LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
Data File : BF098768.D
Acq On : 24 Sep 2017 5:58
Operator : SJ/JU
Sample : I5298-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-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	2.240	21	26	38	rVB	293189	399068	10.71%	1.616%
2	5.146	517	520	530	rVB	242044	241488	6.48%	0.978%
3	5.540	583	587	590	rBV	1630939	1393614	37.39%	5.644%
4	6.534	752	756	760	rBV	1076296	933338	25.04%	3.780%
5	6.563	760	761	765	rVB	58755	45746	1.23%	0.185%
6	6.687	778	782	786	rBV	2422741	2363865	63.42%	9.574%
7	6.922	818	822	826	rBV	1022118	821678	22.05%	3.328%
8	7.081	845	849	852	rBV	3432721	3104291	83.29%	12.572%
9	7.487	912	918	921	rBV	2357561	2363427	63.41%	9.572%
10	8.204	1036	1040	1043	rBV	1207059	958124	25.71%	3.880%
11	9.281	1217	1223	1226	rBV	4192287	3727220	100.00%	15.095%
12	9.663	1285	1288	1292	rBV	81191	70040	1.88%	0.284%
13	9.957	1334	1338	1342	rBV	926582	814084	21.84%	3.297%
14	10.745	1468	1472	1475	rBV	1346385	1124915	30.18%	4.556%
15	11.445	1587	1591	1594	rBV	875621	710956	19.07%	2.879%
16	12.845	1825	1829	1832	rBV	89006	78147	2.10%	0.316%
17	13.033	1856	1861	1864	rBV	3139048	2920124	78.35%	11.826%
18	13.545	1945	1948	1951	rBV2	67029	56242	1.51%	0.228%
19	13.916	2008	2011	2015	rBV2	35258	45604	1.22%	0.185%
20	14.086	2036	2040	2043	rBV	807452	763192	20.48%	3.091%
21	15.204	2226	2230	2234	rBV2	61164	74462	2.00%	0.302%
22	15.580	2288	2294	2303	rVB	483747	738561	19.82%	2.991%
23	16.045	2368	2373	2380	rBV	115518	181040	4.86%	0.733%
24	16.568	2456	2462	2469	rVB2	127651	230070	6.17%	0.932%
