LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100791.D
Acq On : 21 Nov 2017 20:07
Operator : SJ/JU
Sample : I6499-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PG1-2-E(7-8)

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	5.110	510	514	525	rBB	106407	148093	6.56%	0.791%
2	5.498	574	580	583	rBV	1979892	2014461	89.30%	10.765%
3	6.504	745	751	755	rBV	1859770	2085383	92.45%	11.144%
4	6.645	770	775	778	rBV	2171235	2069763	91.75%	11.061%
5	6.869	810	813	817	rVB	491908	442116	19.60%	2.363%
6	7.028	836	840	843	rBV	1798122	1621356	71.87%	8.665%
7	7.433	904	909	912	rBV	1186027	1295104	57.41%	6.921%
8	7.516	918	923	931	rVB	37262	42875	1.90%	0.229%
9	8.151	1027	1031	1035	rBV	685344	575153	25.50%	3.074%
10	9.227	1209	1214	1217	rBV	2454978	2255809	100.00%	12.055%
11	9.616	1277	1280	1283	rBV	171209	146227	6.48%	0.781%
12	9.827	1313	1316	1319	rBV	72040	60363	2.68%	0.323%
13	9.863	1319	1322	1326	rBV	24697	25108	1.11%	0.134%
14	9.910	1326	1330	1333	rVV	678784	613219	27.18%	3.277%
15	10.327	1399	1401	1404	rVB	81612	66499	2.95%	0.355%
16	10.551	1433	1439	1441	rBV	24269	29119	1.29%	0.156%
17	10.698	1460	1464	1467	rBV	1337016	1183429	52.46%	6.324%
18	10.804	1479	1482	1492	rVB	85617	87694	3.89%	0.469%
19	11.251	1554	1558	1560	rBV	60566	45209	2.00%	0.242%
20	11.392	1578	1582	1585	rBV	645286	572522	25.38%	3.060%
21	11.416	1585	1586	1589	rVB	74043	44781	1.99%	0.239%
22	11.910	1664	1670	1679	rBV3	98795	100882	4.47%	0.539%
23	12.604	1785	1788	1792	rBV	118629	95097	4.22%	0.508%
24	12.698	1801	1804	1808	rBV2	27291	29593	1.31%	0.158%
25	12.833	1822	1827	1831	rBV	99271	92658	4.11%	0.495%
26	12.980	1847	1852	1855	rBV	1546570	1493104	66.19%	7.979%
27	13.857	1998	2001	2011	rVB3	123062	149404	6.62%	0.798%
28	14.033	2026	2031	2033	rBV	483793	466291	20.67%	2.492%
29	14.057	2033	2035	2041	rVB	52721	48095	2.13%	0.257%
30	15.068	2203	2207	2210	rBV	62178	85423	3.79%	0.457%
31	15.098	2210	2212	2215	rVB	28573	26307	1.17%	0.141%
32	15.374	2256	2259	2265	rVB	33424	44775	1.98%	0.239%
33	15.439	2266	2270	2275	rVB	49091	60180	2.67%	0.322%
34	15.504	2276	2281	2292	rBV	383334	517582	22.94%	2.766%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100791.D
Acq On : 21 Nov 2017 20:07
Operator : SJ/JU
Sample : I6499-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PG1-2-E(7-8)

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.974	2527	2531	2539	rVB3	22858	42742	1.89%	0.228%
36	17.427	2602	2608	2615	rBV	17197	36077	1.60%	0.193%

