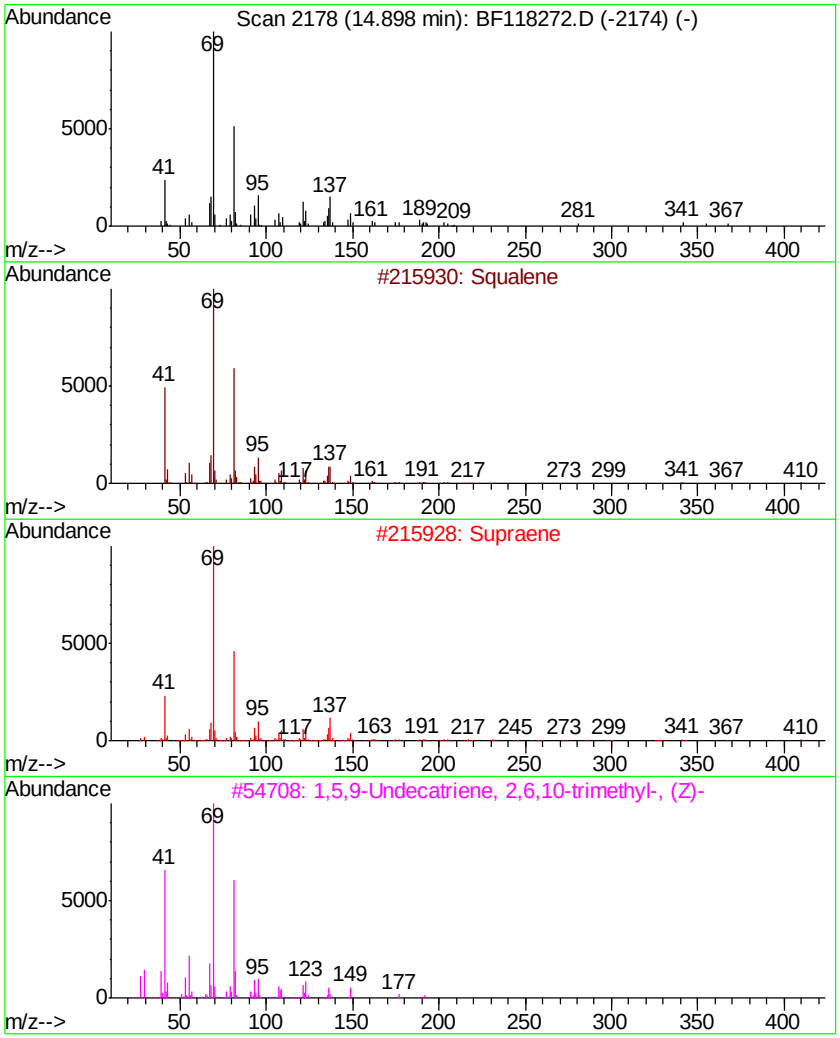
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

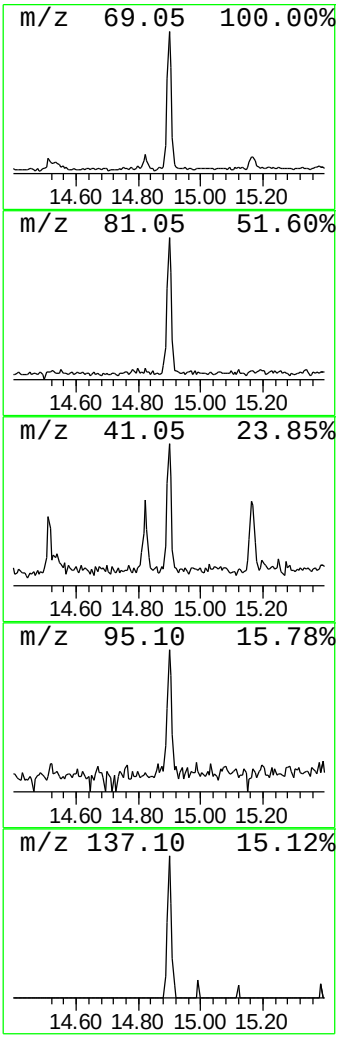
****

Peak Number 7 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.25 ng	88374	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	83
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	81
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
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Operator : JU
Sample : K6357-04
Misc :
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Instrument : BNA_F
ClientSampleId : PF-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

