LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
Data File : BF118377.D
Acq On : 28 Dec 2019 20:49
Operator : JU
Sample : K6439-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF004-01

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-BF122419.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	5.063	502	506	518	rVB	465561	607824	10.92%	1.658%
2	5.475	572	576	602	rBV	3382225	3187128	57.27%	8.693%
3	6.492	744	749	767	rBV	3139697	3418956	61.44%	9.325%
4	6.622	767	771	775	rBV	3726493	3609974	64.87%	9.846%
5	6.851	806	810	818	rVB	787616	652786	11.73%	1.780%
6	7.010	832	837	840	rBV	3084248	2819449	50.66%	7.690%
7	7.416	902	906	922	rBV	1980085	2118896	38.08%	5.779%
8	8.139	1025	1029	1046	rBV	853153	838656	15.07%	2.287%
9	9.216	1208	1212	1215	rBV	5027088	4307831	77.41%	11.749%
10	9.610	1276	1279	1291	rBV	211160	248527	4.47%	0.678%
11	9.898	1324	1328	1341	rBV	1167590	1027431	18.46%	2.802%
12	10.692	1459	1463	1478	rBV	3038332	3198988	57.48%	8.725%
13	11.392	1578	1582	1592	rBV	1234161	1124858	20.21%	3.068%
14	11.916	1668	1671	1684	rBV	242418	279867	5.03%	0.763%
15	12.704	1802	1805	1812	rBV2	41938	61422	1.10%	0.168%
16	12.986	1848	1853	1856	rBV	5985398	5564946	100.00%	15.178%
17	13.874	2001	2004	2017	rBV	404104	663238	11.92%	1.809%
18	14.045	2029	2033	2044	rVB	1144021	1139668	20.48%	3.108%
19	14.498	2107	2110	2112	rBV	68228	65731	1.18%	0.179%
20	14.810	2157	2163	2166	rBV2	83465	102116	1.83%	0.279%
21	15.151	2217	2221	2225	rBV	84031	97234	1.75%	0.265%
22	15.539	2281	2287	2298	rBV	840259	1139573	20.48%	3.108%
23	15.974	2357	2361	2368	rVB	55728	85318	1.53%	0.233%
24	16.057	2369	2375	2388	rBV8	53050	172525	3.10%	0.471%
25	16.492	2443	2449	2454	rBV5	31687	58777	1.06%	0.160%
26	16.745	2486	2492	2498	rBV6	37501	72279	1.30%	0.197%