Sum of corrected areas: 18712493

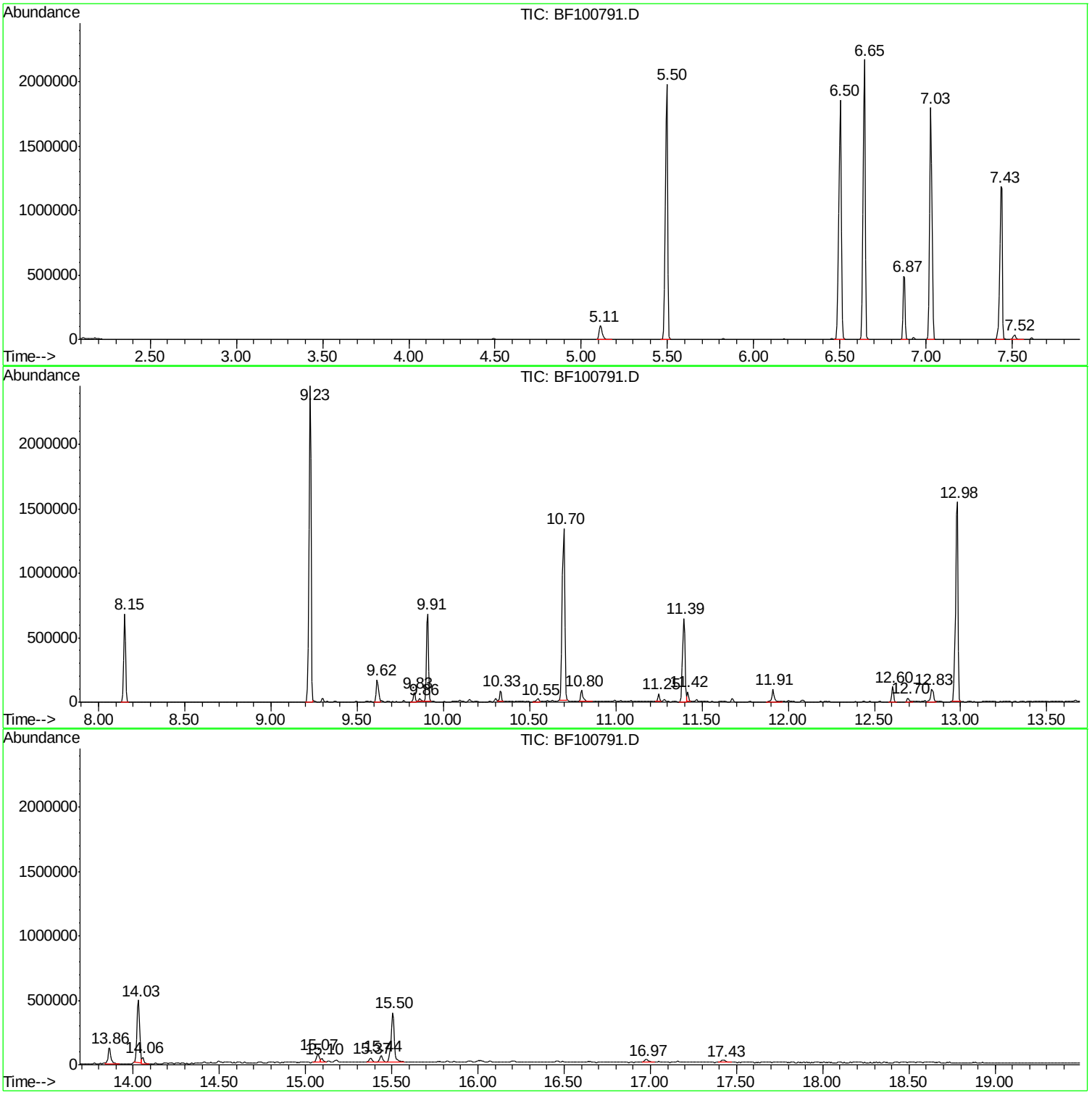
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100791.D
Acq On : 21 Nov 2017 20:07
Operator : SJ/JU
Sample : I6499-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PG1-2-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100791.D
Acq On : 21 Nov 2017 20:07
Operator : SJ/JU
Sample : I6499-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PG1-2-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