25	17.180	2560	2566	2574	rBV	98830	207989	5.58%	0.842%
26	17.915	2684	2691	2701	rVB	78383	193034	5.18%	0.782%
27	18.774	2832	2837	2849	rVB3	47283	131257	3.52%	0.532%

Sum of corrected areas: 24691576

LSC Report - Integrated Chromatogram

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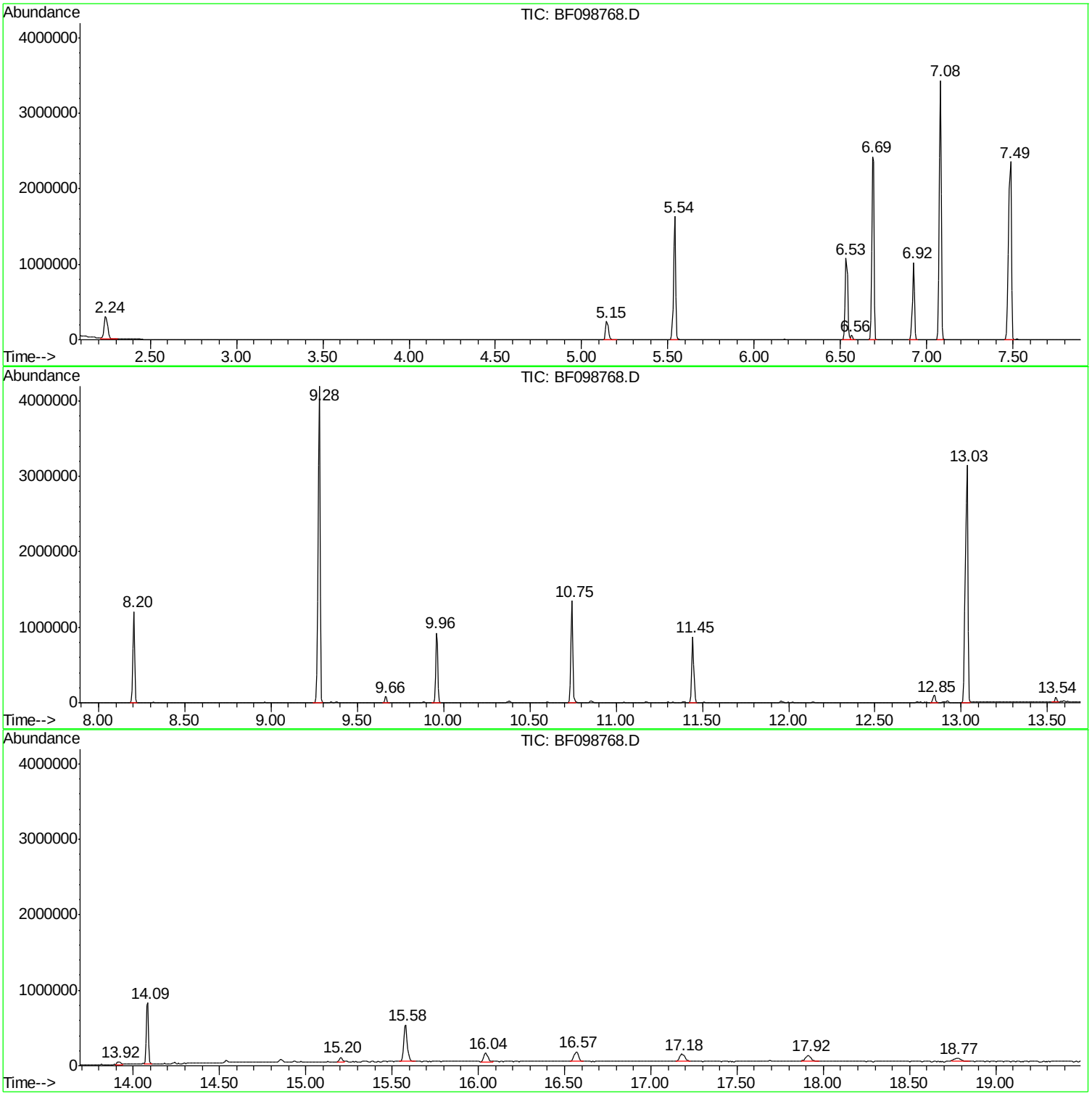
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091817-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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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

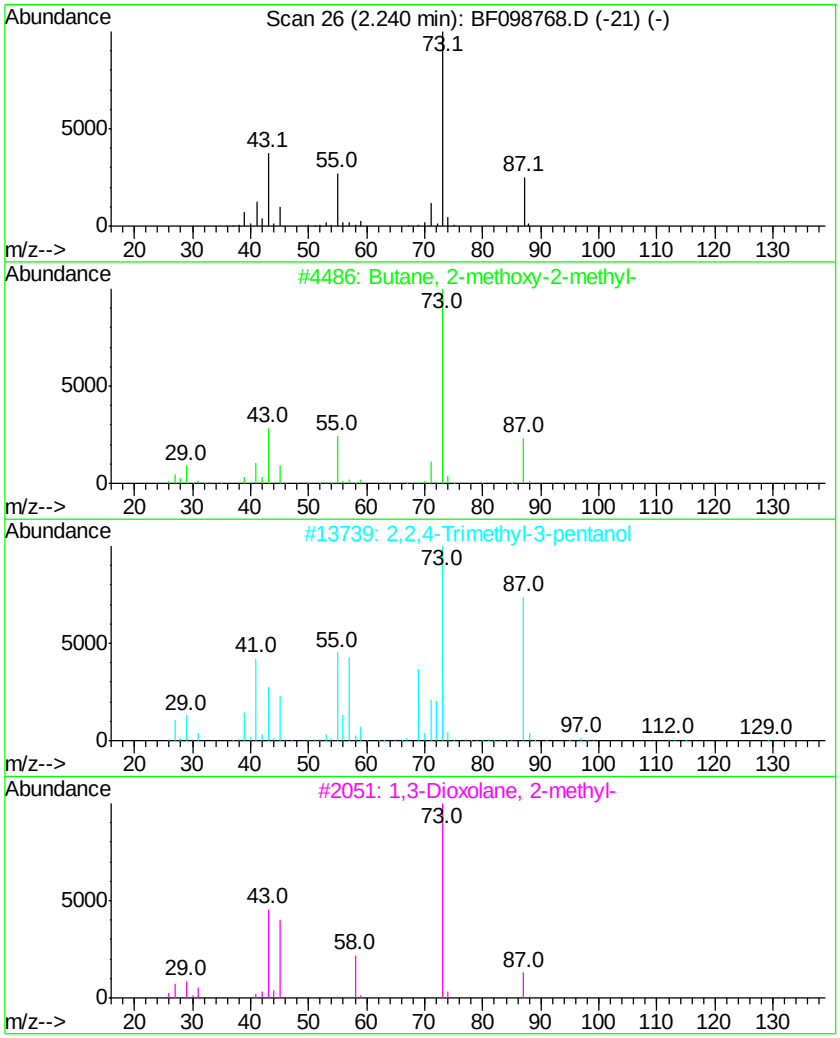
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

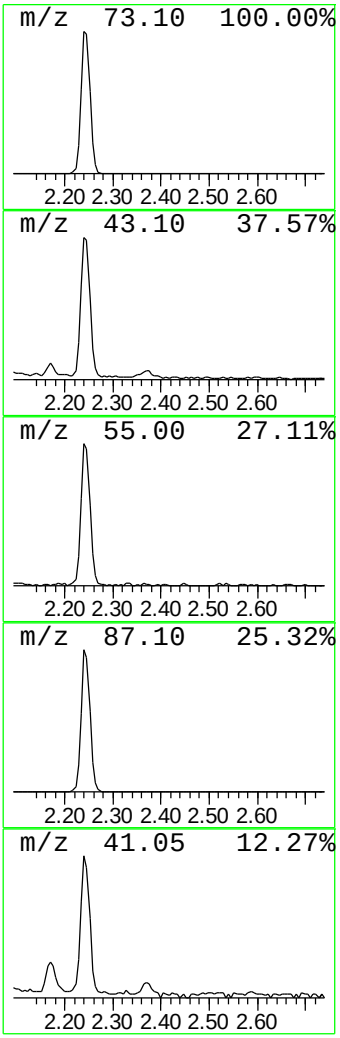