Sum of corrected areas: 36663998

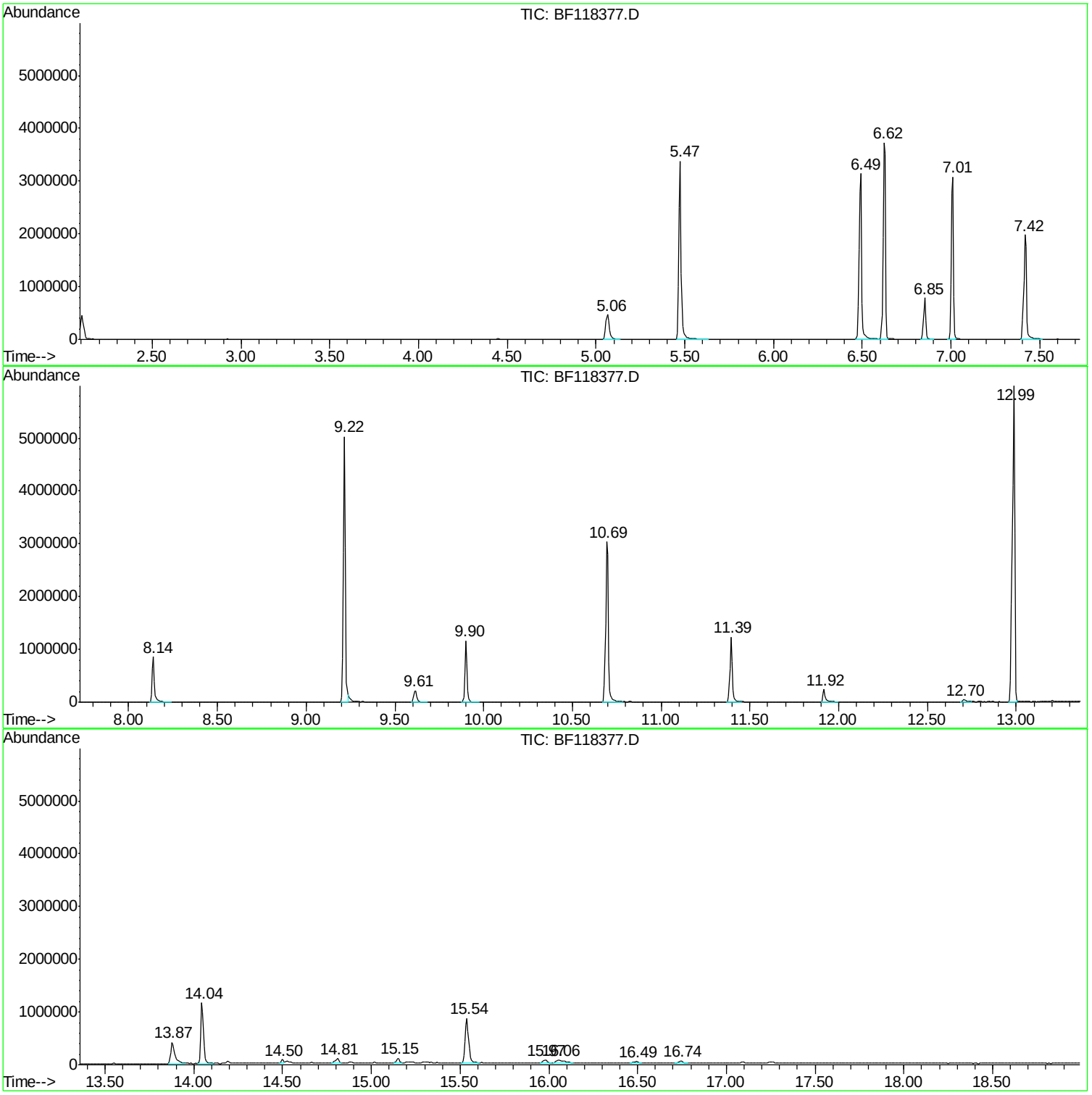
LSC Report - Integrated Chromatogram

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
Data File : BF118377.D
Acq On : 28 Dec 2019 20:49
Operator : JU
Sample : K6439-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIED-BF004-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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\BF122819\
Data File : BF118377.D
Acq On : 28 Dec 2019 20:49
Operator : JU
Sample : K6439-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF004-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

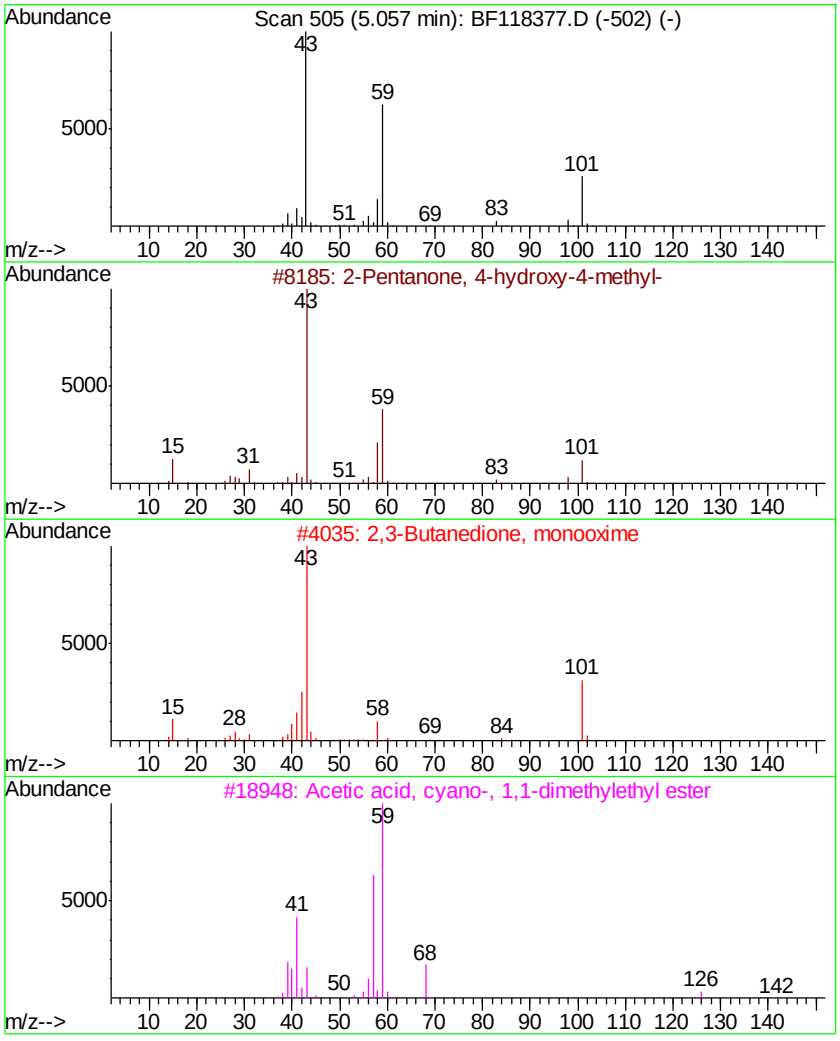
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

