LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

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-BF091418.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	4.902	433	436	447	rVB	298394	323682	18.76%	2.208%
2	5.331	505	509	518	rBV	719650	669065	38.77%	4.564%
3	5.666	564	566	573	rBV	38749	39002	2.26%	0.266%
4	6.354	679	683	702	rBV3	1485687	1725578	100.00%	11.770%
5	6.490	702	706	709	rBV	1109553	981594	56.88%	6.695%
6	6.719	742	745	749	rBV	892606	742680	43.04%	5.066%
7	6.878	768	772	775	rBV	1485299	1181986	68.50%	8.062%
8	7.278	836	840	843	rBV	978227	777590	45.06%	5.304%
9	7.913	944	948	959	rBV	264124	258045	14.95%	1.760%
10	8.001	959	963	966	rBV	1126436	873571	50.62%	5.959%
11	8.637	1068	1071	1081	rVB	162661	142487	8.26%	0.972%
12	9.078	1142	1146	1149	rBV	1576455	1211598	70.21%	8.264%
13	9.472	1209	1213	1219	rBV	149441	128829	7.47%	0.879%
14	9.754	1257	1261	1264	rBV	895526	803523	46.57%	5.481%
15	10.531	1390	1393	1403	rBV	282885	267499	15.50%	1.825%
16	11.230	1508	1512	1514	rBV	851233	737804	42.76%	5.032%
17	11.248	1514	1515	1518	rVB	45692	32676	1.89%	0.223%
18	12.436	1714	1717	1721	rVB	37470	35163	2.04%	0.240%
19	12.660	1749	1755	1759	rBV	39047	43088	2.50%	0.294%
20	12.807	1777	1780	1784	rBV	1151132	925508	53.63%	6.313%
21	13.054	1818	1822	1825	rBV	30837	27330	1.58%	0.186%
22	13.277	1858	1860	1867	rVB6	16701	25637	1.49%	0.175%
23	13.395	1878	1880	1882	rBV	43586	32010	1.86%	0.218%
24	13.724	1932	1936	1942	rBV	78964	86093	4.99%	0.587%
25	13.854	1954	1958	1961	rBV	1091742	945198	54.78%	6.447%
26	14.036	1986	1989	1994	rVB	68344	64647	3.75%	0.441%
27	14.342	2038	2041	2046	rBV	87192	76376	4.43%	0.521%
28	14.636	2088	2091	2095	rBV	97530	87169	5.05%	0.595%
29	14.707	2100	2103	2108	rVB	65498	59526	3.45%	0.406%
30	14.954	2142	2145	2150	rBV	99461	103374	5.99%	0.705%
31	15.260	2192	2197	2201	rBV	710156	806343	46.73%	5.500%
32	15.307	2202	2205	2210	rVB	91597	114803	6.65%	0.783%
33	15.713	2270	2274	2280	rVB	90032	118713	6.88%	0.810%
34	16.113	2338	2342	2346	rVB6	33155	45598	2.64%	0.311%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

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-BF091418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.177	2349	2353	2359	rVB2	63276	120000	6.95%	0.819%
36	16.724	2442	2446	2453	rVB2	26518	47118	2.73%	0.321%

