LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
Data File : BF097126.D
Acq On : 27 Jul 2017 16:56
Operator : SJ/JU
Sample : PB101001BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB101001BL

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-BF072517.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	4.645	464	469	480	rBV	318728	476156	16.97%	2.208%
2	5.098	541	546	563	rBV	2182579	2380278	84.82%	11.039%
3	6.151	719	725	728	rBV	2185597	2499269	89.06%	11.591%
4	6.263	739	744	747	rBV	2333228	2293655	81.73%	10.637%
5	6.486	778	782	790	rBV	619359	530359	18.90%	2.460%
6	6.639	804	808	812	rBV	2053611	2036604	72.57%	9.445%
7	7.051	874	878	892	rBV	1531510	1657345	59.06%	7.686%
8	7.769	996	1000	1008	rBV	912410	783659	27.92%	3.634%
9	8.851	1178	1184	1187	rBV	2656999	2806359	100.00%	13.015%
10	9.516	1292	1297	1306	rVB	781553	762519	27.17%	3.536%
11	10.304	1426	1431	1441	rBV	1296240	1338669	47.70%	6.208%
12	10.986	1543	1547	1551	rBV	734274	630449	22.47%	2.924%
13	12.574	1812	1817	1820	rBV	2166320	2139513	76.24%	9.922%
14	13.610	1989	1993	1997	rBV	620316	538655	19.19%	2.498%
15	14.956	2218	2222	2227	rBV	358808	417369	14.87%	1.936%
16	15.009	2228	2231	2235	rVB	26172	34027	1.21%	0.158%
17	15.368	2288	2292	2296	rBV	32123	45212	1.61%	0.210%
18	15.998	2396	2399	2400	rBV3	23175	29279	1.04%	0.136%
19	16.845	2541	2543	2548	rVB6	27649	34295	1.22%	0.159%
20	17.150	2593	2595	2599	rBV4	24861	33788	1.20%	0.157%
21	17.621	2672	2675	2677	rBV3	32949	48873	1.74%	0.227%