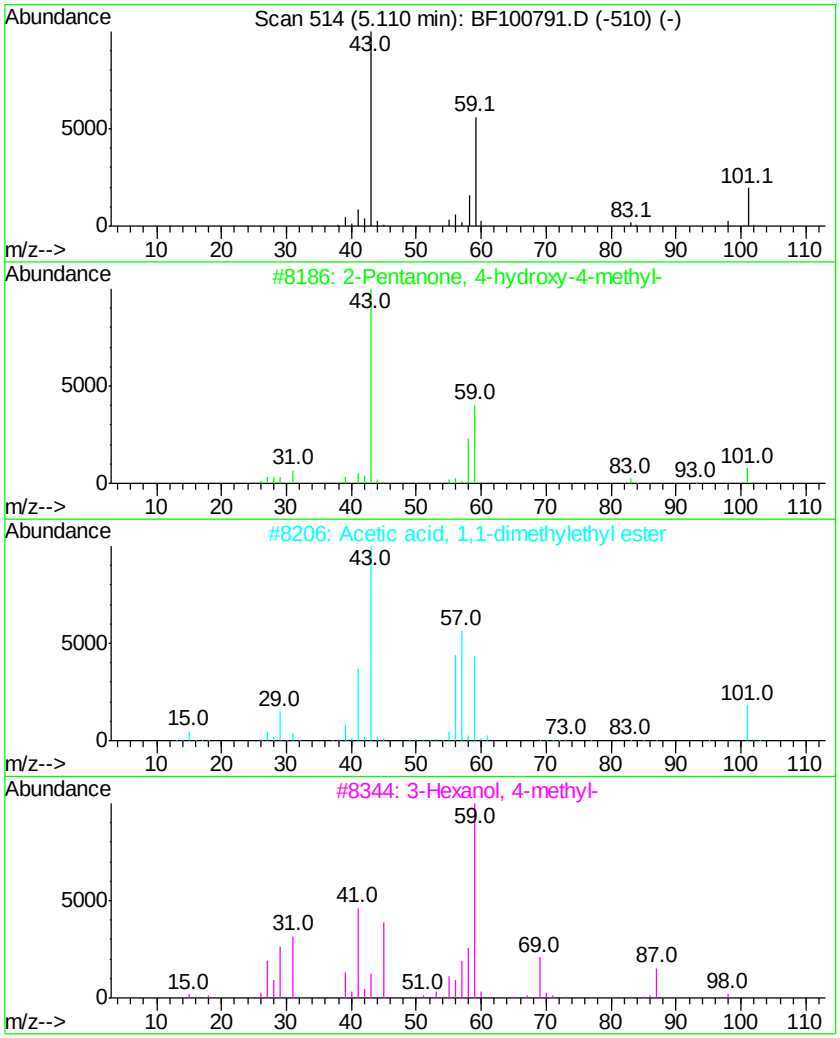
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

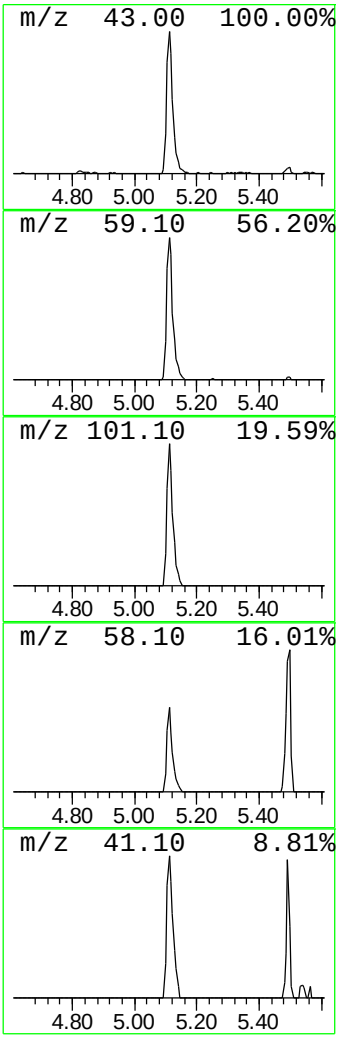
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	6.70 ng	148093	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100791.D
Acq On : 21 Nov 2017 20:07
Operator : SJ/JU
Sample : I6499-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PG1-2-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