Sum of corrected areas: 14660903

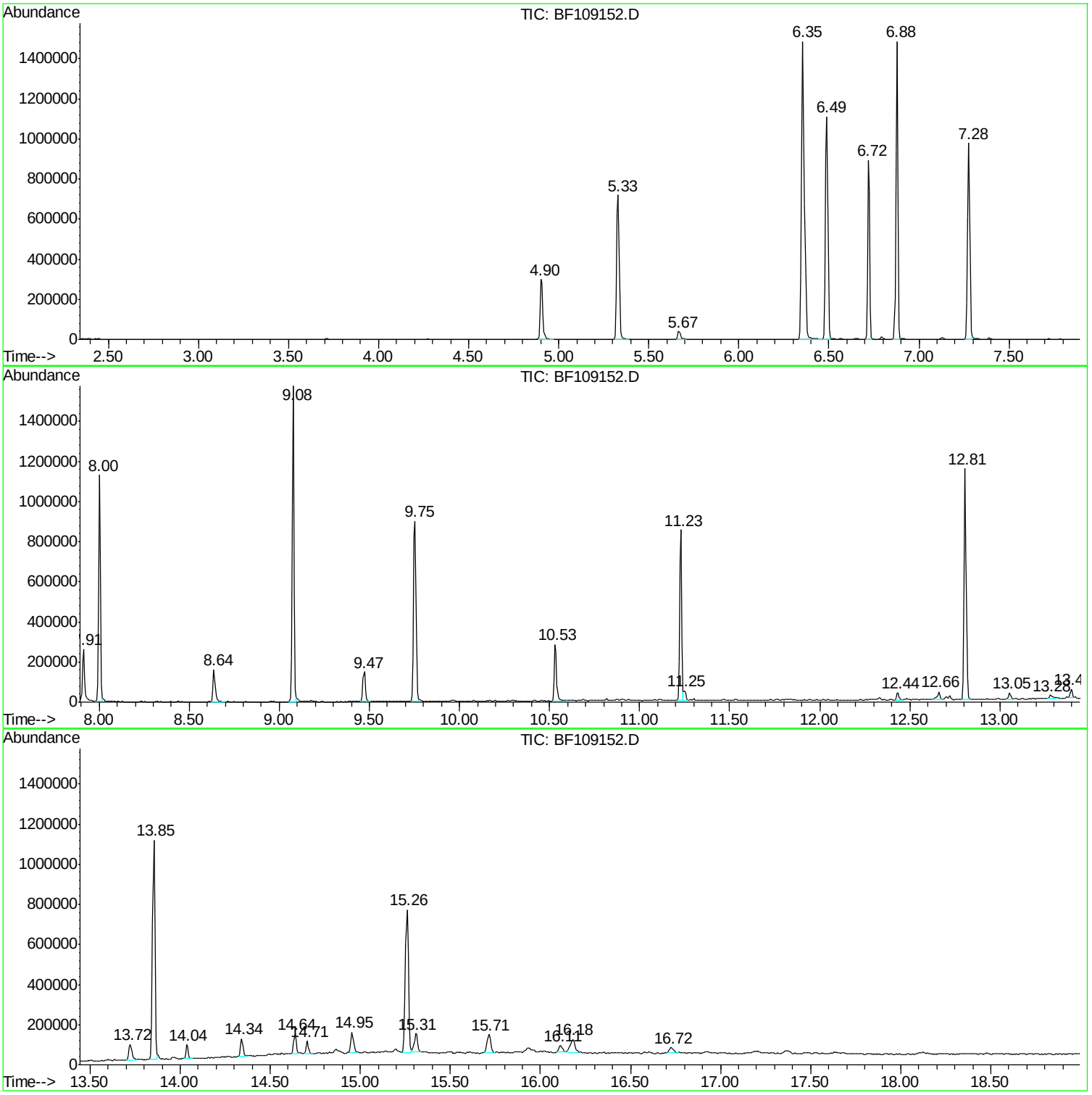
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

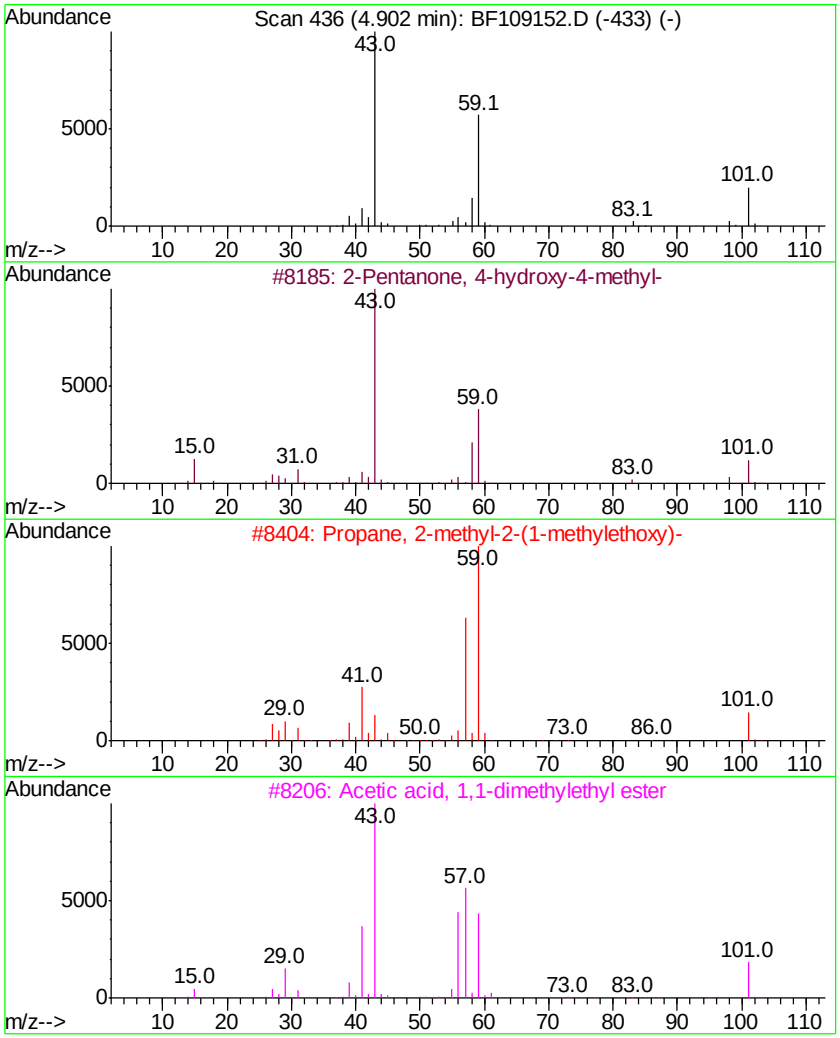
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

