LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098848.D
Acq On : 26 Sep 2017 22:41
Operator : SJ/JU
Sample : I5427-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-U-B

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-BF092317.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	2.204	15	20	26	rVB	281545	355309	7.69%	1.299%
2	5.134	514	518	528	rVB	228774	246708	5.34%	0.902%
3	5.528	581	585	588	rBV	1606676	1378966	29.84%	5.041%
4	6.528	751	755	758	rBV	1215007	950486	20.57%	3.474%
5	6.681	776	781	784	rBV	2795793	2416288	52.29%	8.832%
6	6.910	817	820	824	rBV	986356	832695	18.02%	3.044%
7	7.069	843	847	851	rBV	3280794	3131586	67.77%	11.447%
8	7.475	911	916	919	rBV	2386657	2626984	56.85%	9.603%
9	8.192	1034	1038	1042	rBV	1281295	1137902	24.62%	4.159%
10	9.274	1216	1222	1225	rBV	4522791	4620977	100.00%	16.891%
11	9.657	1284	1287	1290	rVB	95727	69279	1.50%	0.253%
12	9.951	1333	1337	1341	rBV	1469240	1213044	26.25%	4.434%
13	10.739	1466	1471	1474	rBV	1855660	1648535	35.68%	6.026%
14	11.439	1586	1590	1593	rBV	1229030	1105809	23.93%	4.042%
15	13.021	1854	1859	1863	rBV	3423034	3604133	78.00%	13.174%