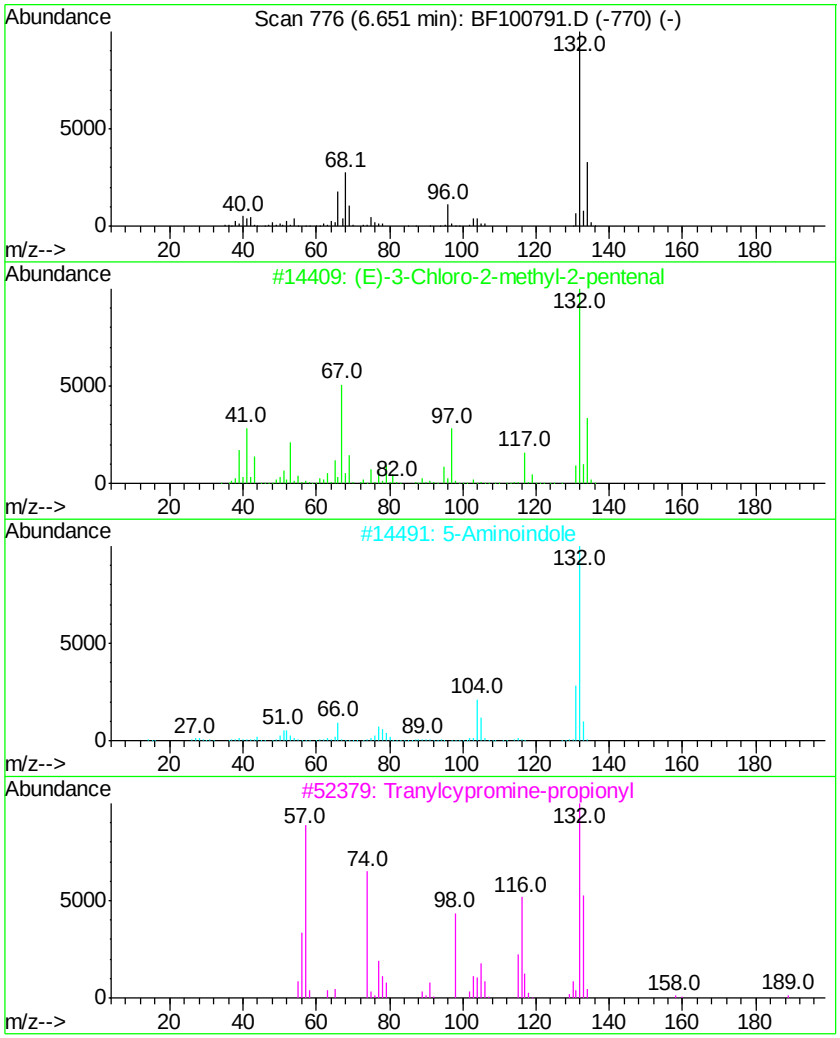
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

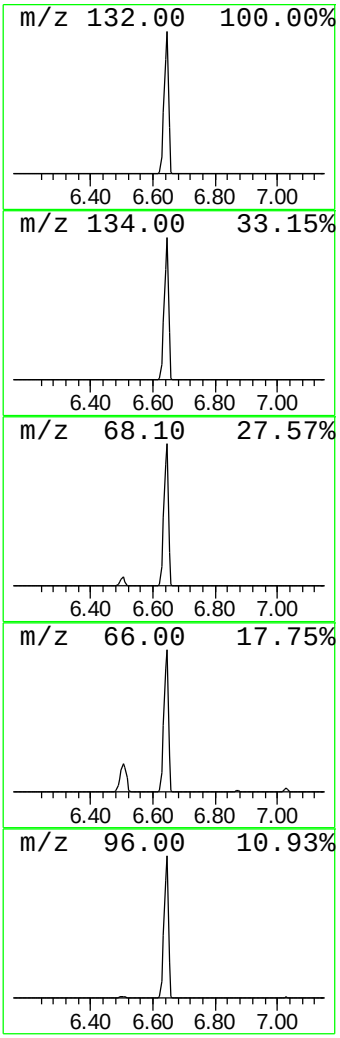
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	93.63 ng	2069760	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100791.D
Acq On : 21 Nov 2017 20:07
Operator : SJ/JU
Sample : I6499-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PG1-2-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