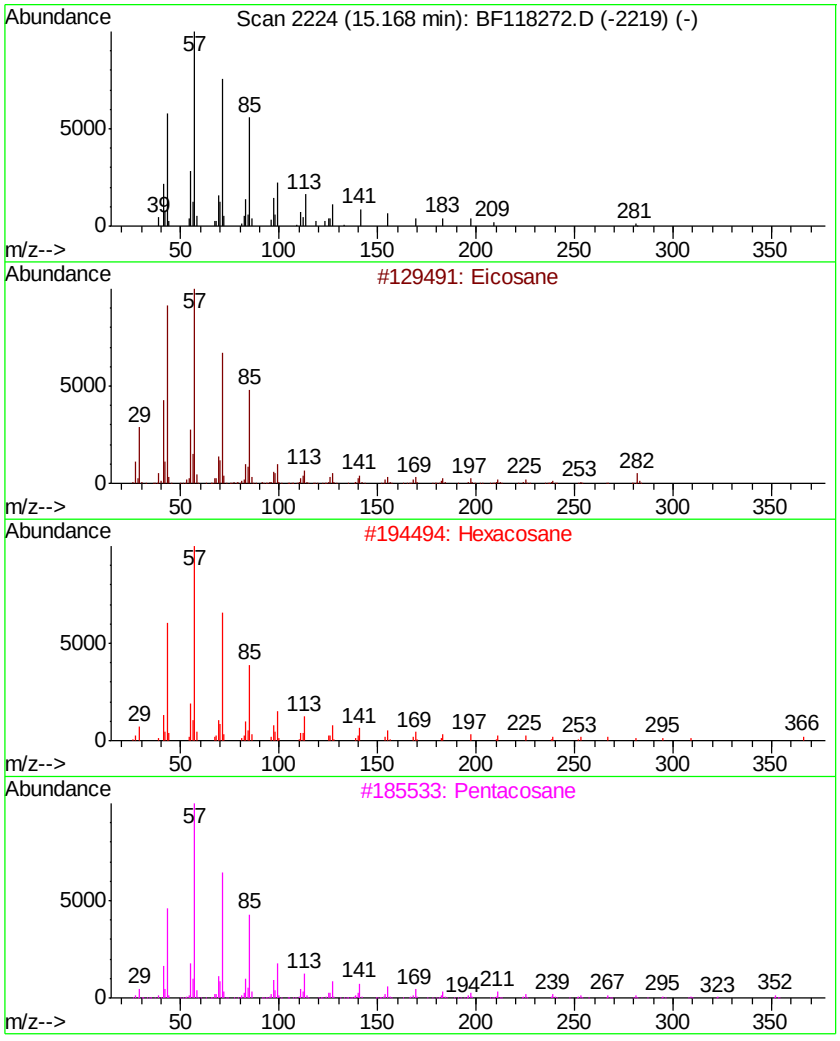
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

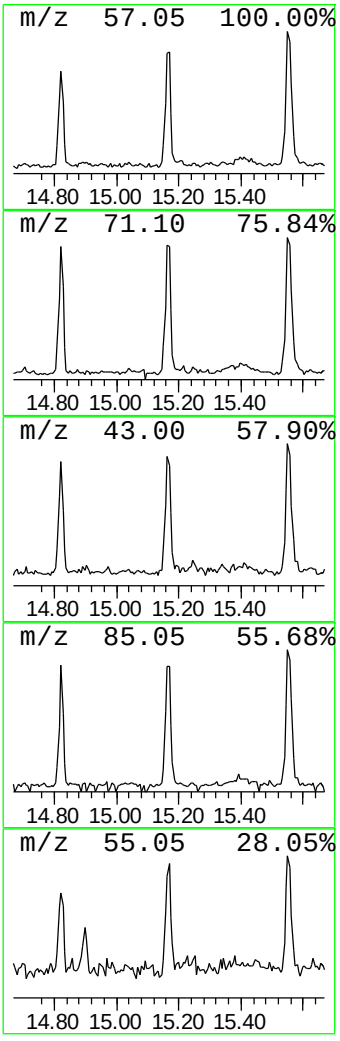
****

Peak Number 8 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.15 ng	84300	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Octacosane	394	C28H58	000630-02-4	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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Misc :
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Instrument : BNA_F
ClientSampleId : PF-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