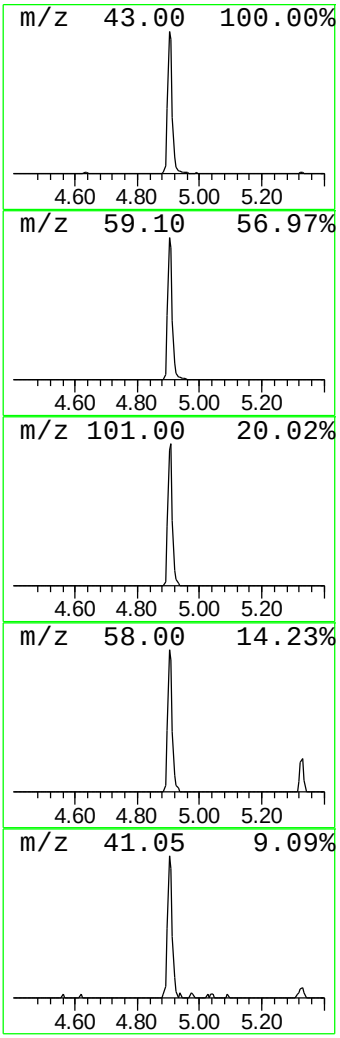
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	8.72 ng	323682	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

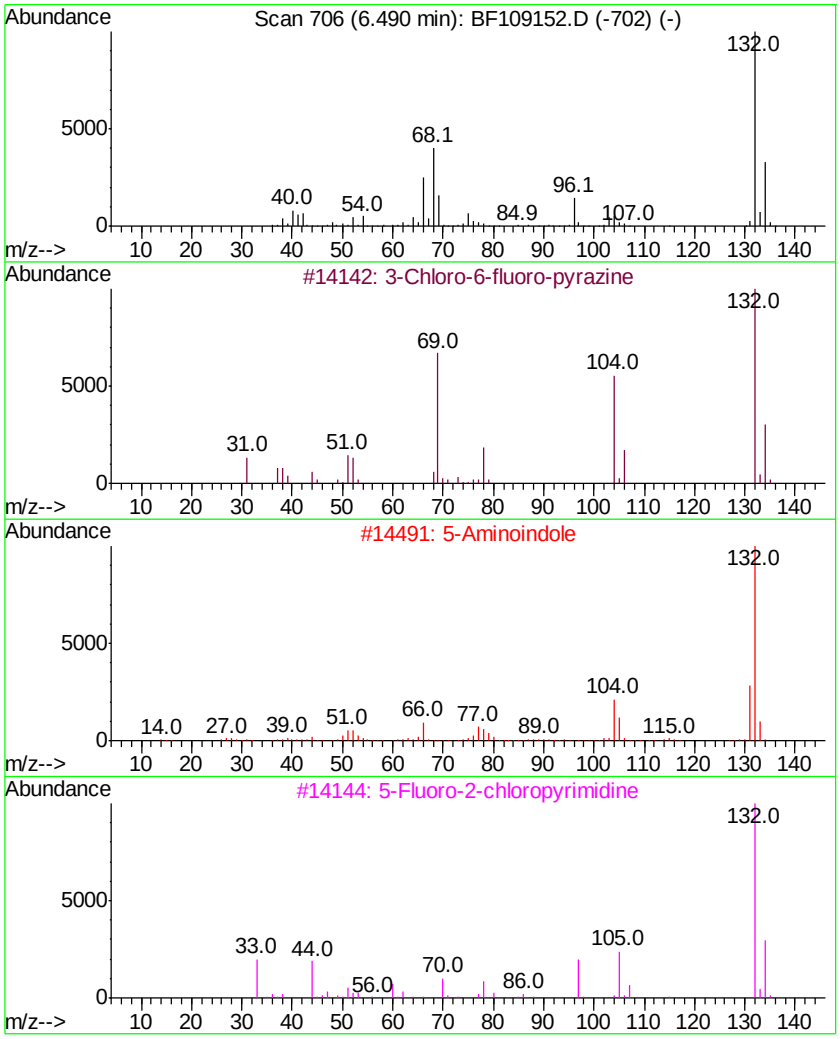
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