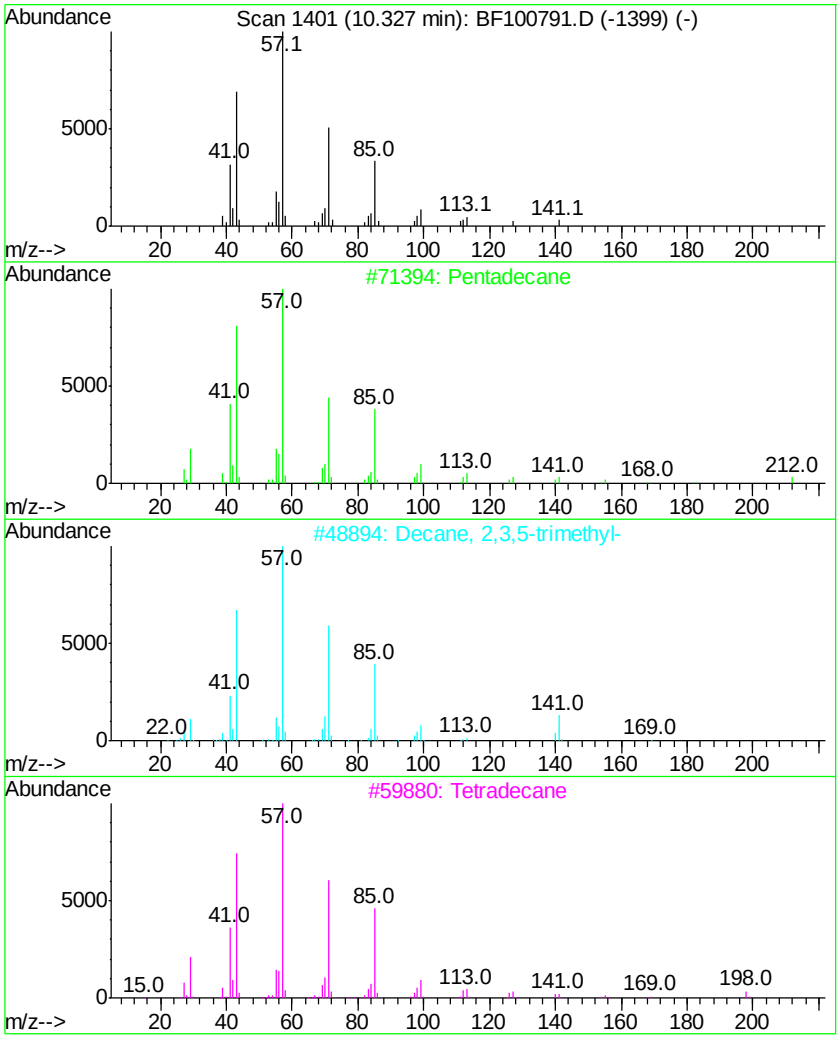
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

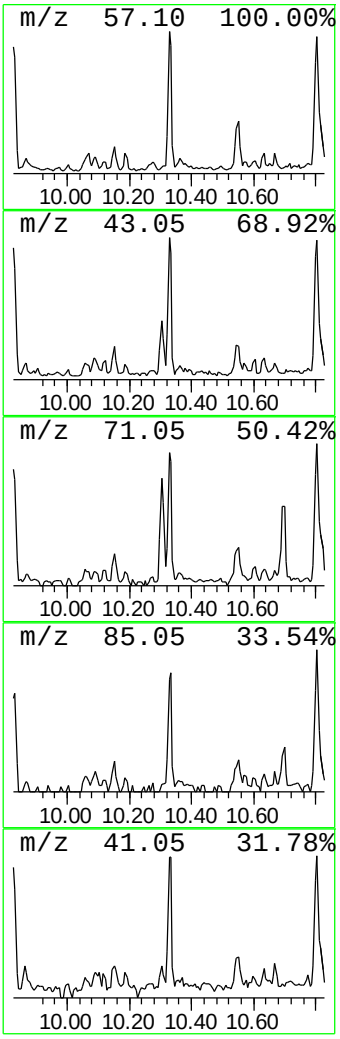
****

Peak Number 4 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.17 ng	66499	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
3	Tetradecane	198	C14H30	000629-59-4	90
4	Tridecane	184	C13H28	000629-50-5	90
5	Hexadecane	226	C16H34	000544-76-3	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100791.D
Acq On : 21 Nov 2017 20:07
Operator : SJ/JU
Sample : I6499-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PG1-2-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