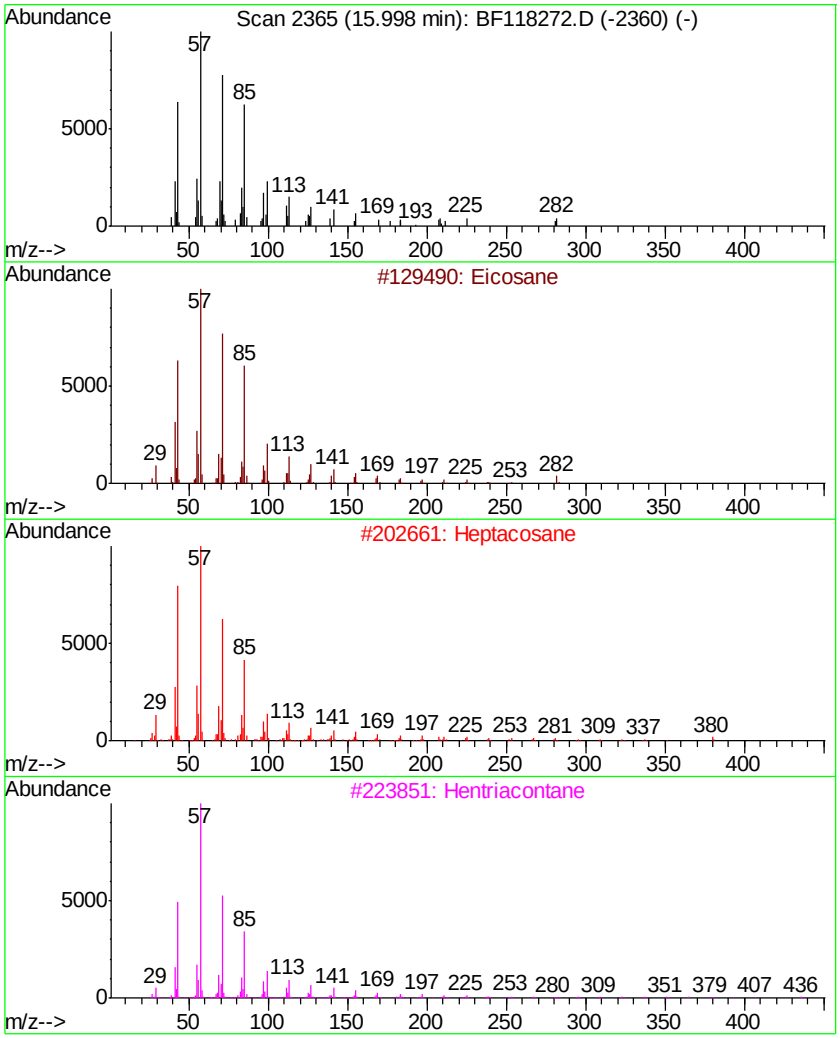
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

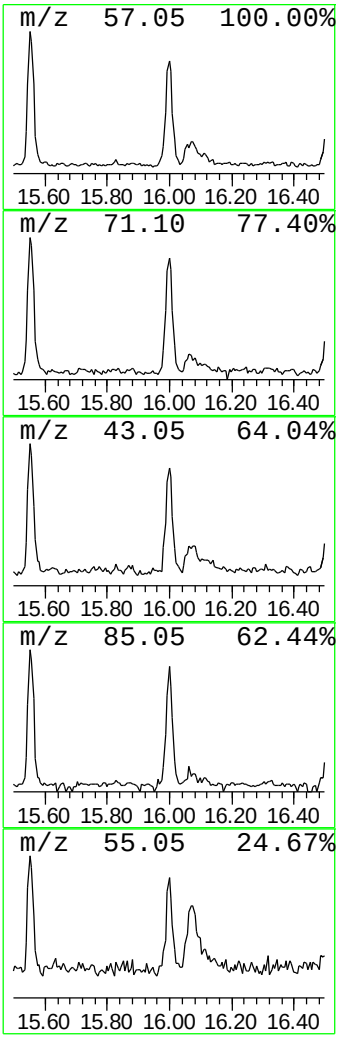
****

Peak Number 9 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.77 ng	108577	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Hexacosane	366	C26H54	000630-01-3	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
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Acq On : 18 Dec 2019 21:26
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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