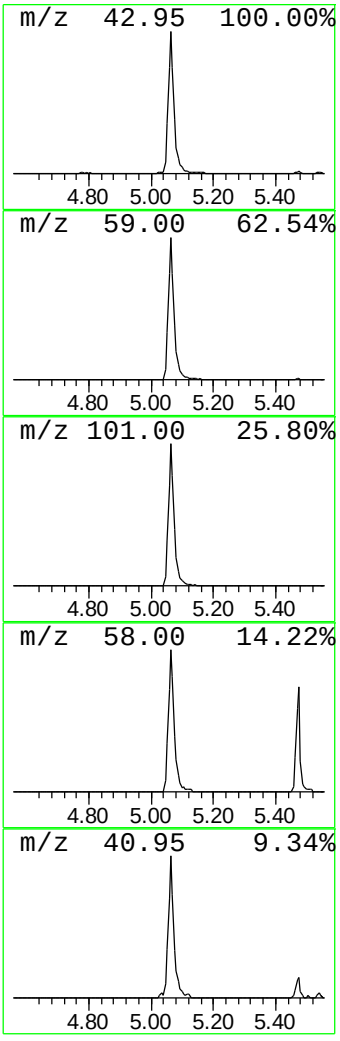
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	18.62 ng	607824	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
Data File : BF118377.D
Acq On : 28 Dec 2019 20:49
Operator : JU
Sample : K6439-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF004-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