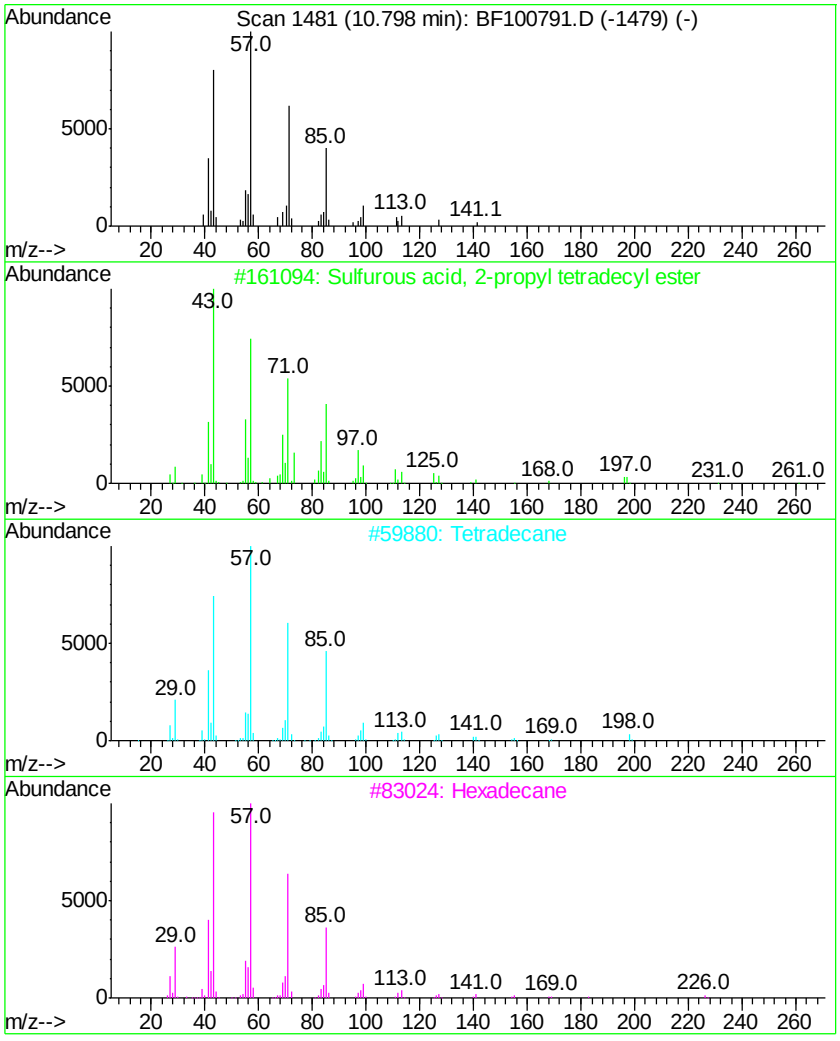
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

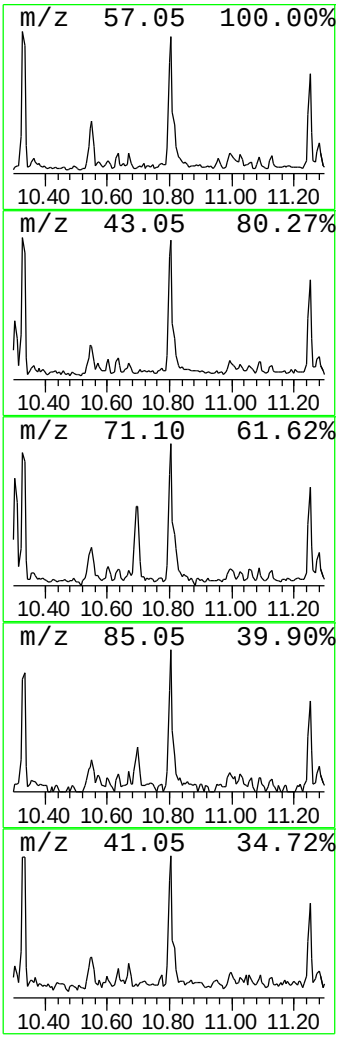
****

Peak Number 5 Sulfurous acid, 2-propyl te... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	3.06 ng	87694	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100791.D
Acq On : 21 Nov 2017 20:07
Operator : SJ/JU
Sample : I6499-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PG1-2-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