22	18.886	2887	2890	2893	rBV4	29783	46028	1.64%	0.213%

Sum of corrected areas: 21562360

LSC Report - Integrated Chromatogram

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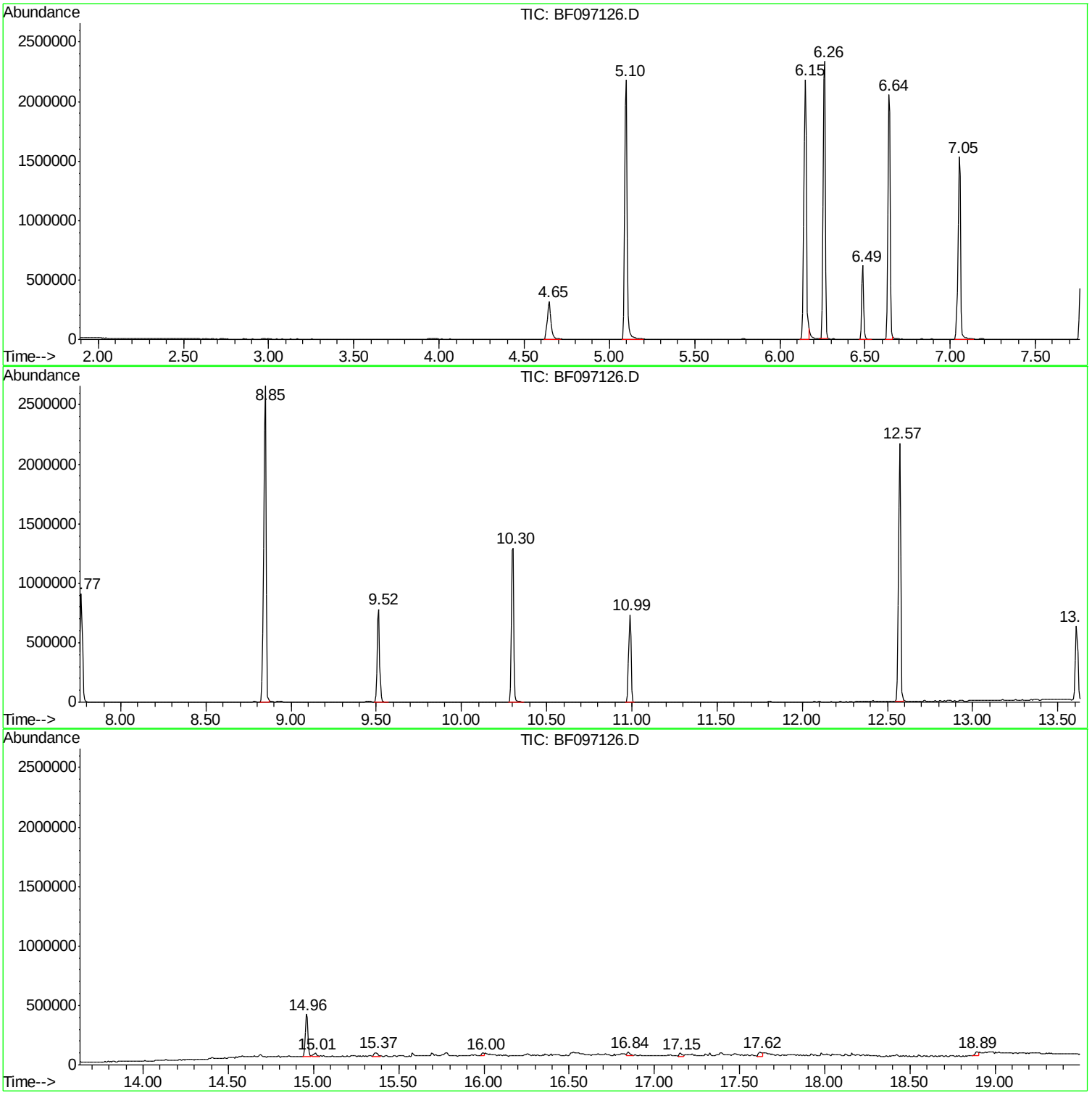
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB101001BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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

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Acq On : 27 Jul 2017 16:56
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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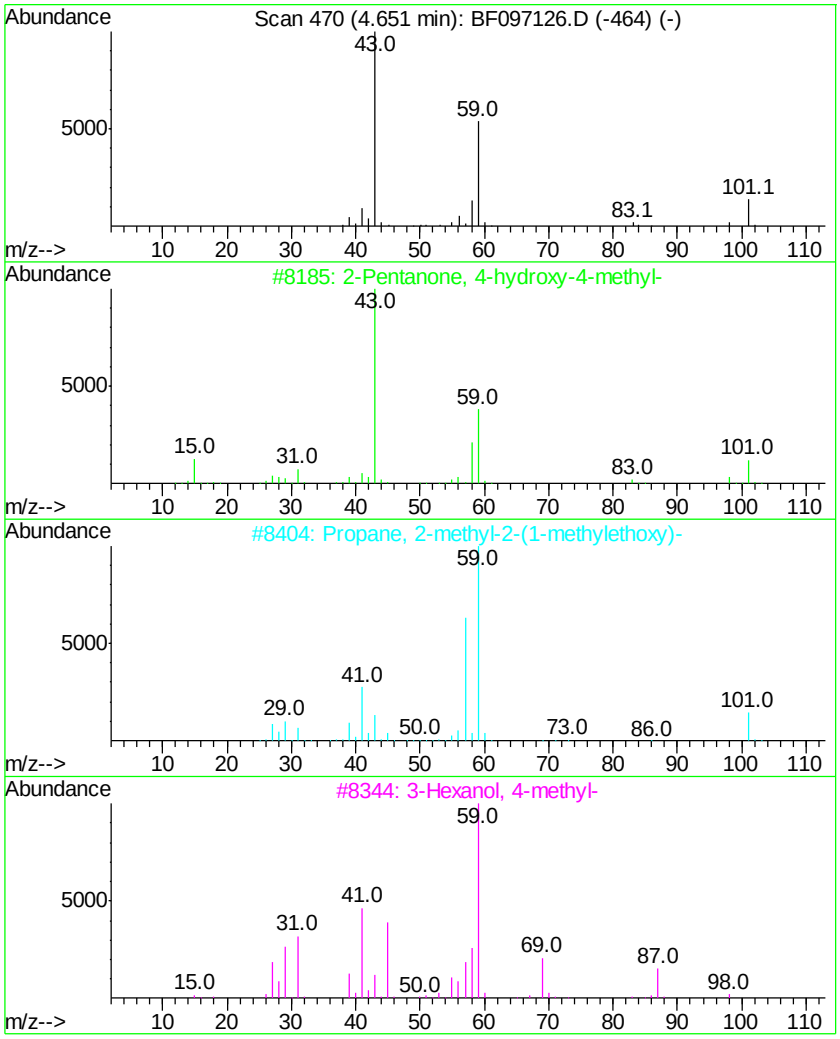
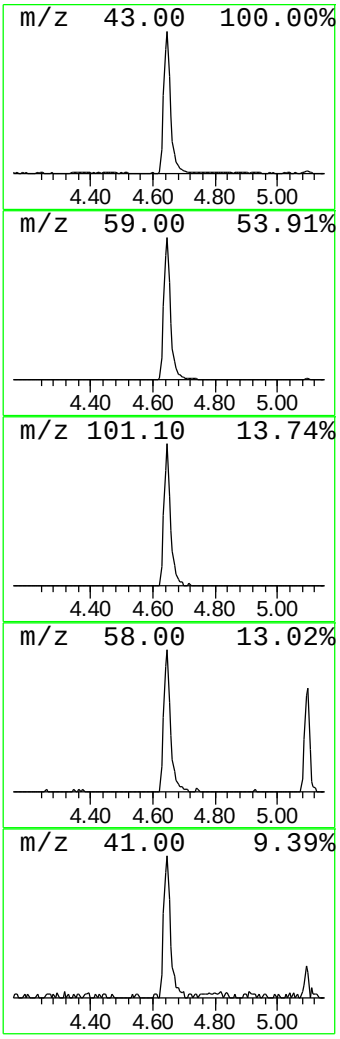