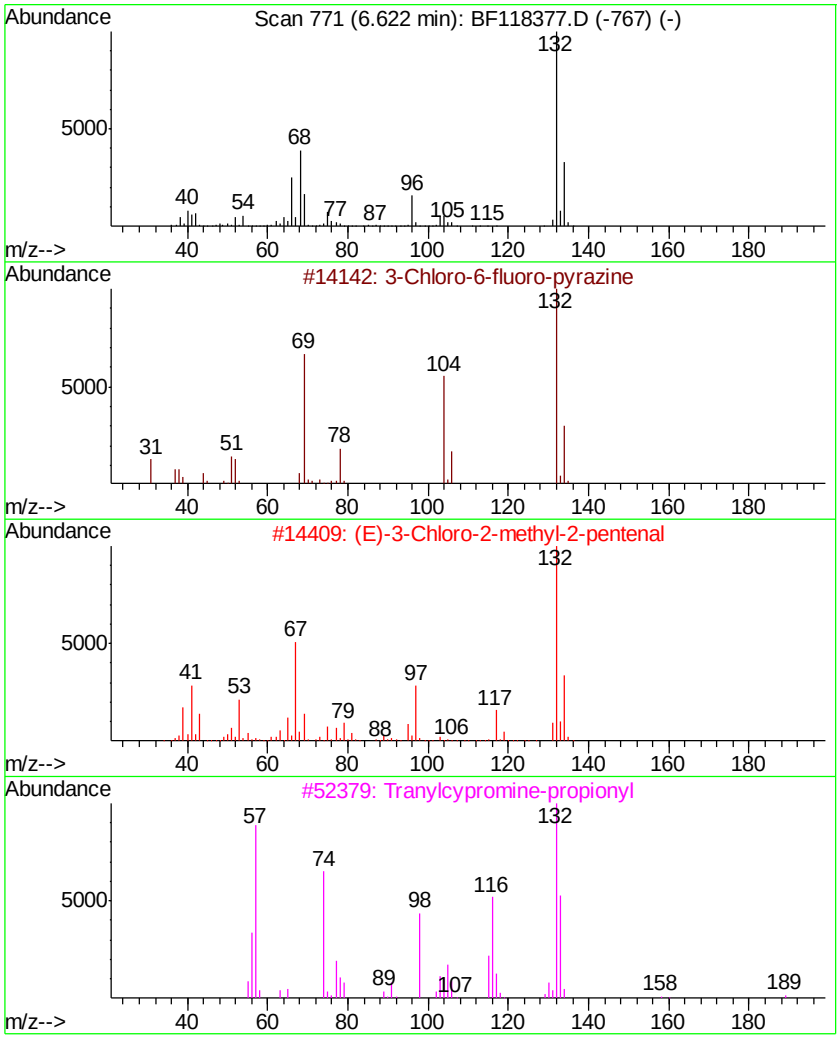
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

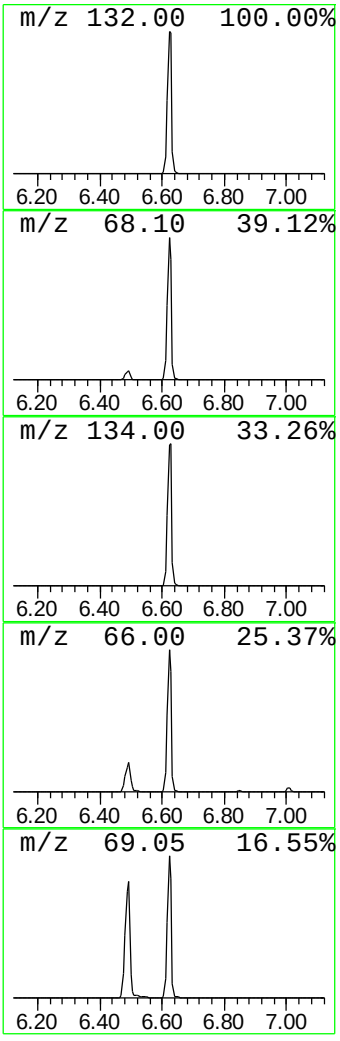
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	110.60 ng	3609970	1,4-Dichlorobenzene-d4	6.85

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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\BF122819\
Data File : BF118377.D
Acq On : 28 Dec 2019 20:49
Operator : JU
Sample : K6439-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF004-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