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	9.71 ng	399068	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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Sample : I5298-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-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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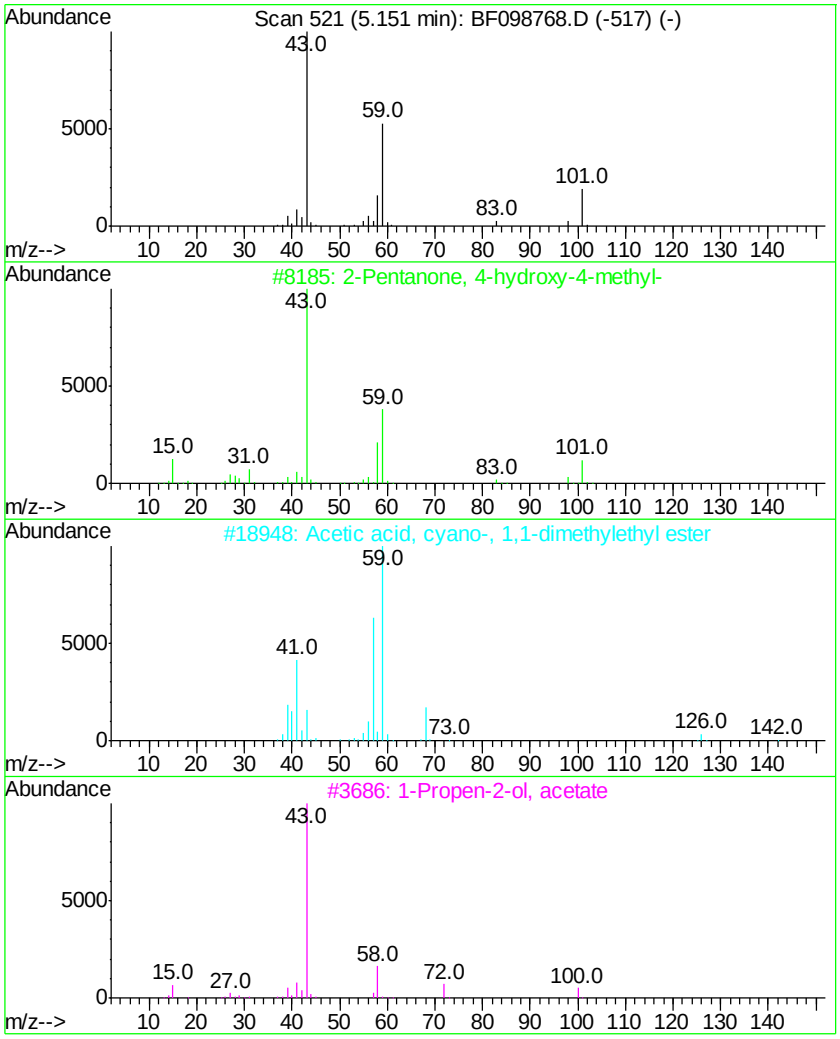
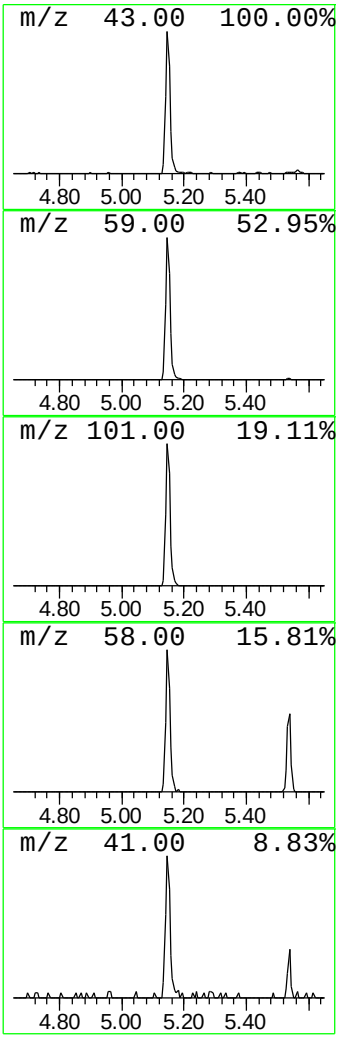
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	5.88 ng	241488	1,4-Dichlorobenzene-d4	6.92

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	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 24 Sep 2017 5:58
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Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-B

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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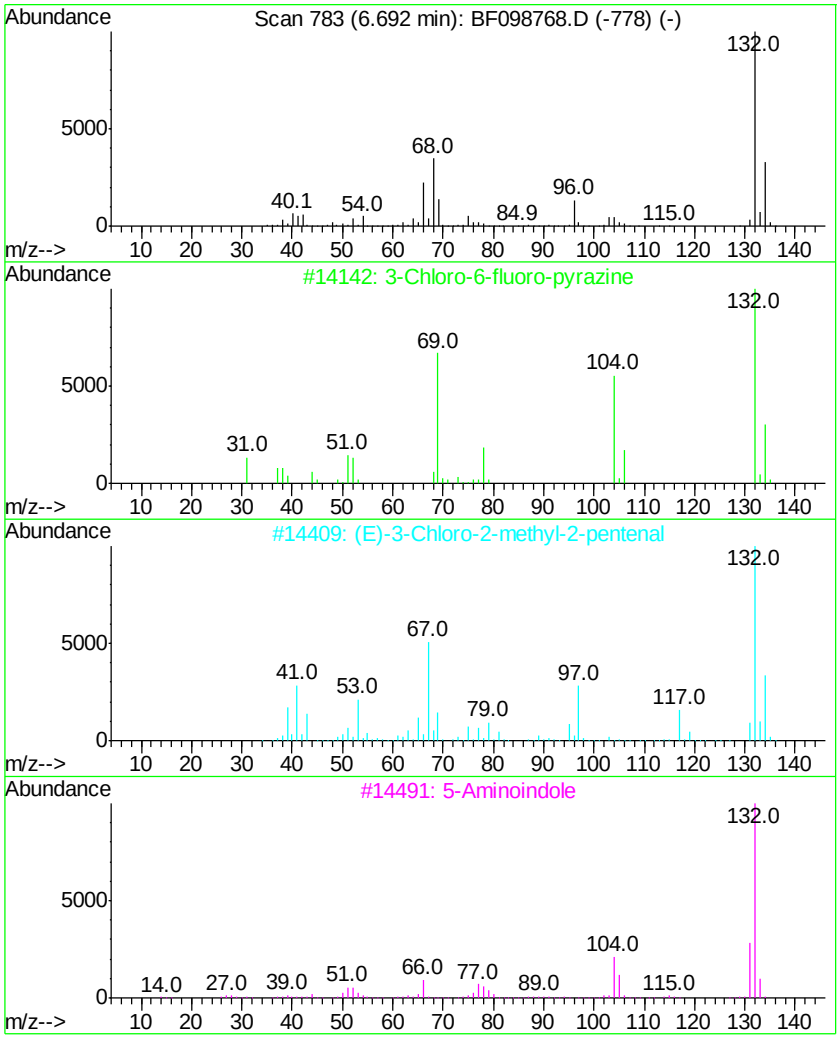