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	17.96 ng	476156	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Sample : PB101001BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB101001BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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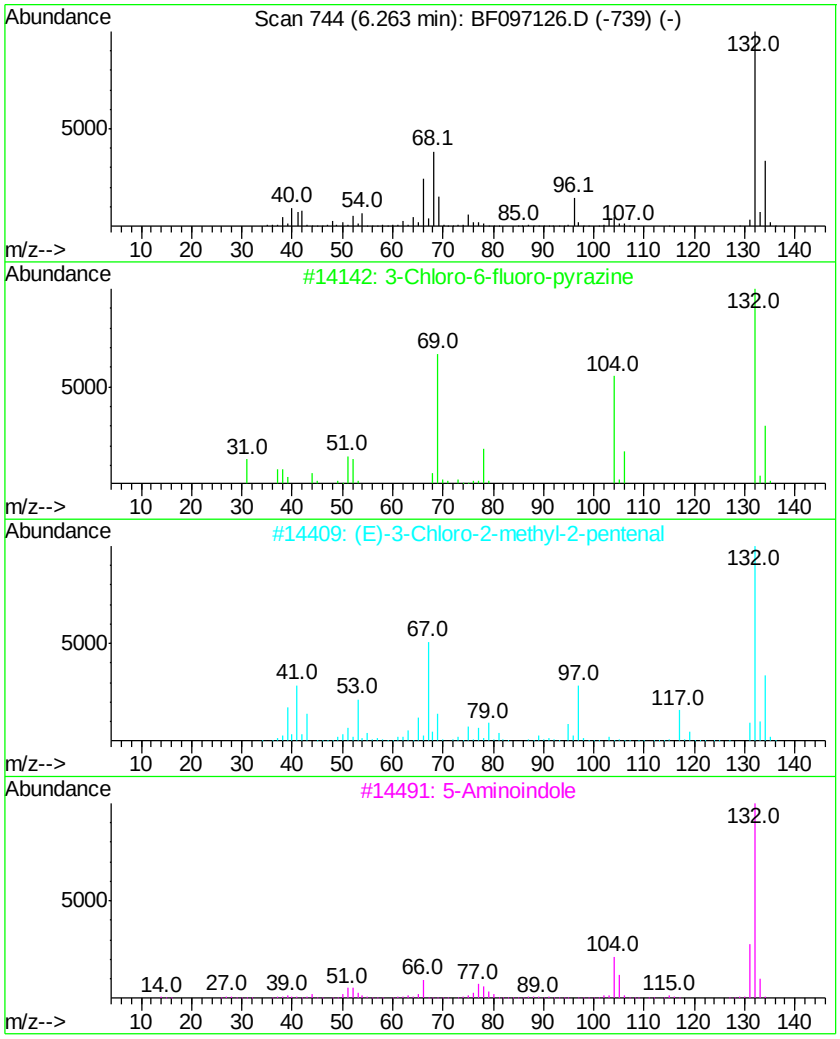
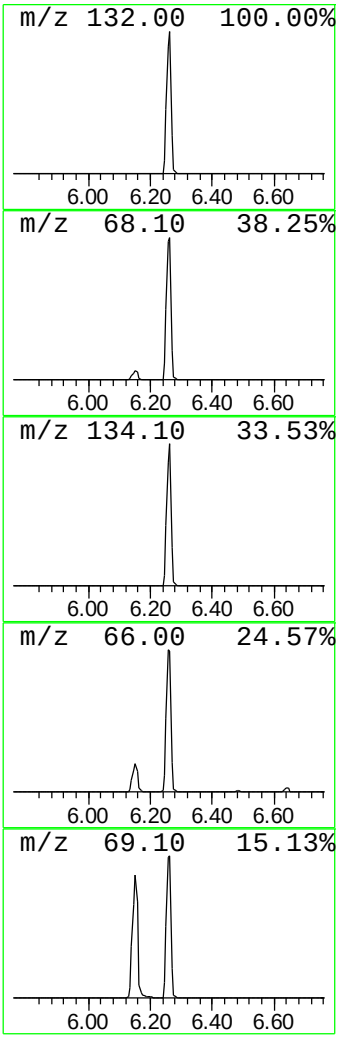
Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	86.49 ng	2293660	1,4-Dichlorobenzene-d4	6.49

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : PB101001BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB101001BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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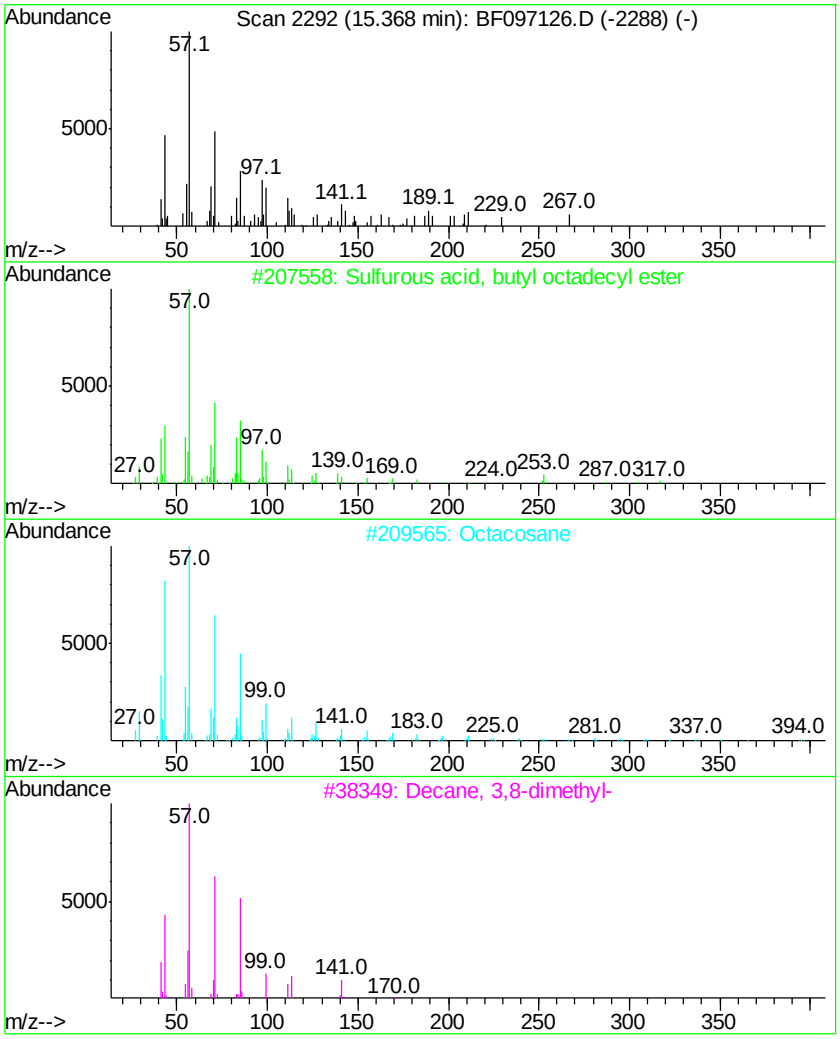
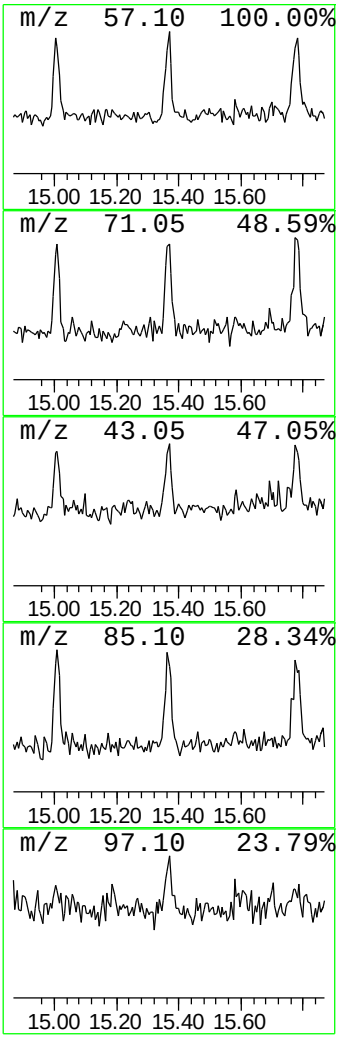