16	14.074	2034	2038	2042	rVB	973213	808905	17.51%	2.957%
17	15.568	2286	2292	2300	rBV	597239	814187	17.62%	2.976%
18	16.027	2365	2370	2374	rBV	50523	71258	1.54%	0.260%
19	16.550	2453	2459	2465	rVB3	52492	99062	2.14%	0.362%
20	17.156	2557	2562	2568	rVB2	45053	80731	1.75%	0.295%
21	17.880	2679	2685	2695	rVB5	35117	86303	1.87%	0.315%
22	18.744	2825	2832	2839	rBV5	23637	58093	1.26%	0.212%

Sum of corrected areas: 27357240

LSC Report - Integrated Chromatogram

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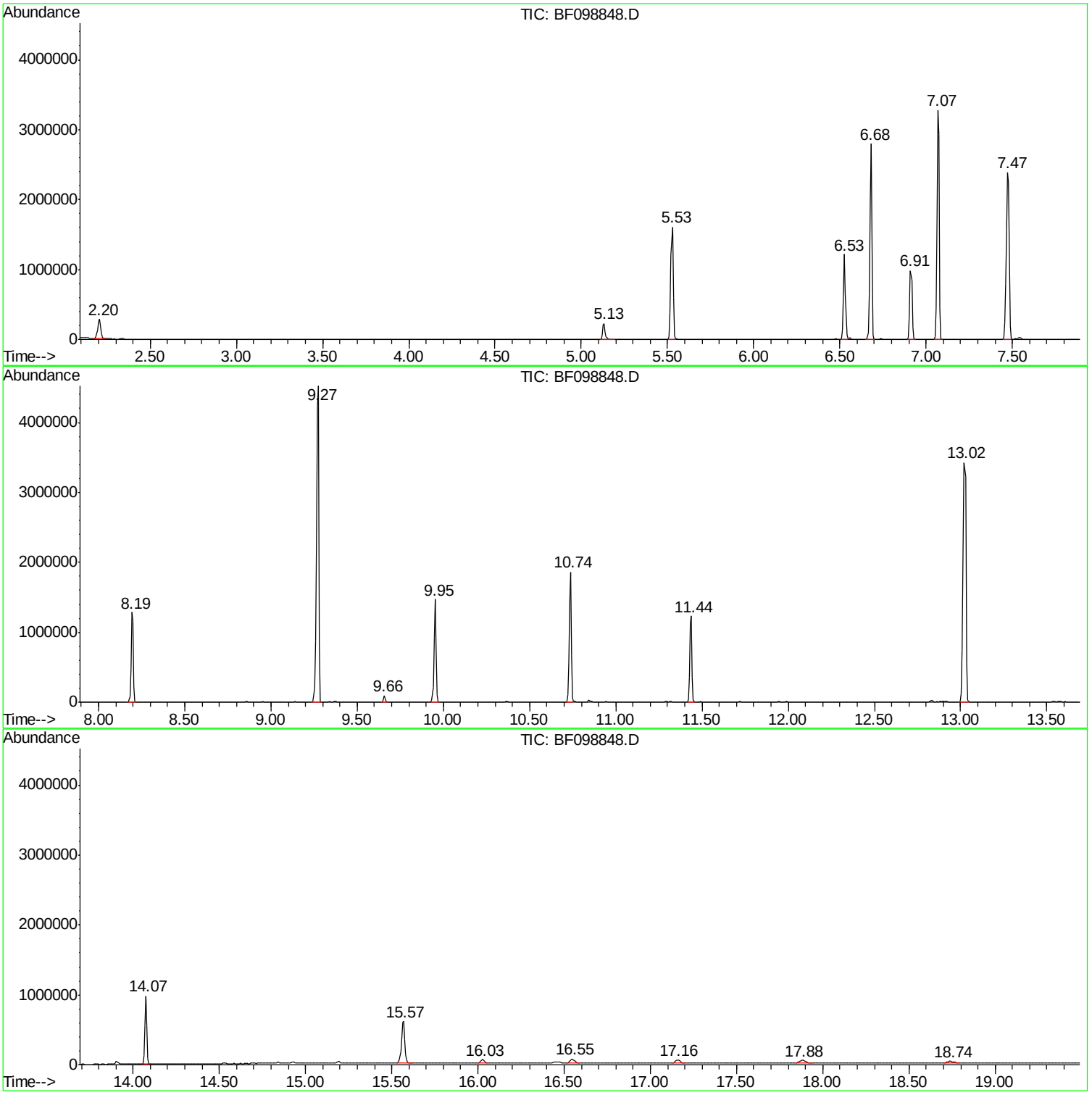
Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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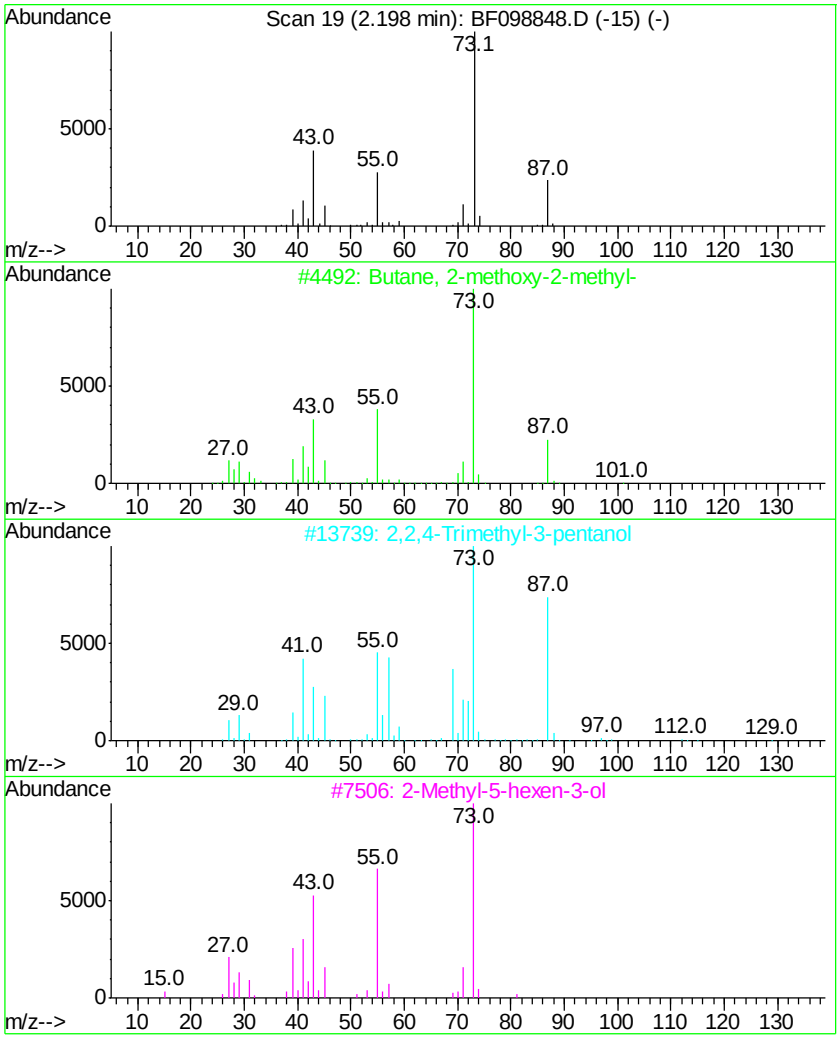
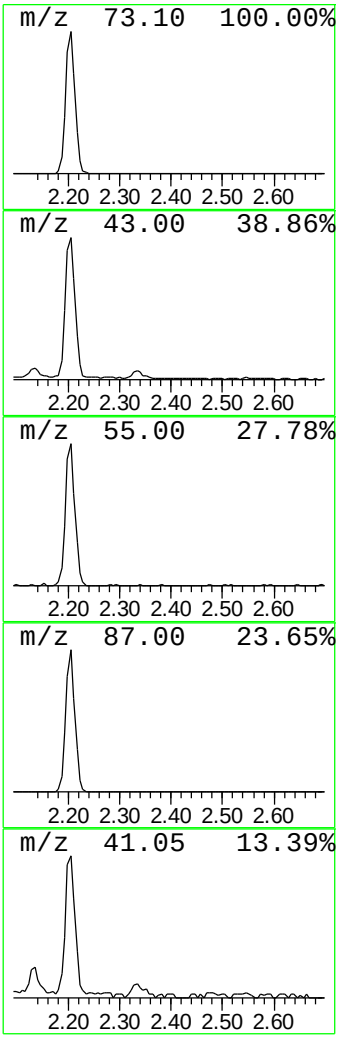
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	8.53 ng	355309	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
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Acq On : 26 Sep 2017 22:41
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Sample : I5427-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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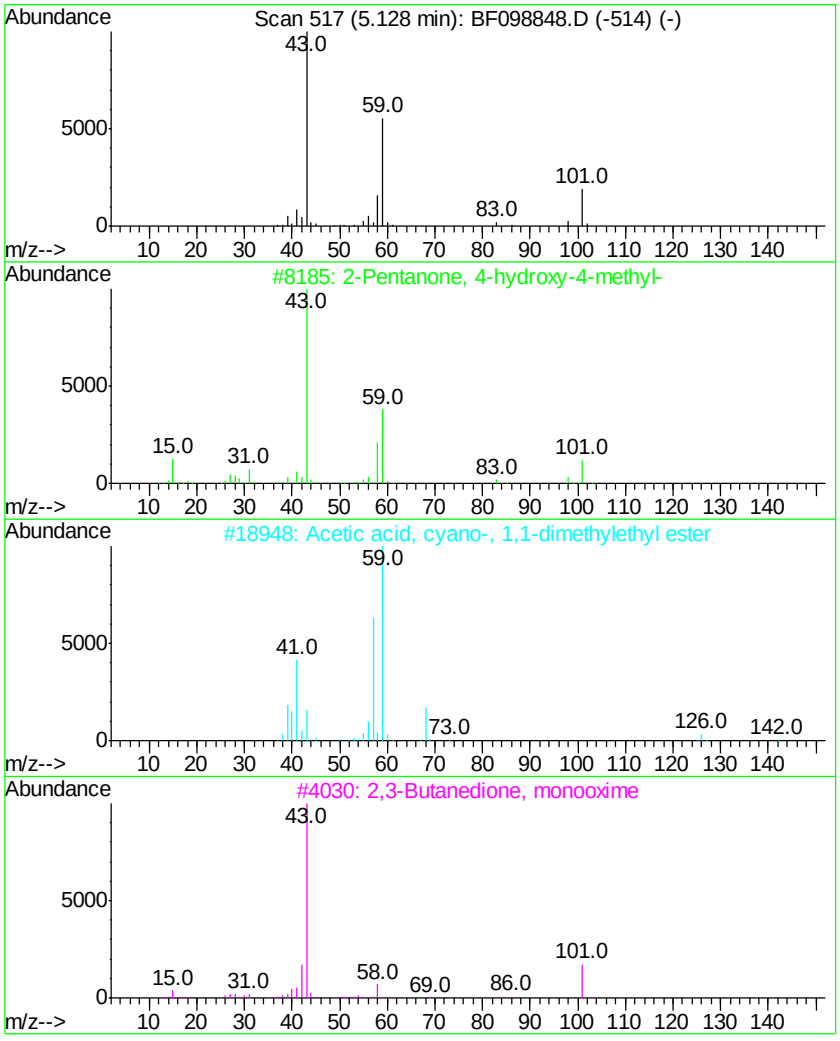