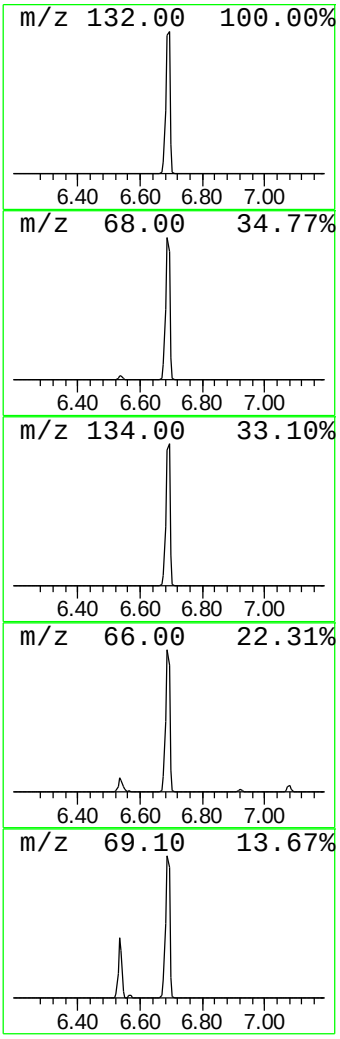
Peak Number 3 unknown6.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	57.54 ng	2363870	1,4-Dichlorobenzene-d4	6.92

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Sample : I5298-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-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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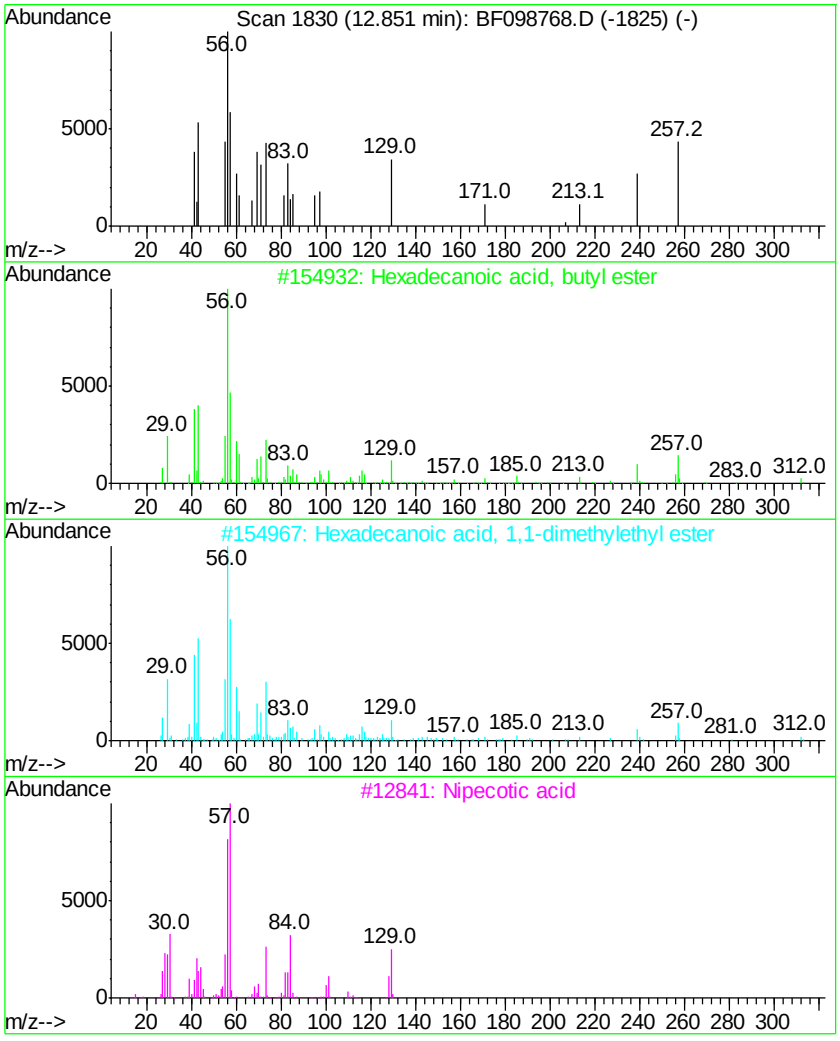
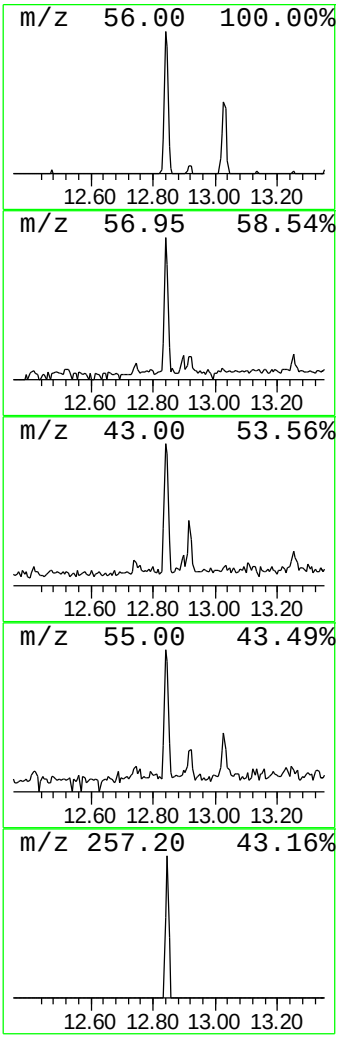
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	2.05 ng	78147	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	68
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Cyclobutane, 1,2-diethyl-	112	C8H16	061141-83-1	27