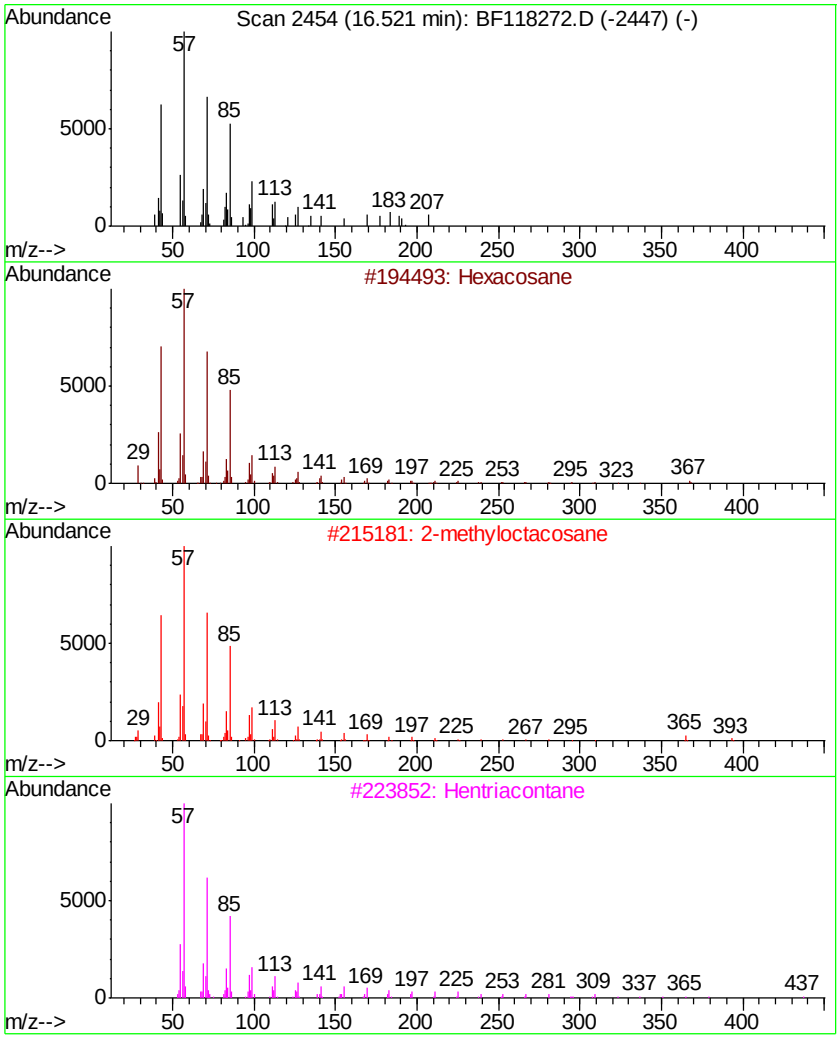
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

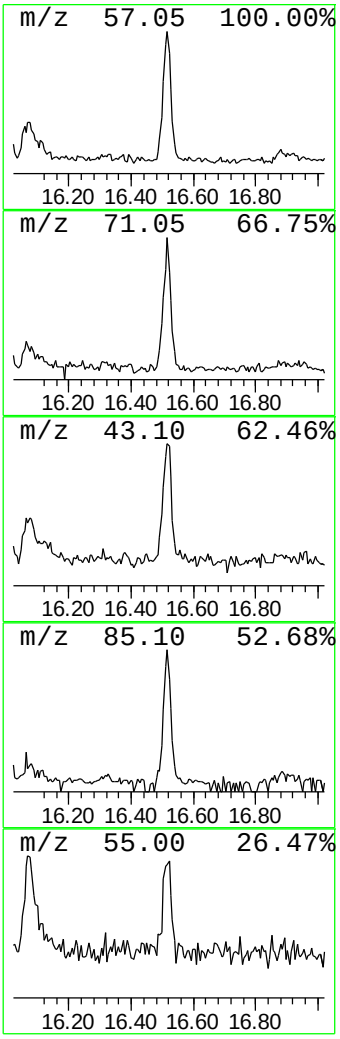
****

Peak Number 10 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.52	2.27 ng	89187	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Octacosane	394	C28H58	000630-02-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121819\
Data File : BF118272.D
Acq On : 18 Dec 2019 21:26
Operator : JU
Sample : K6357-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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
Butane, 2-methoxy...	2.11	6.9	ng	192774	1	6.86	560210	20.0
2-Pentanone, 4-hy...	5.06	12.9	ng	361096	1	6.86	560210	20.0
unknown6.63	6.63	78.7	ng	2205520	1	6.86	560210	20.0
n-Hexadecanoic acid	11.92	3.9	ng	175057	4	11.40	907466	20.0
Trifluoroacetoxy ...	13.89	10.5	ng	395905	5	14.06	756744	20.0
Squalene	14.90	2.3	ng	88374	6	15.54	784857	20.0
Eicosane	15.17	2.1	ng	84300	6	15.54	784857	20.0
Heptacosane	16.00	2.8	ng	108577	6	15.54	784857	20.0
Hexacosane	16.52	2.3	ng	89187	6	15.54	784857	20.0