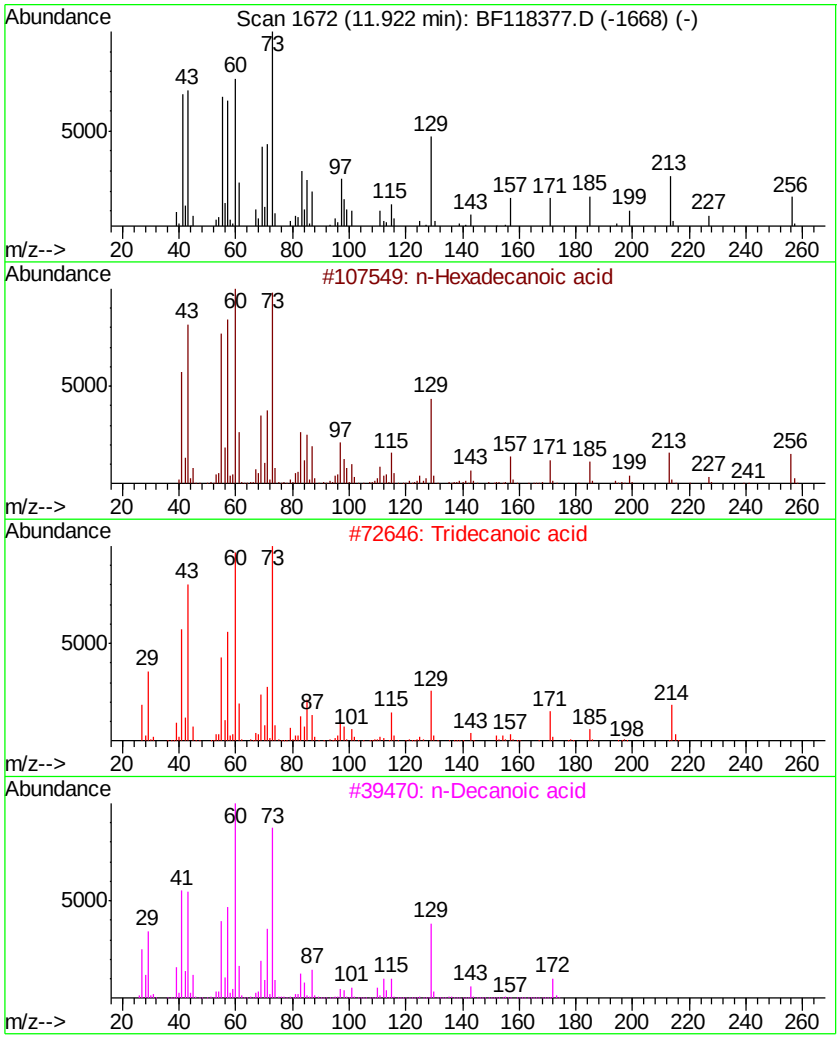
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

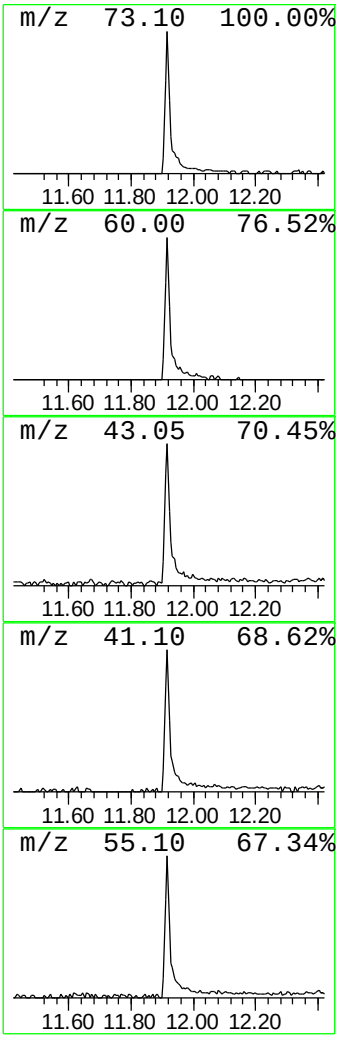
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.98 ng	279867	Phenanthrene-d10	11.39

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	91
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	74





Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
Data File : BF118377.D
Acq On : 28 Dec 2019 20:49
Operator : JU
Sample : K6439-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF004-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