Peak Number 4 Sulfurous acid, butyl octad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	2.17 ng	45212	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	50
2	Octacosane	394	C28H58	000630-02-4	50
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	50
4	Tridecane, 3-methyl-	198	C14H30	006418-41-3	47
5	Heptacosane	380	C27H56	000593-49-7	47





Library Search Compound Report

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Sample : PB101001BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB101001BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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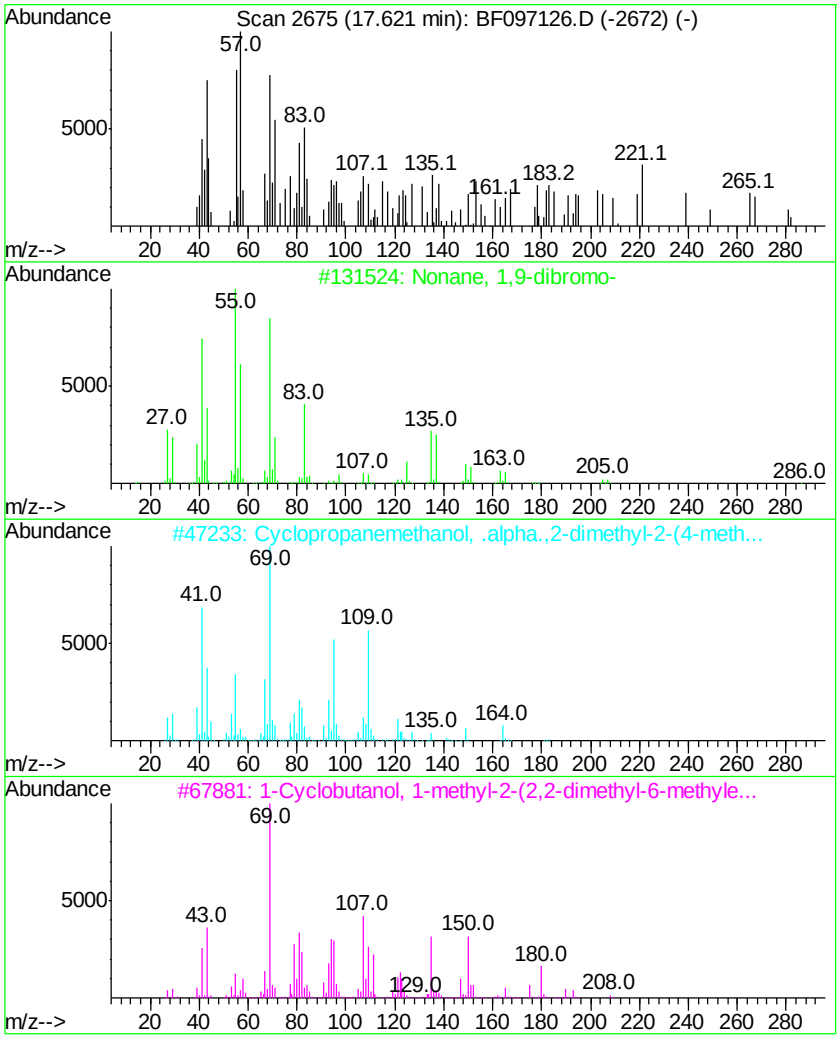
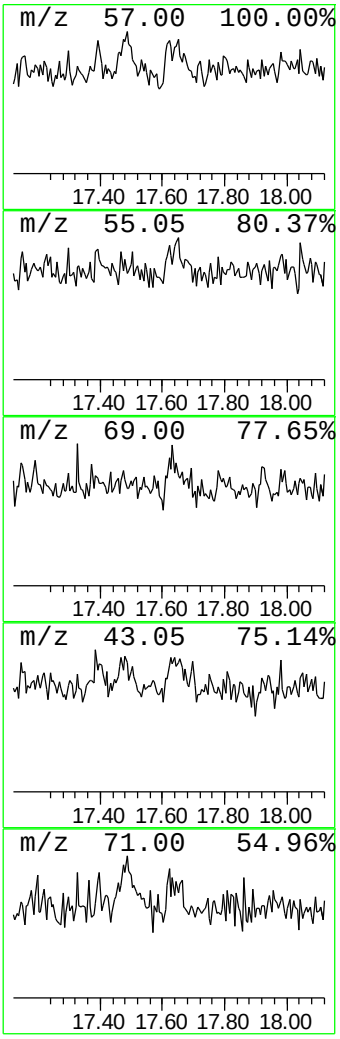