5	2-Methyl-1-tetradecene	210	C15H30	052254-38-3	27





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Sample : I5298-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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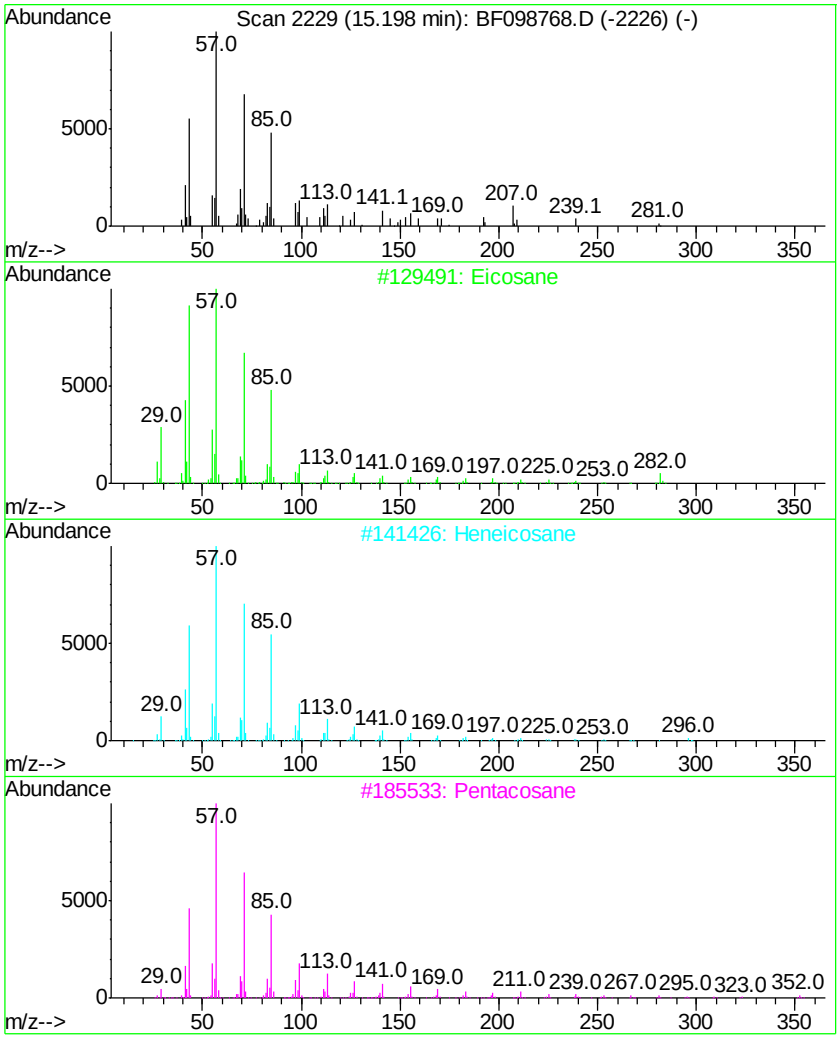
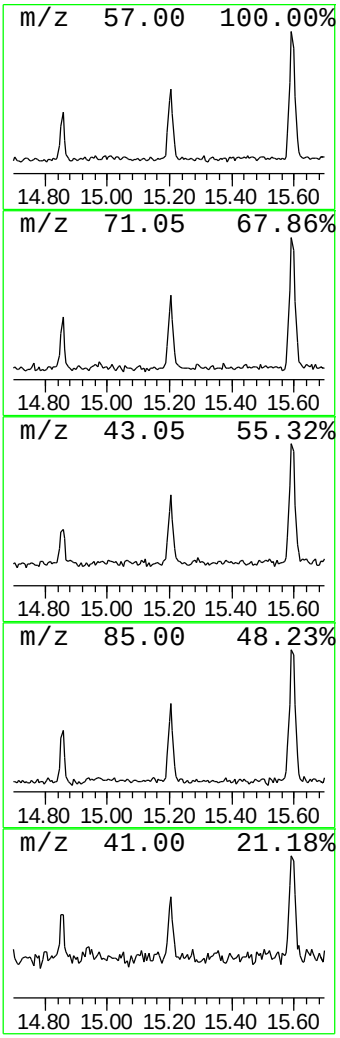
Peak Number 6 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	2.02 ng	74462	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Pentacosane	352	C25H52	000629-99-2	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





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Instrument : BNA_F
ClientSampleId : 091817-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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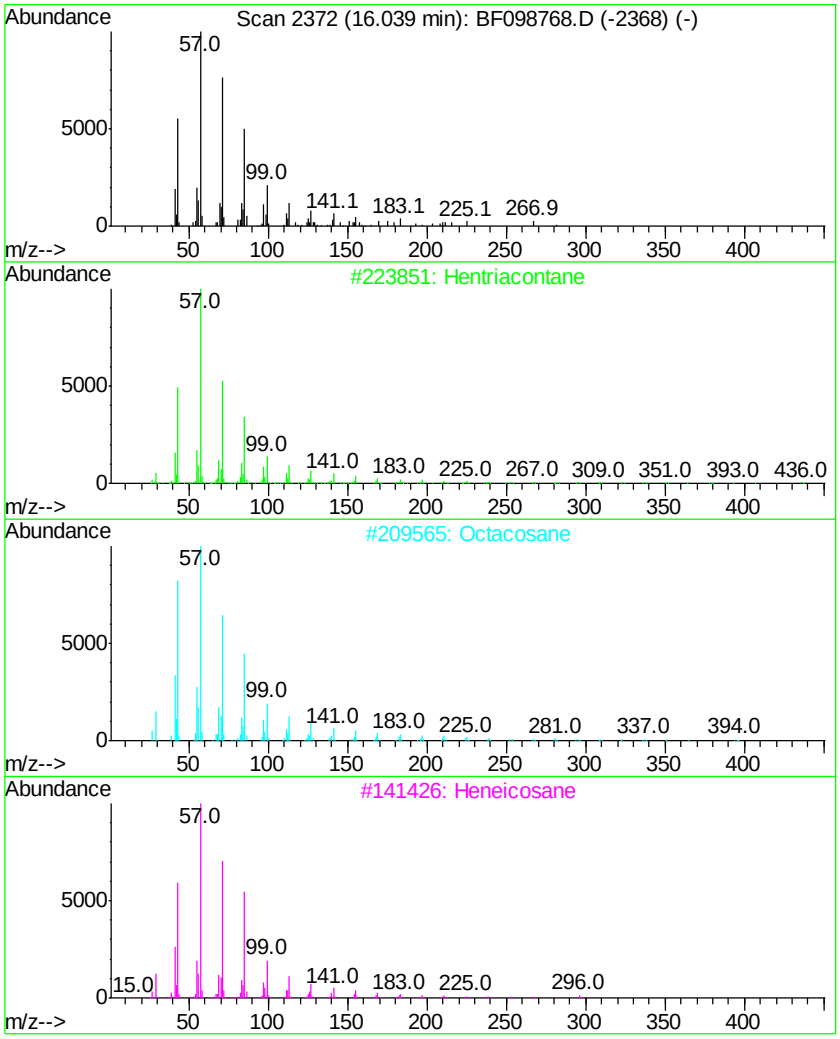