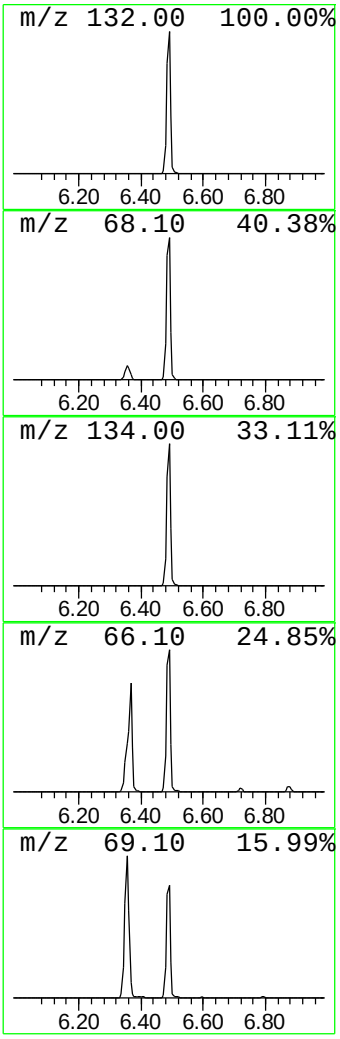
****

Peak Number 2 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	26.43 ng	981594	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

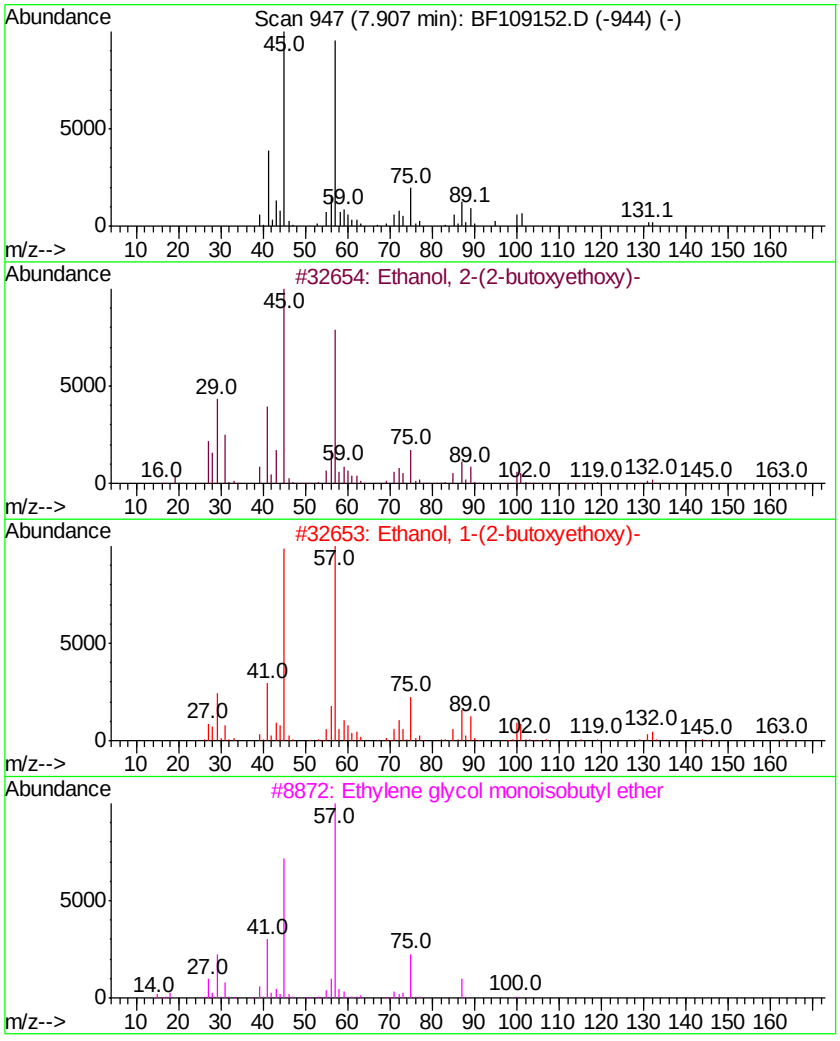
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

