LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099182.D
Acq On : 7 Oct 2017 7:58
Operator : SJ/JU
Sample : I5675-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RI-MW-2-GW

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	2.169	8	14	21	rVB	578499	746708	19.11%	2.783%
2	3.222	188	193	201	rVB2	29995	52222	1.34%	0.195%
3	5.093	507	511	519	rBV	254403	297857	7.62%	1.110%
4	5.487	574	578	582	rBV	2096835	2012426	51.50%	7.500%
5	6.493	745	749	752	rBV	1589142	1355355	34.69%	5.051%
6	6.634	769	773	776	rBV	3025200	2989778	76.52%	11.143%
7	6.863	808	812	815	rBV	971383	762042	19.50%	2.840%
8	7.022	834	839	842	rBV	3004488	2742859	70.20%	10.222%
9	7.428	903	908	911	rVB	2048351	2210906	56.58%	8.240%
10	8.145	1026	1030	1033	rBV	1236070	1045734	26.76%	3.897%
11	9.222	1207	1213	1216	rBV	4039383	3907406	100.00%	14.562%
12	9.610	1276	1279	1281	rBV	116795	85426	2.19%	0.318%
13	9.898	1324	1328	1332	rBV2	1298822	1098235	28.11%	4.093%
14	10.692	1458	1463	1466	rBV	1869506	1894307	48.48%	7.060%
15	10.792	1477	1480	1484	rVB	50419	46812	1.20%	0.174%
16	11.386	1577	1581	1584	rBV	1153954	975373	24.96%	3.635%
17	12.969	1845	1850	1853	rBV	2787878	2745974	70.28%	10.234%
18	13.851	1997	2000	2006	rBV	48459	54356	1.39%	0.203%
19	14.021	2025	2029	2035	rVB	672185	577302	14.77%	2.152%
20	15.498	2274	2280	2291	rBV	541652	700415	17.93%	2.610%
21	15.933	2348	2354	2361	rBV	62923	104175	2.67%	0.388%
22	16.439	2434	2440	2448	rVB	70262	127873	3.27%	0.477%
23	17.033	2534	2541	2547	rBV3	52477	107538	2.75%	0.401%
24	17.727	2652	2659	2671	rBV3	47269	119655	3.06%	0.446%
25	18.562	2794	2801	2810	rVB5	24372	71425	1.83%	0.266%

Sum of corrected areas: 26832159

LSC Report - Integrated Chromatogram

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Operator : SJ/JU
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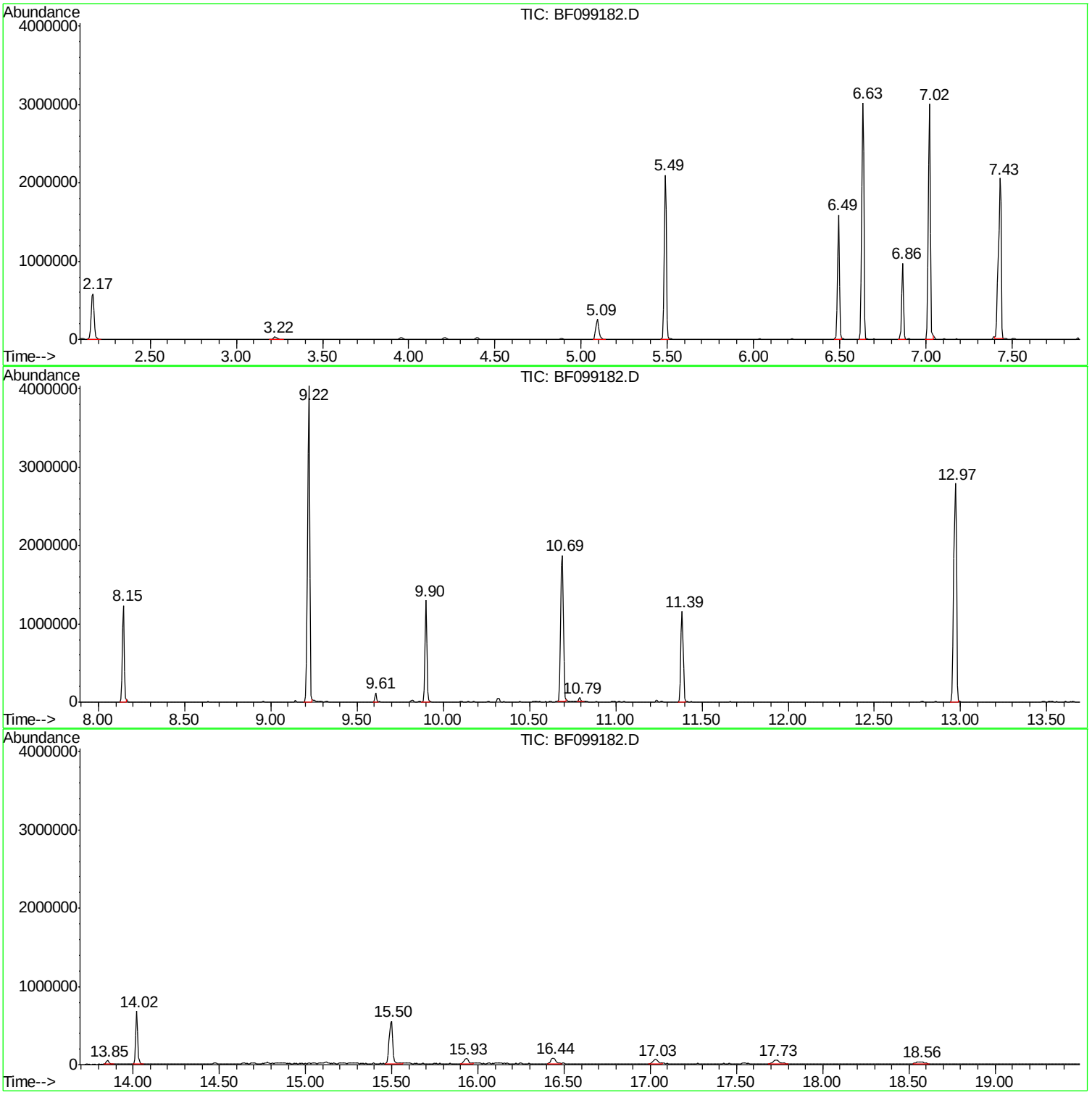
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RI-MW-2-GW