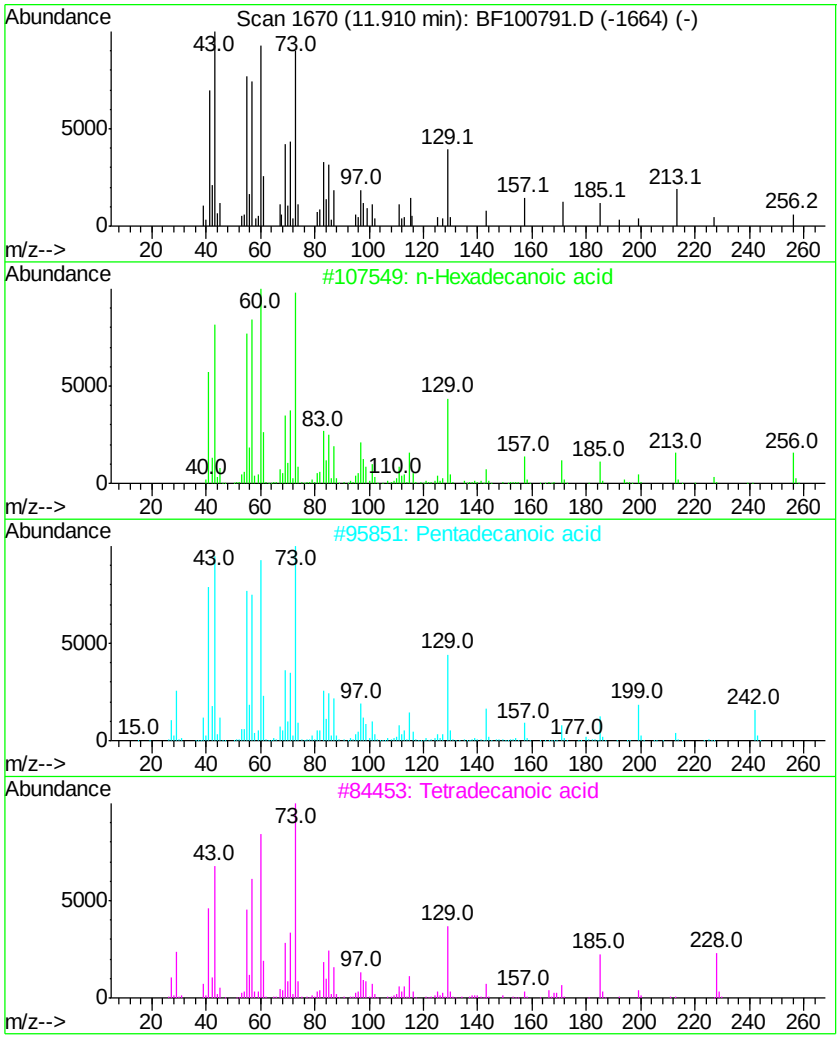
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

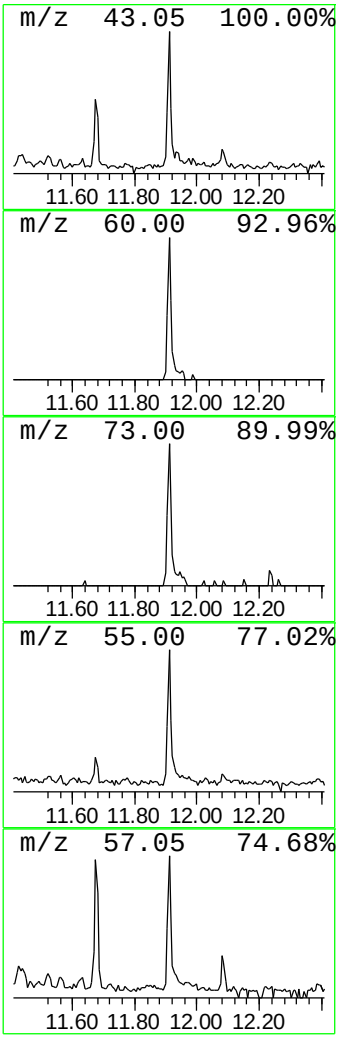
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	3.52 ng	100882	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Tridecane	184	C13H28	000629-50-5	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100791.D
Acq On : 21 Nov 2017 20:07
Operator : SJ/JU
Sample : I6499-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PG1-2-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

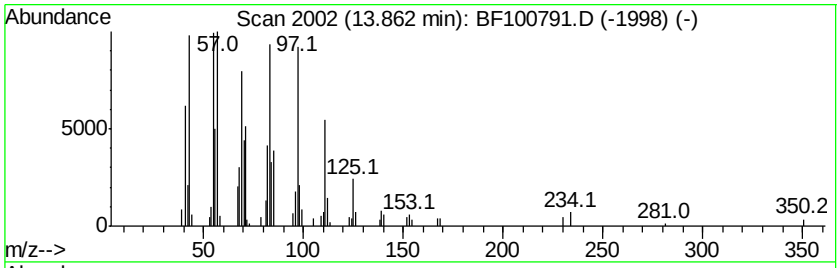
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