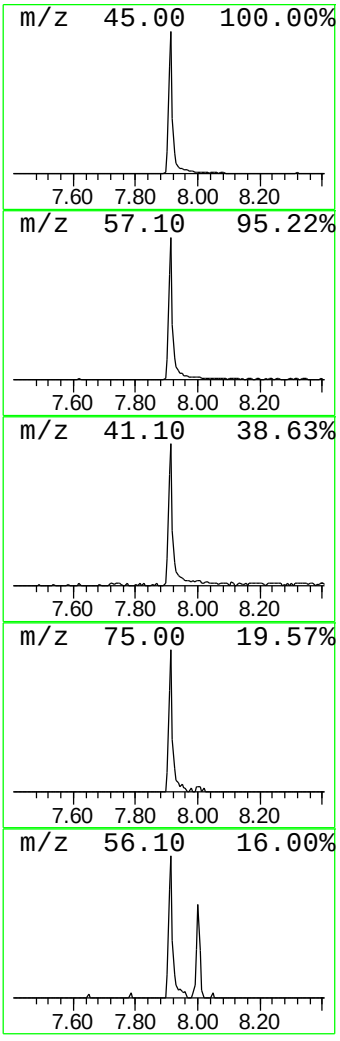
****

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.91	5.91 ng	258045	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5	Di-sec-butyl ether	130	C8H18O	006863-58-7	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

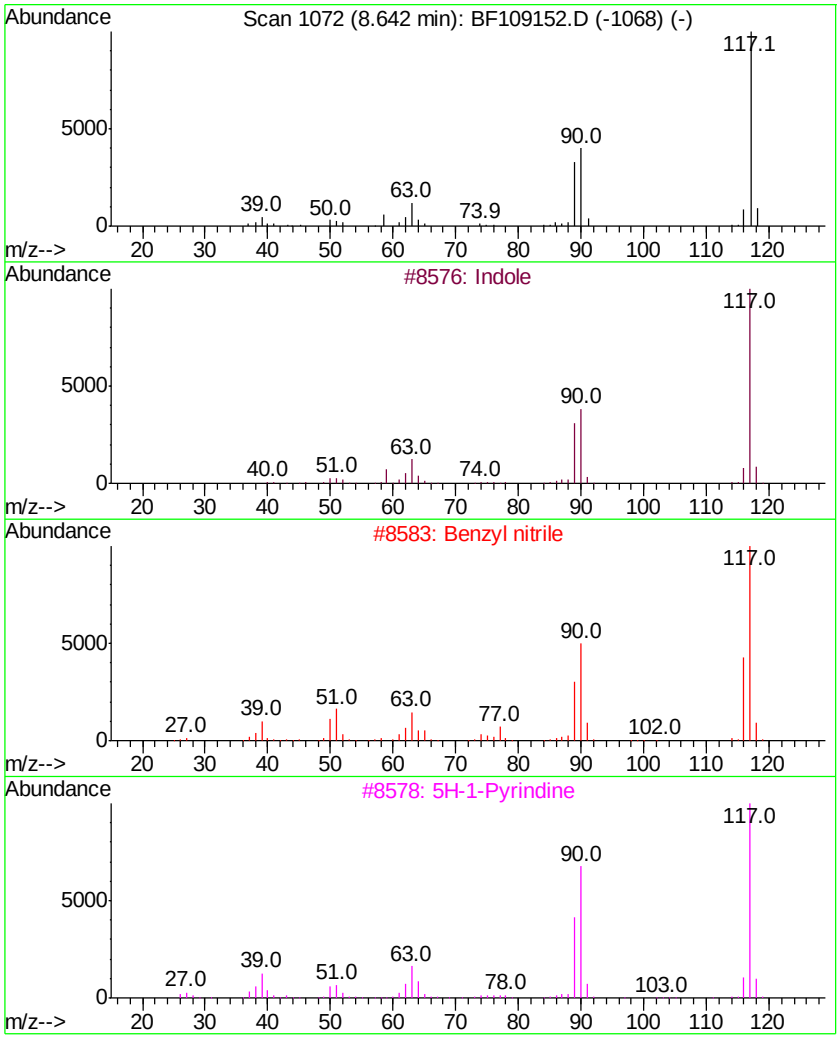
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

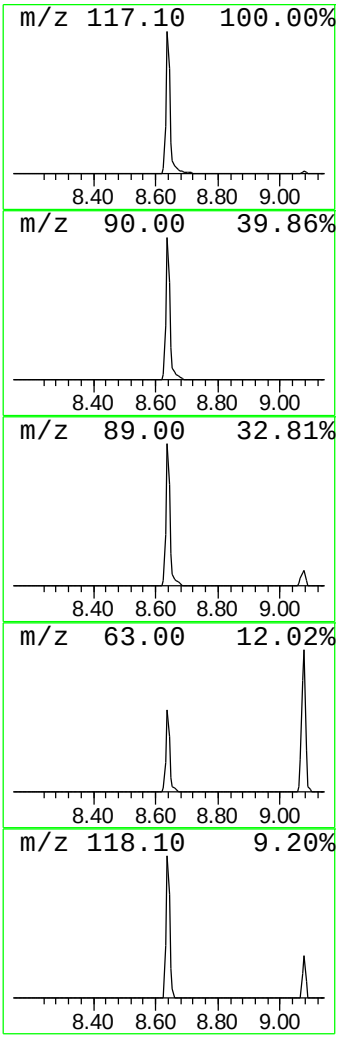
****

Peak Number 5 Indole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.64	3.26 ng	142487	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole	117	C8H7N	000120-72-9	97
2	Benzyl nitrile	117	C8H7N	000140-29-4	91
3	5H-1-Pyrindine	117	C8H7N	000270-91-7	91
4	Indolizine	117	C8H7N	000274-40-8	90
5	Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