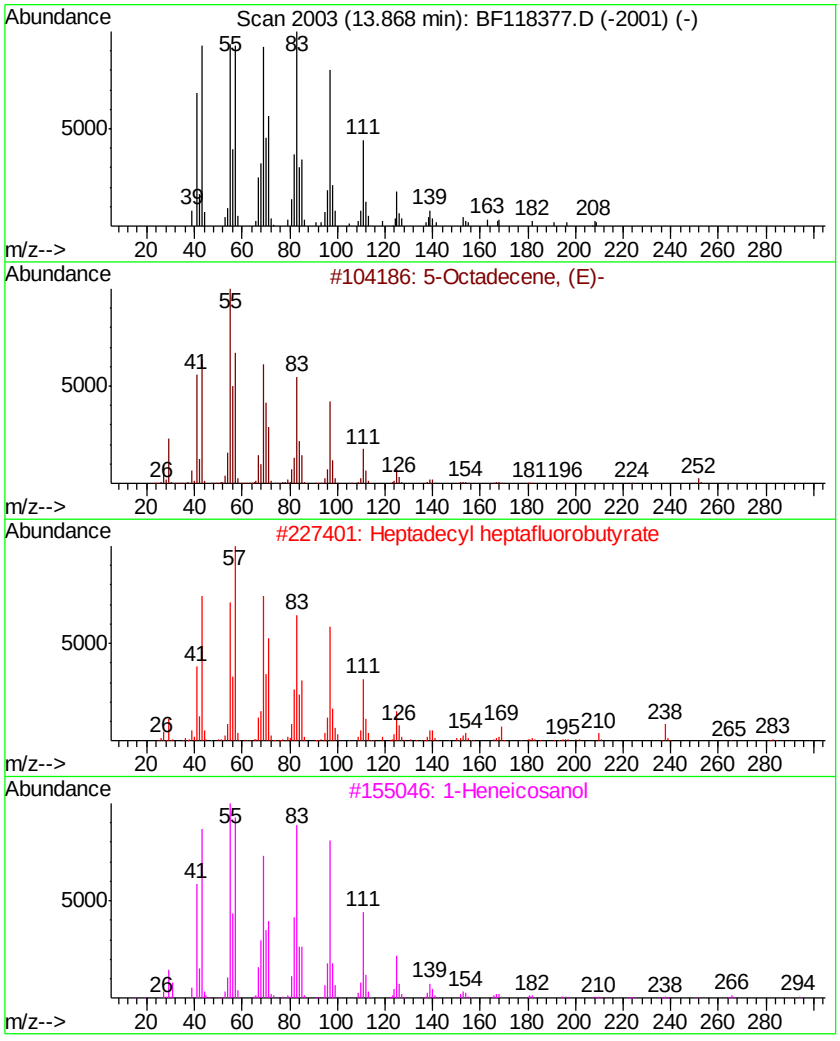
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

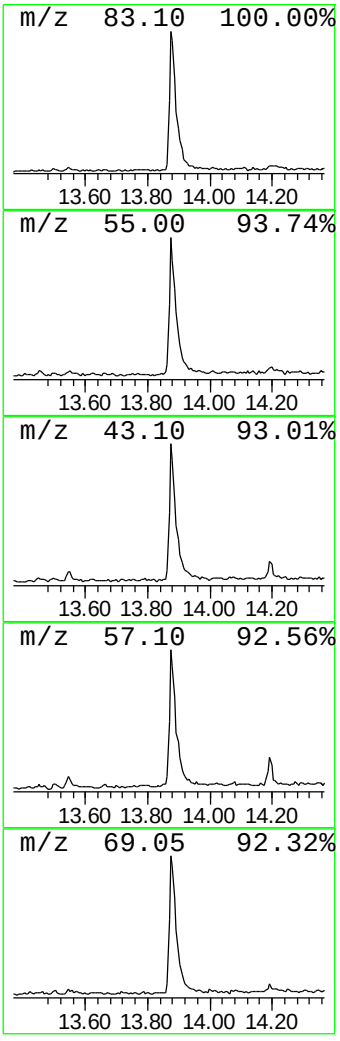
****

Peak Number 5 5-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	11.64 ng	663238	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93





Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
Data File : BF118377.D
Acq On : 28 Dec 2019 20:49
Operator : JU
Sample : K6439-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF004-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