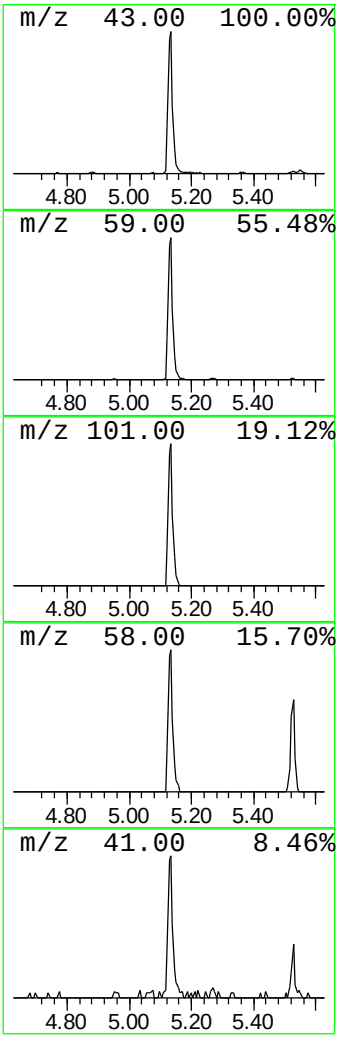
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	5.93 ng	246708	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : I5427-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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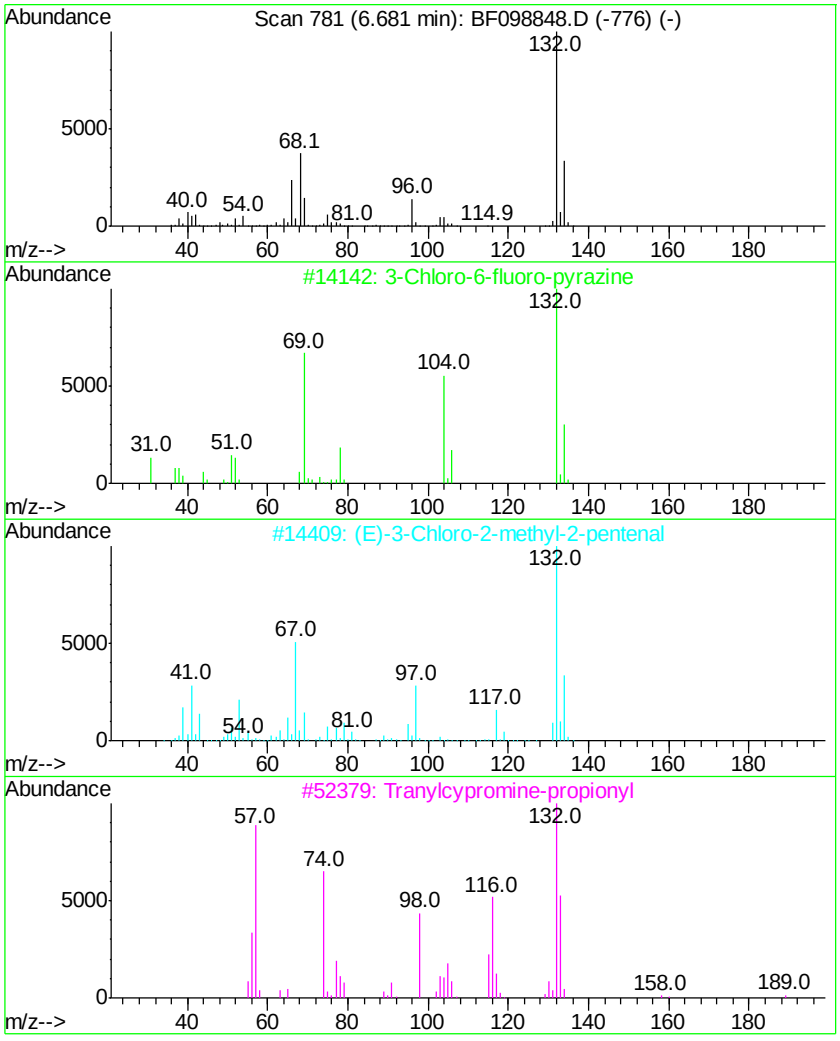
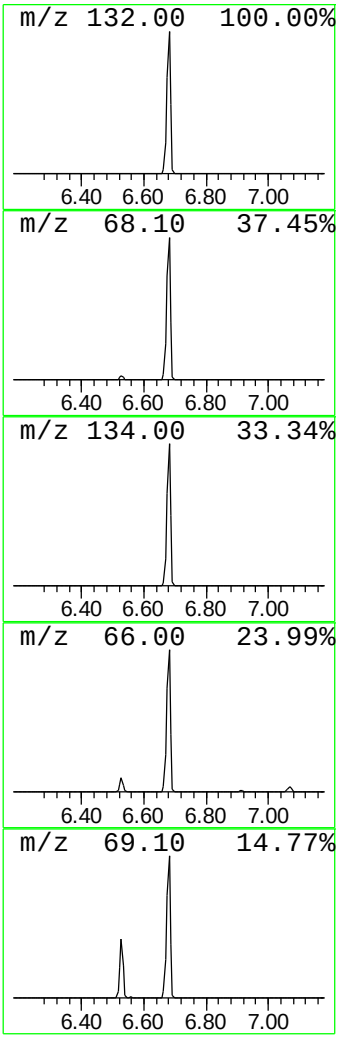
Peak Number 3 unknown6.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	58.04 ng	2416290	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : I5427-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