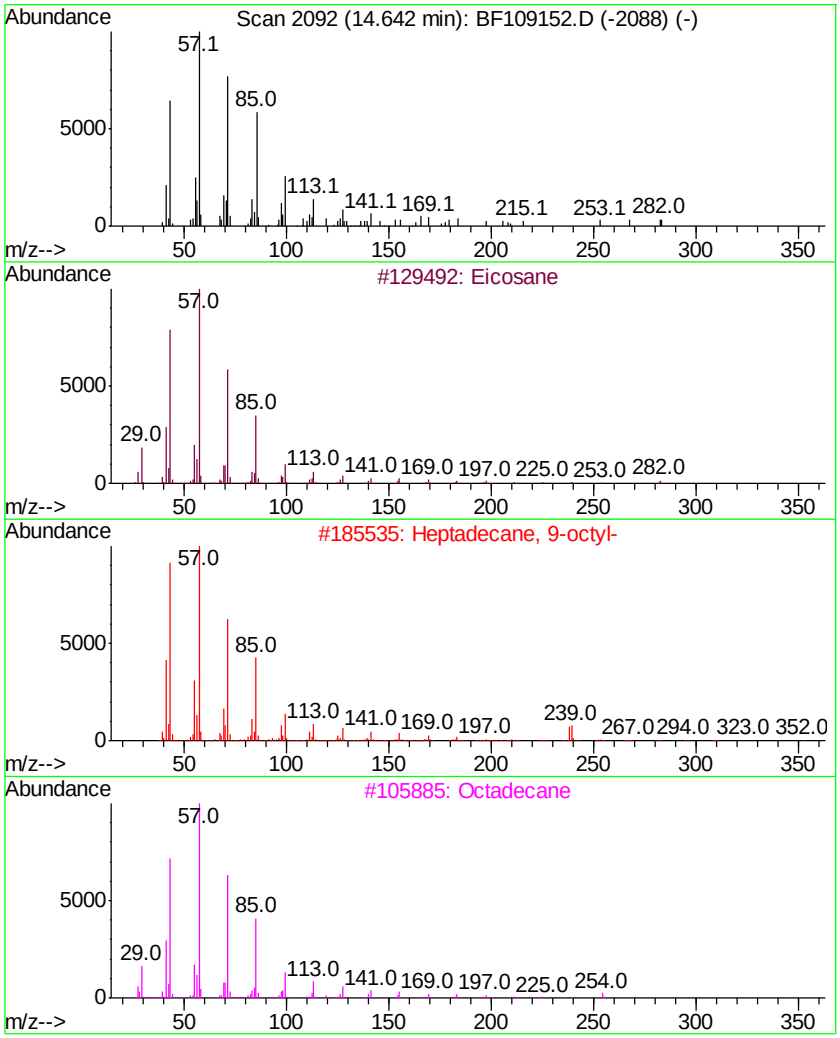
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

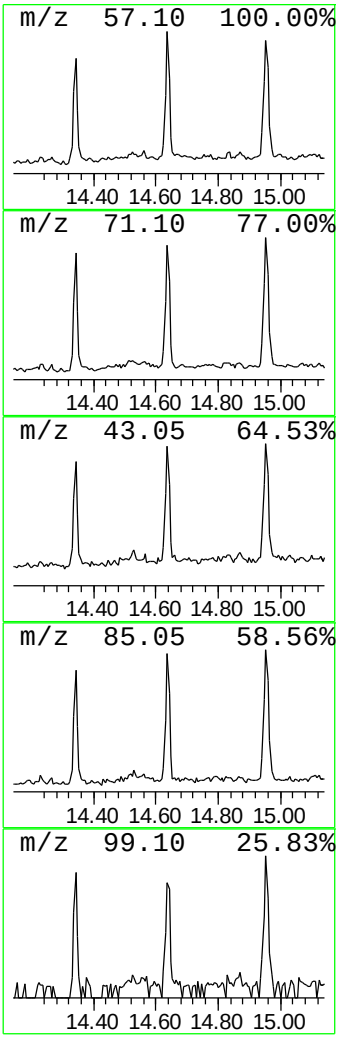
****

Peak Number 6 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.16 ng	87169	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Octadecane	254	C18H38	000593-45-3	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Triacontane	422	C30H62	000638-68-6	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