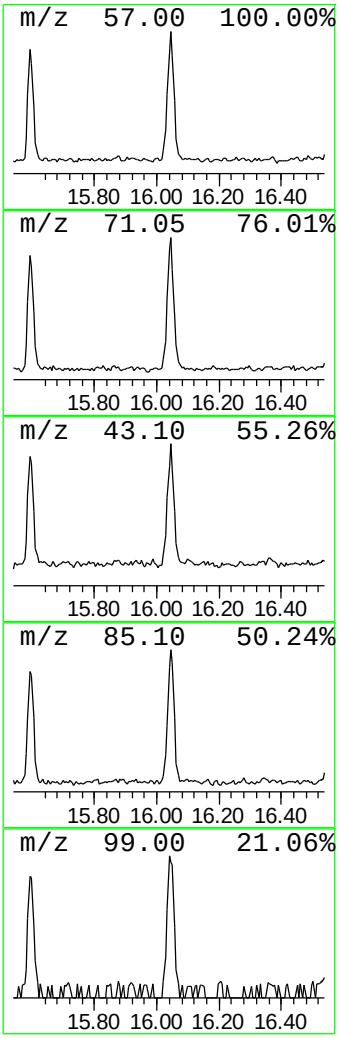
Peak Number 7 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	4.90 ng	181040	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Docosane	310	C22H46	000629-97-0	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





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Instrument : BNA_F
ClientSampleId : 091817-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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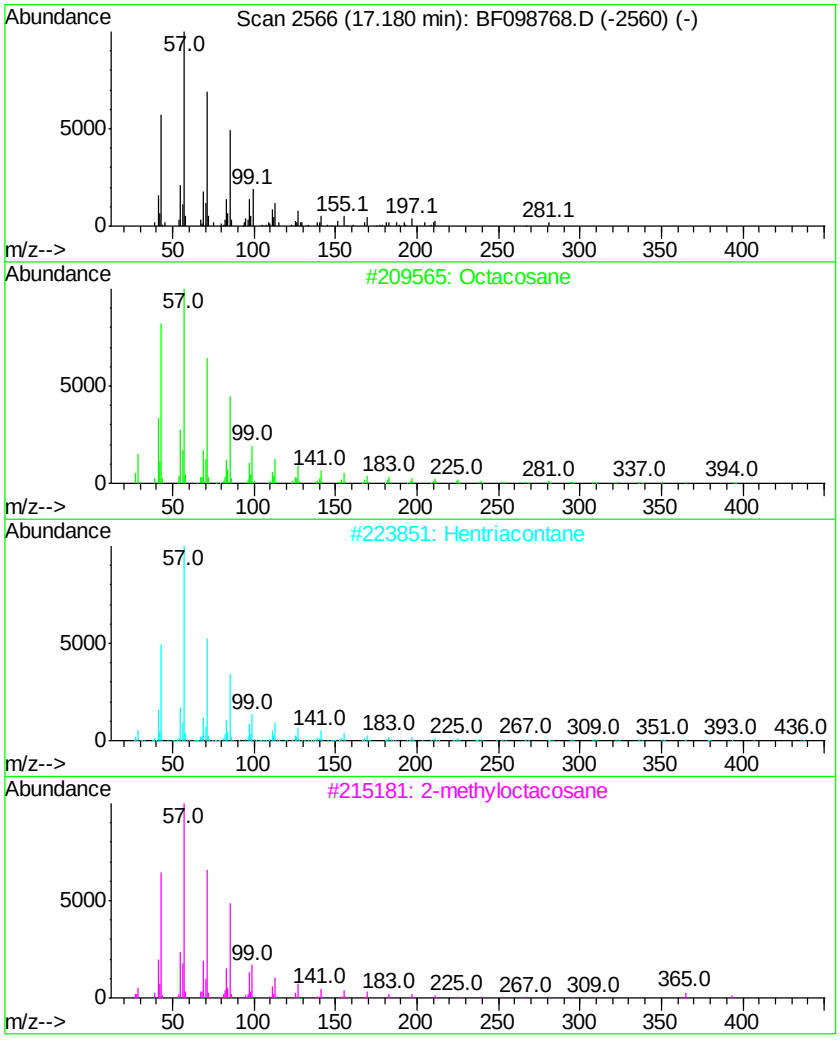
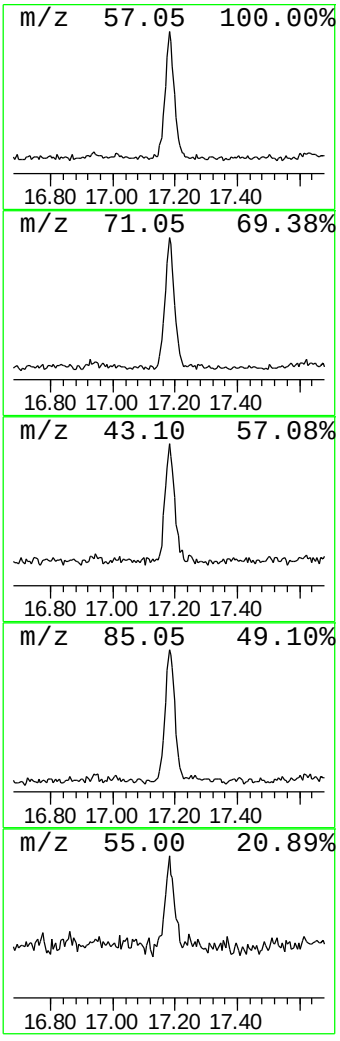
Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.18	5.63 ng	207989	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Heneicosane	296	C21H44	000629-94-7	90





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