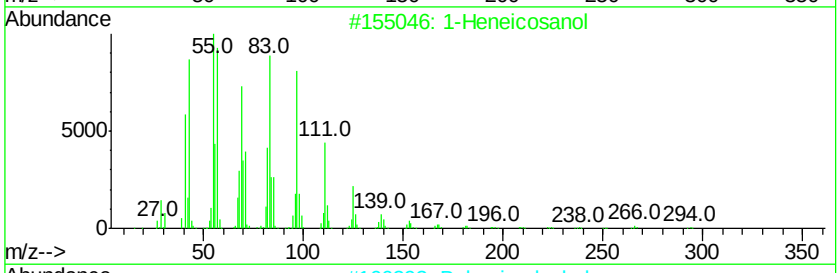
****

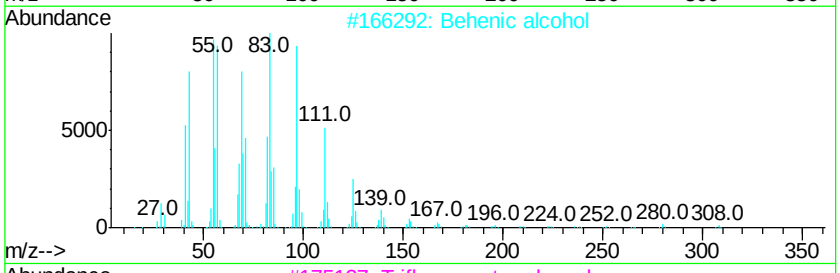
Peak Number 7 1-Heneicosanol Concentration Rank 4

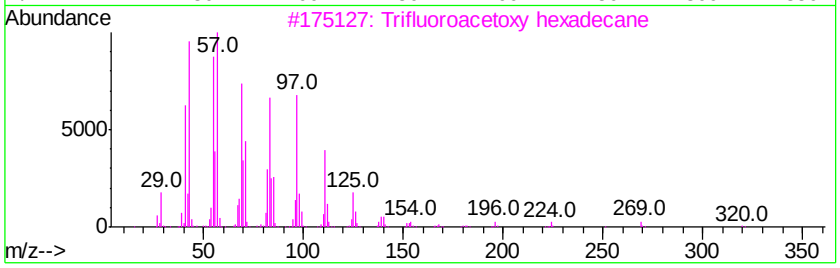
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	6.41 ng	149404	Chrysene-d12	14.03

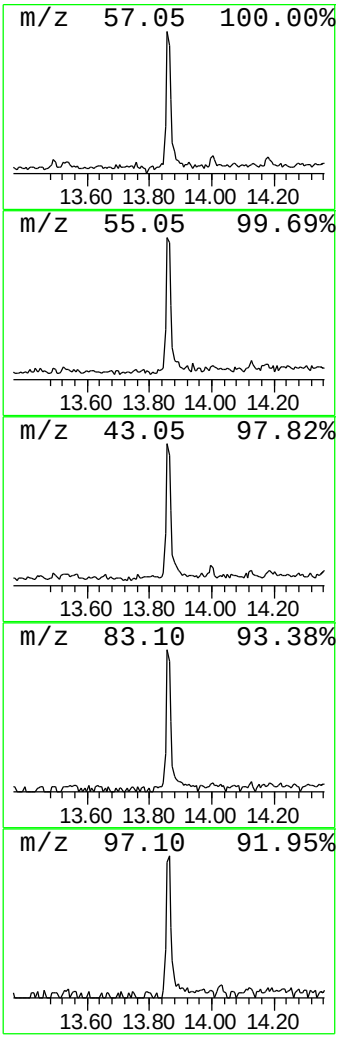
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94











Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
Data File : BF100791.D
Acq On : 21 Nov 2017 20:07
Operator : SJ/JU
Sample : I6499-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PG1-2-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.11	6.7	ng	148093	1	6.87	442116	20.0
unknown6.65	6.65	93.6	ng	2069760	1	6.87	442116	20.0
Pentadecane	10.33	2.2	ng	66499	3	9.91	613219	20.0
Sulfurous acid, 2...	10.80	3.1	ng	87694	4	11.39	572522	20.0
n-Hexadecanoic acid	11.91	3.5	ng	100882	4	11.39	572522	20.0
1-Heneicosanol	13.86	6.4	ng	149404	5	14.03	466291	20.0