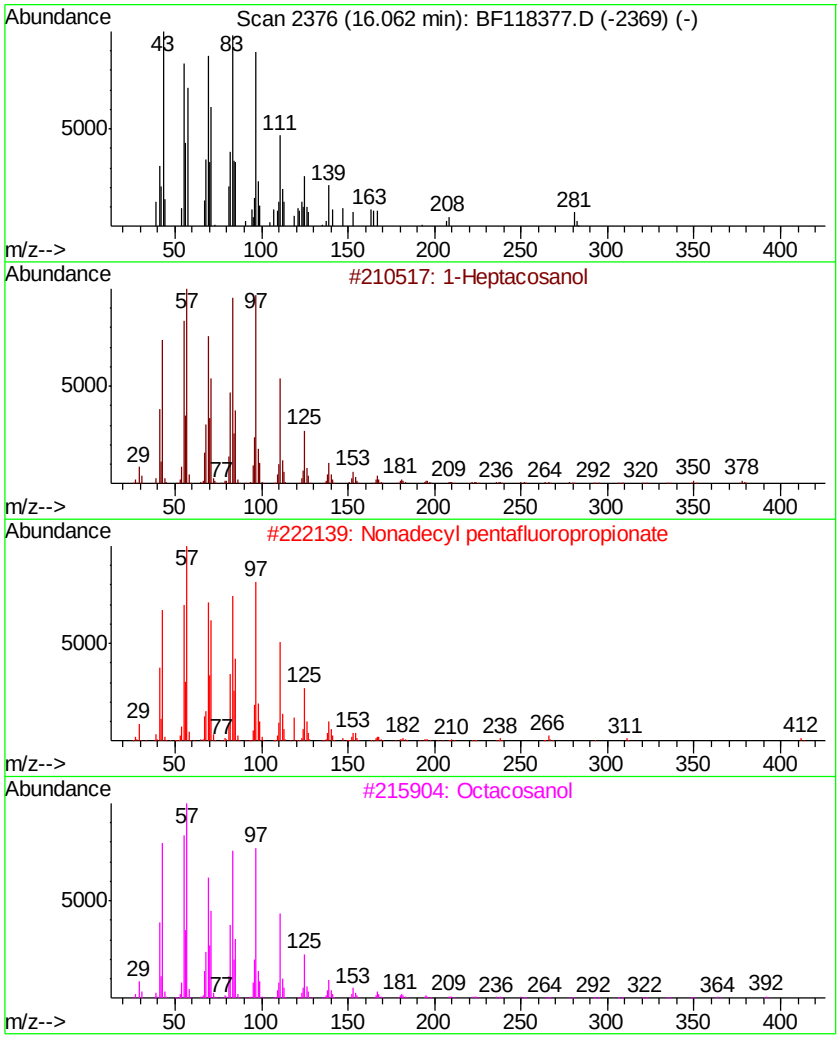
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

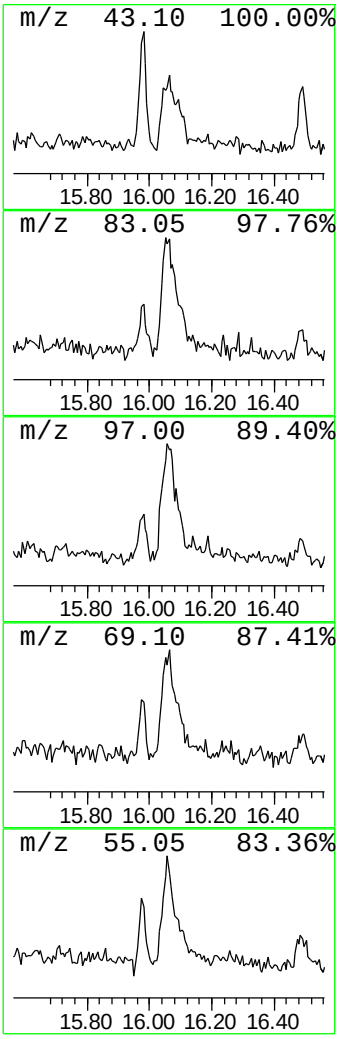
****

Peak Number 6 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	3.03 ng	172525	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
3	Octacosanol	410	C28H58O	000557-61-9	87
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	86
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122819\
Data File : BF118377.D
Acq On : 28 Dec 2019 20:49
Operator : JU
Sample : K6439-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF004-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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
2-Pentanone, 4-hy...	5.06	18.6	ng	607824	1	6.85	652786	20.0
unknown6.62	6.62	110.6	ng	3609970	1	6.85	652786	20.0
n-Hexadecanoic acid	11.92	5.0	ng	279867	4	11.39	1124860	20.0
5-Octadecene, (E)-	13.87	11.6	ng	663238	5	14.04	1139670	20.0
1-Heptacosanol	16.06	3.0	ng	172525	6	15.54	1139570	20.0