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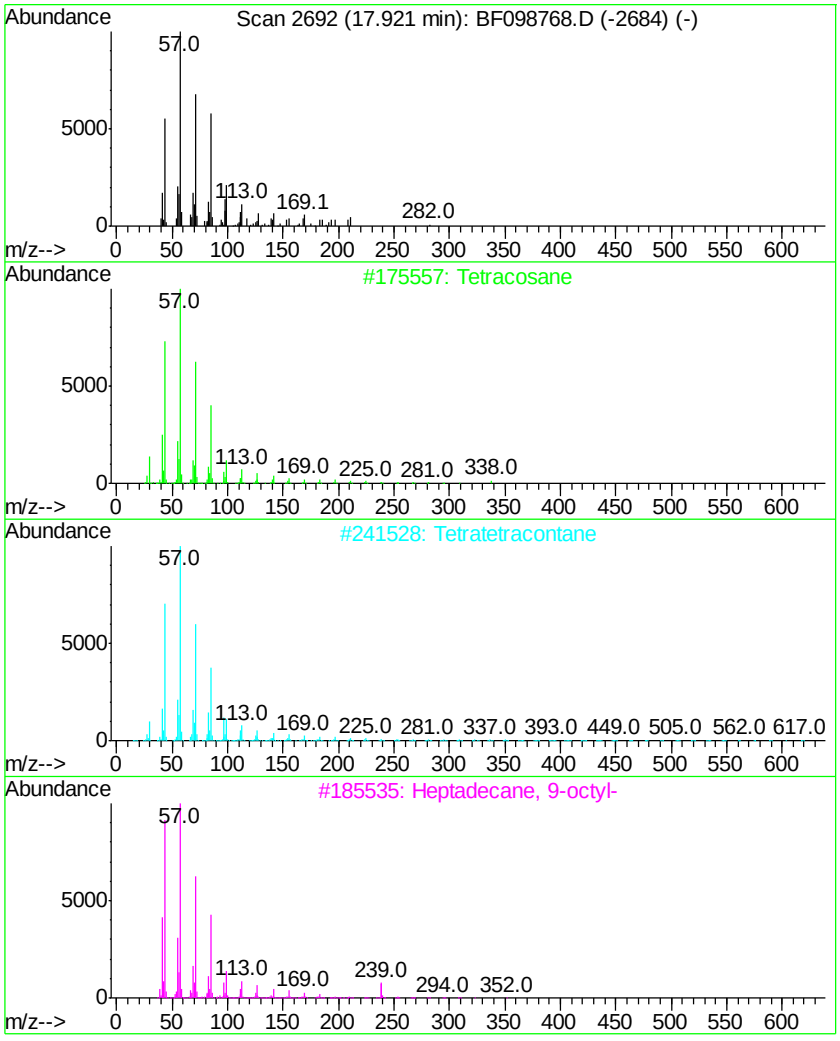
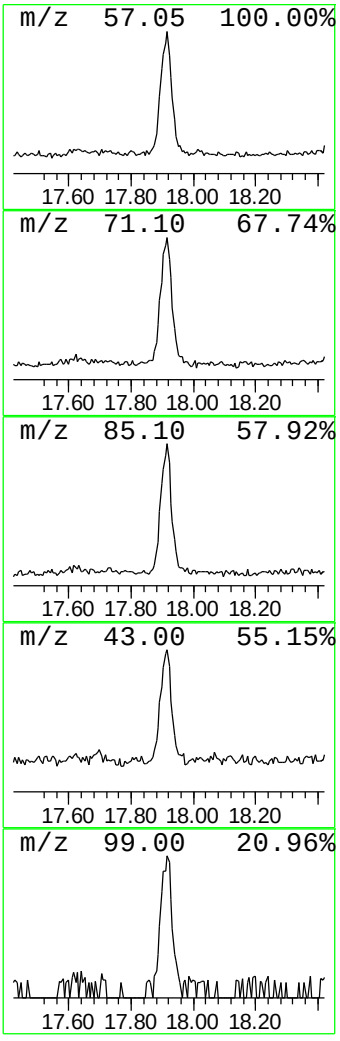
Peak Number 10 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.92	5.23 ng	193034	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heneicosane	296	C21H44	000629-94-7	90





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...	2.24	9.7	ng	399068	1	6.92	821678	20.0
2-Pentanone, 4-hy...	5.15	5.9	ng	241488	1	6.92	821678	20.0
unknown6.69	6.69	57.5	ng	2363870	1	6.92	821678	20.0
Hexadecanoic acid...	12.85	2.0	ng	78147	5	14.09	763192	20.0
Eicosane	15.20	2.0	ng	74462	6	15.58	738561	20.0
Hentriacontane	16.04	4.9	ng	181040	6	15.58	738561	20.0
Octacosane	17.18	5.6	ng	207989	6	15.58	738561	20.0
Tetracosane	17.92	5.2	ng	193034	6	15.58	738561	20.0