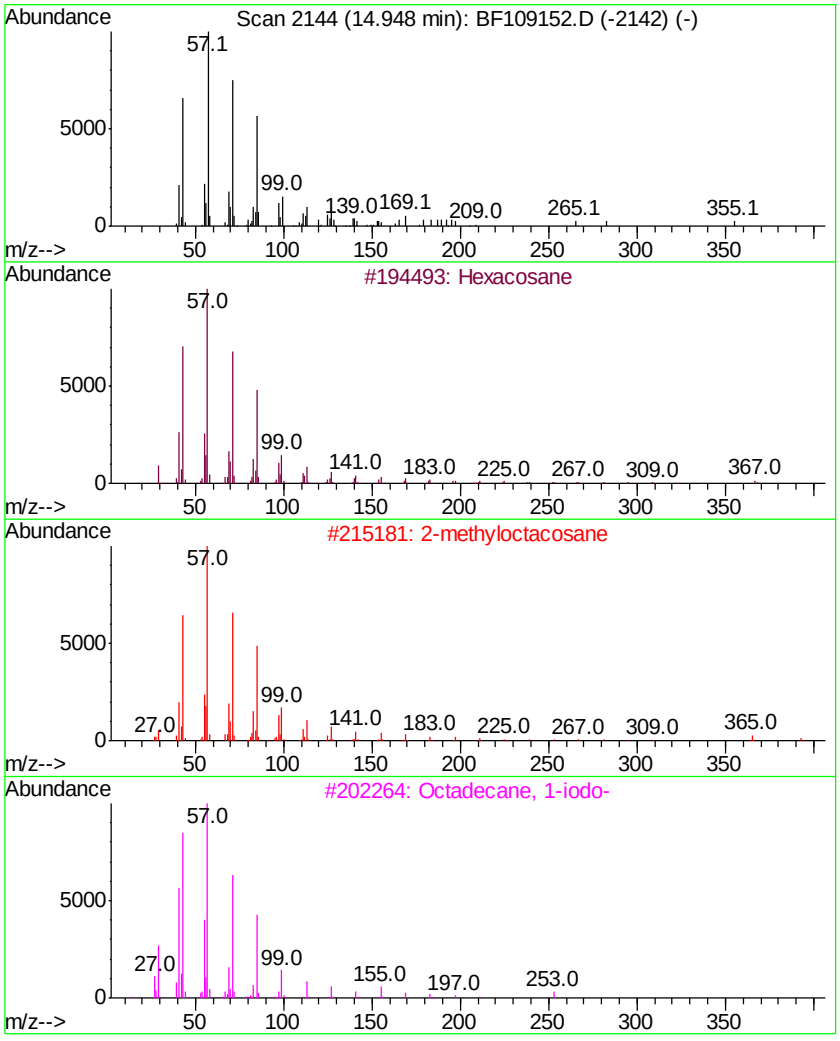
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

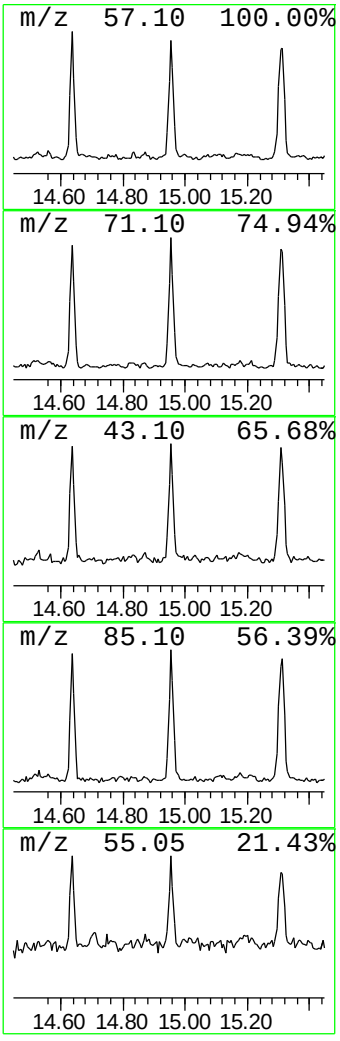
****

Peak Number 7 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.56 ng	103374	Perylene-d12	15.26

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	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Heneicosane	296	C21H44	000629-94-7	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