Peak Number 5 unknown17.62 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.62	2.34 ng	48873	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 1,9-dibromo-	284	C9H18Br2	004549-33-1	27
2	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	22
3	1-Cyclobutanol, 1-methyl-2-(2,2-...	208	C14H24O	1000197-21-8	22
4	Phosphetane, 1-chloro-2,2,3,4,4-...	194	C8H16ClOP	029276-11-7	22
5	2,6,11,15-Tetramethyl-hexadeca-2...	272	C20H32	038259-79-9	22





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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB101001BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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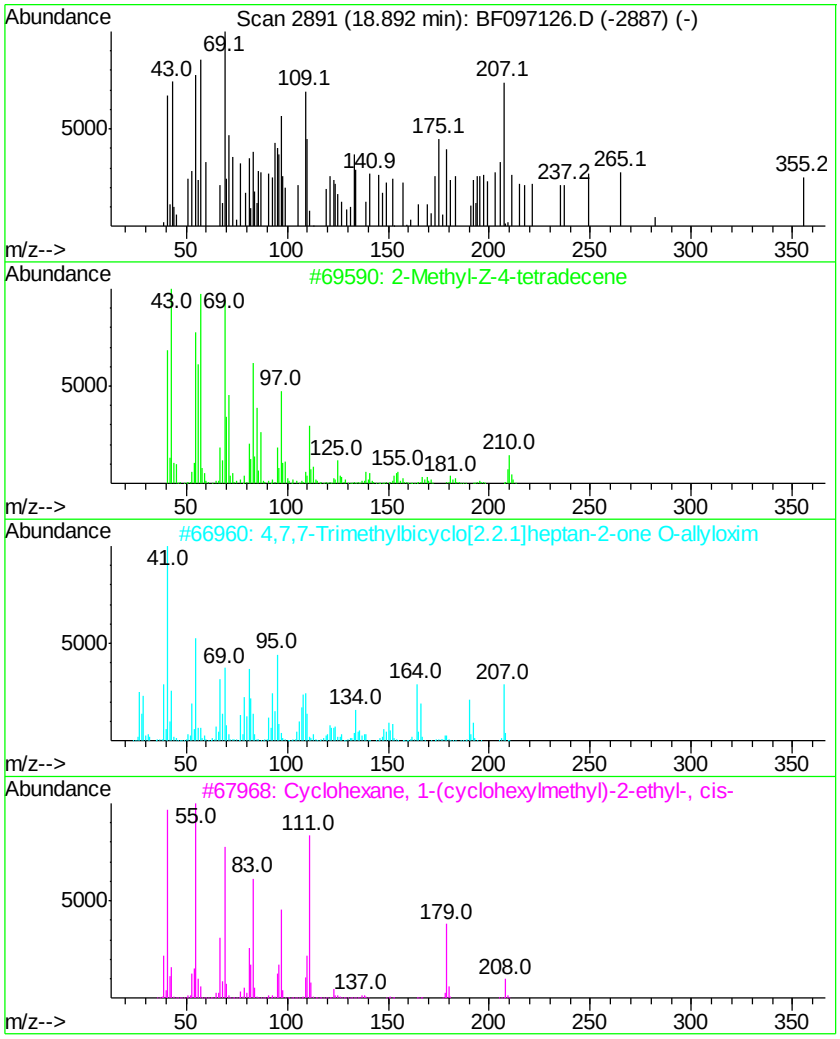
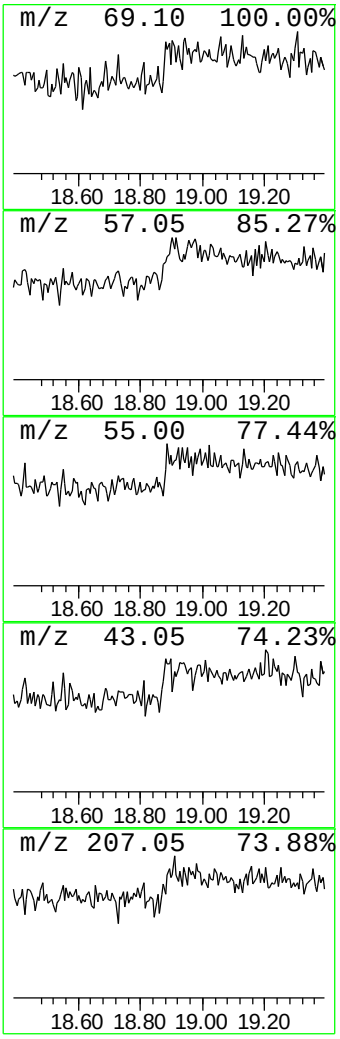
Peak Number 6 unknown18.89 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.89	2.21 ng	46028	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-Z-4-tetradecene	210	C15H30	1000130-78-3	41
2	4,7,7-Trimethylbicyclo[2.2.1]hep...	207	C13H21NO	1000210-89-8	27
3	Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-93-9	15
4	1,3-Cyclohexanedipropanoic acid,...	270	C14H22O5	1000137-90-0	11
5	5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	11





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.65	18.0	ng	476156	1	6.49	530359	20.0
unknown6.26	6.26	86.5	ng	2293660	1	6.49	530359	20.0
Sulfurous acid, b...	15.37	2.2	ng	45212	6	14.96	417369	20.0
unknown17.62	17.62	2.3	ng	48873	6	14.96	417369	20.0
unknown18.89	18.89	2.2	ng	46028	6	14.96	417369	20.0