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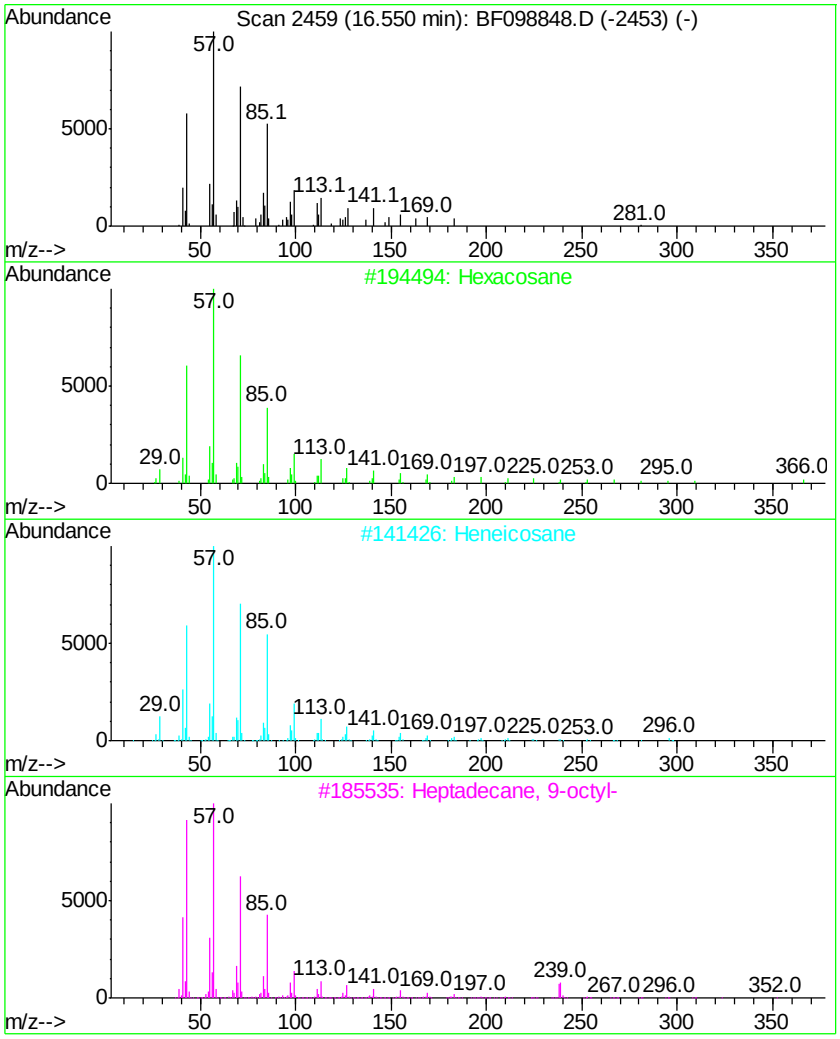
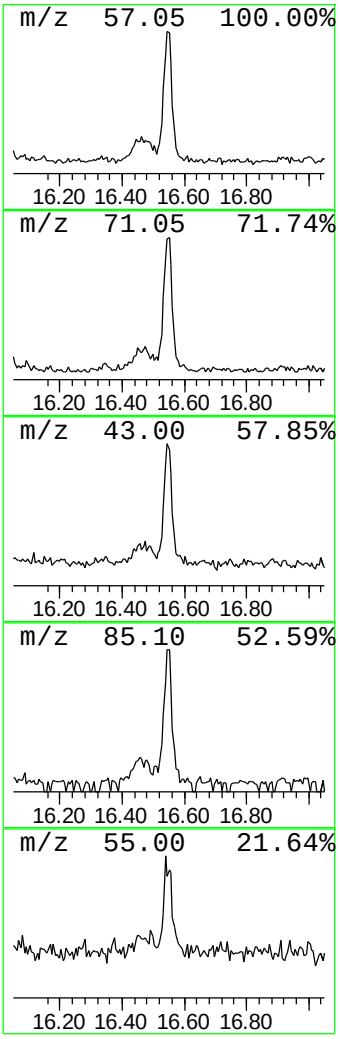
Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	2.43 ng	99062	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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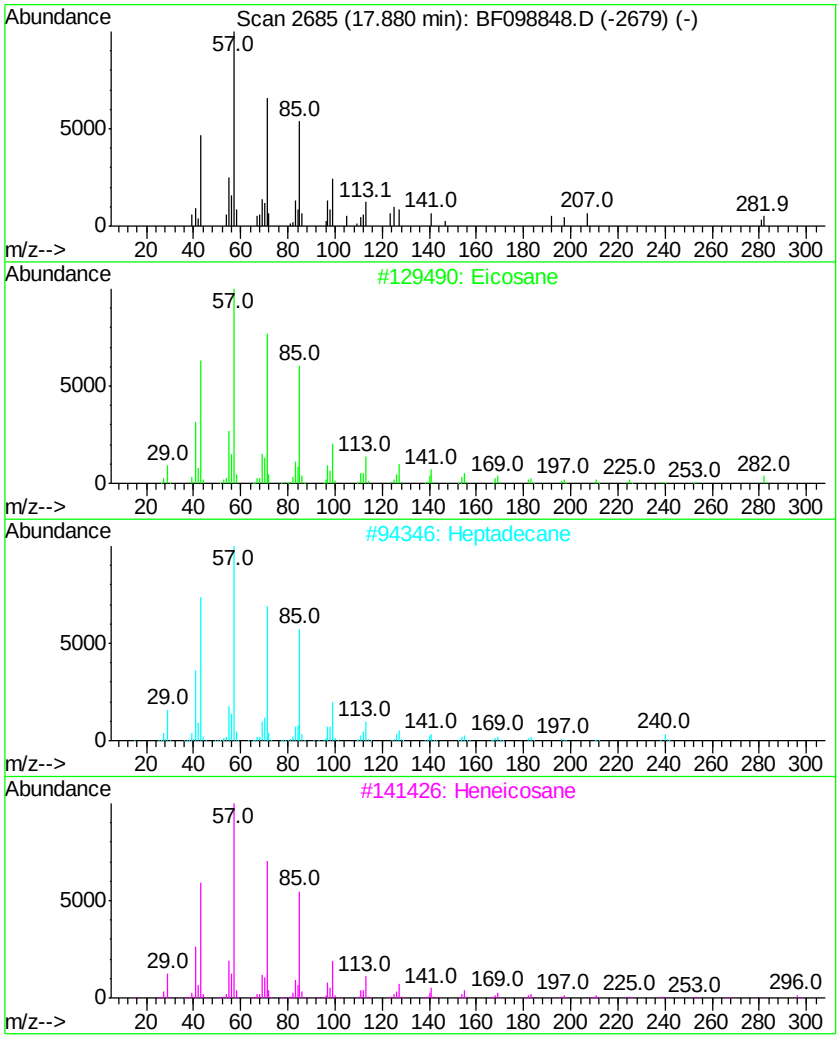
TIC Integration Parameters: LSCINT.P

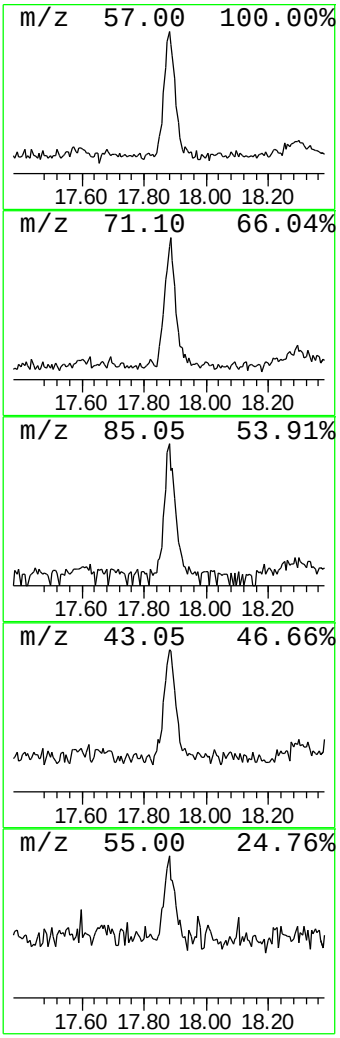
****

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.88	2.12 ng	86303	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Heptadecane	240	C17H36	000629-78-7	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octacosane	394	C28H58	000630-02-4	83
5	Pentacosane	352	C25H52	000629-99-2	80





Tentatively Identified Compound (LSC) summary

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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...	2.20	8.5	ng	355309	1	6.91	832695	20.0
2-Pentanone, 4-hy...	5.13	5.9	ng	246708	1	6.91	832695	20.0
unknown6.68	6.68	58.0	ng	2416290	1	6.91	832695	20.0
Hexacosane	16.55	2.4	ng	99062	6	15.57	814187	20.0
Eicosane	17.88	2.1	ng	86303	6	15.57	814187	20.0