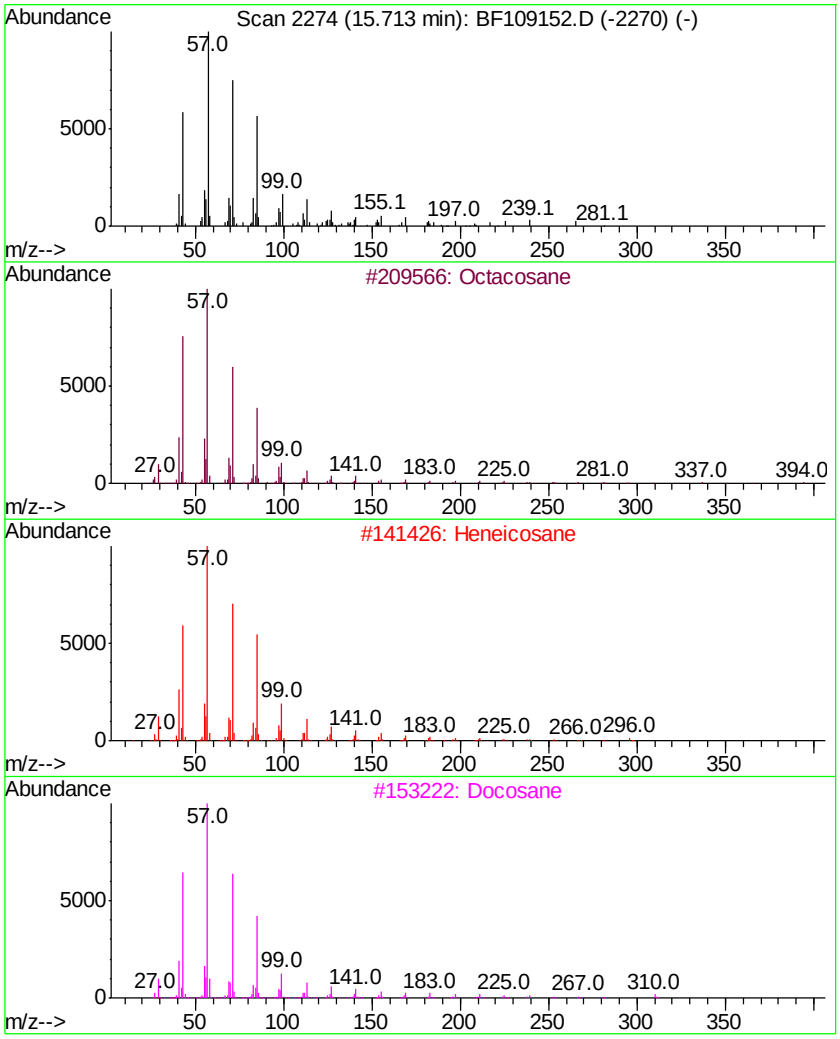
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

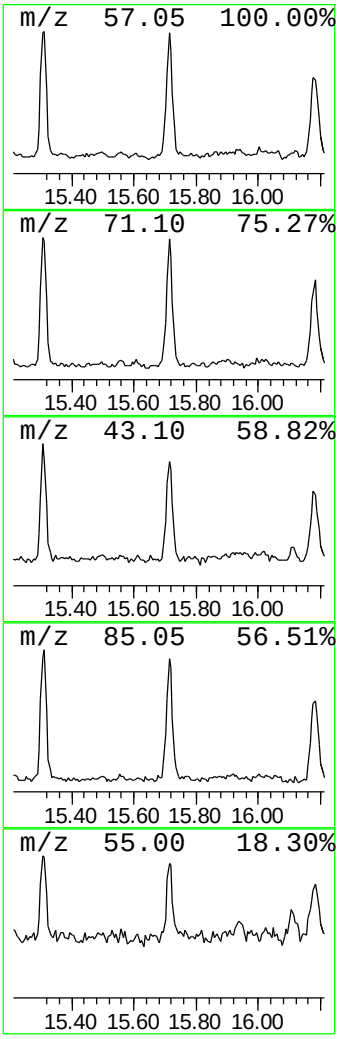
****

Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.94 ng	118713	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Docosane	310	C22H46	000629-97-0	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Hexacosane	366	C26H54	000630-01-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091918\
Data File : BF109152.D
Acq On : 19 Sep 2018 19:09
Operator : JU/SJ
Sample : J4975-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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...	4.90	8.7	ng	323682	1	6.72	742680	20.0
unknown6.49	6.49	26.4	ng	981594	1	6.72	742680	20.0
Ethanol, 2-(2-but...	7.91	5.9	ng	258045	2	8.00	873571	20.0
Indole	8.64	3.3	ng	142487	2	8.00	873571	20.0
Eicosane	14.64	2.2	ng	87169	6	15.26	806343	20.0
Hexacosane	14.95	2.6	ng	103374	6	15.26	806343	20.0
Octacosane	15.71	2.9	ng	118713	6	15.26	806343	20.0