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099182.D
Acq On : 7 Oct 2017 7:58
Operator : SJ/JU
Sample : I5675-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RI-MW-2-GW

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

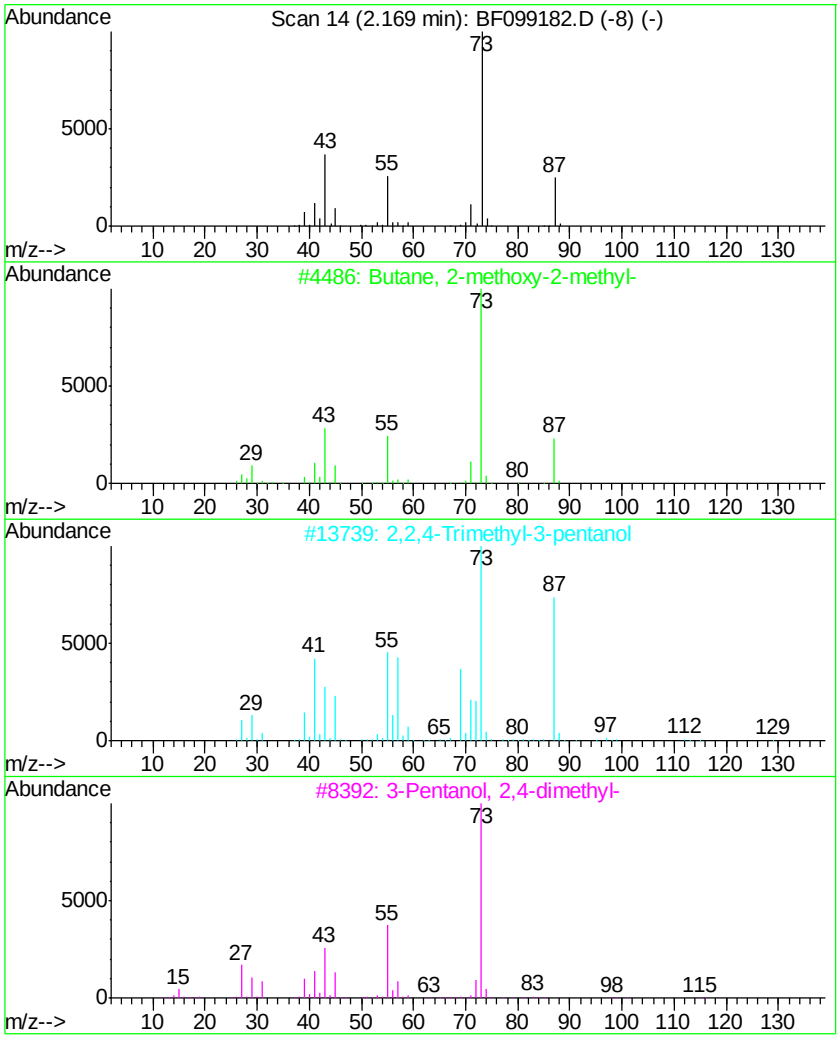
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

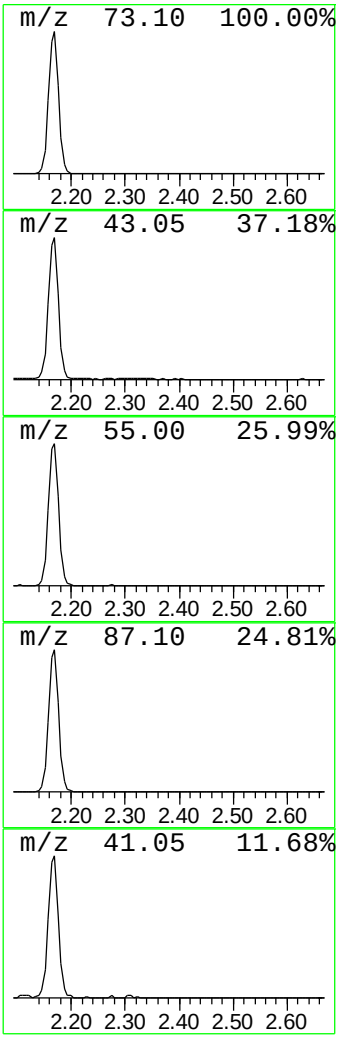
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	19.60 ng	746708	1,4-Dichlorobenzene-d4	6.86

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Operator : SJ/JU
Sample : I5675-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RI-MW-2-GW

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

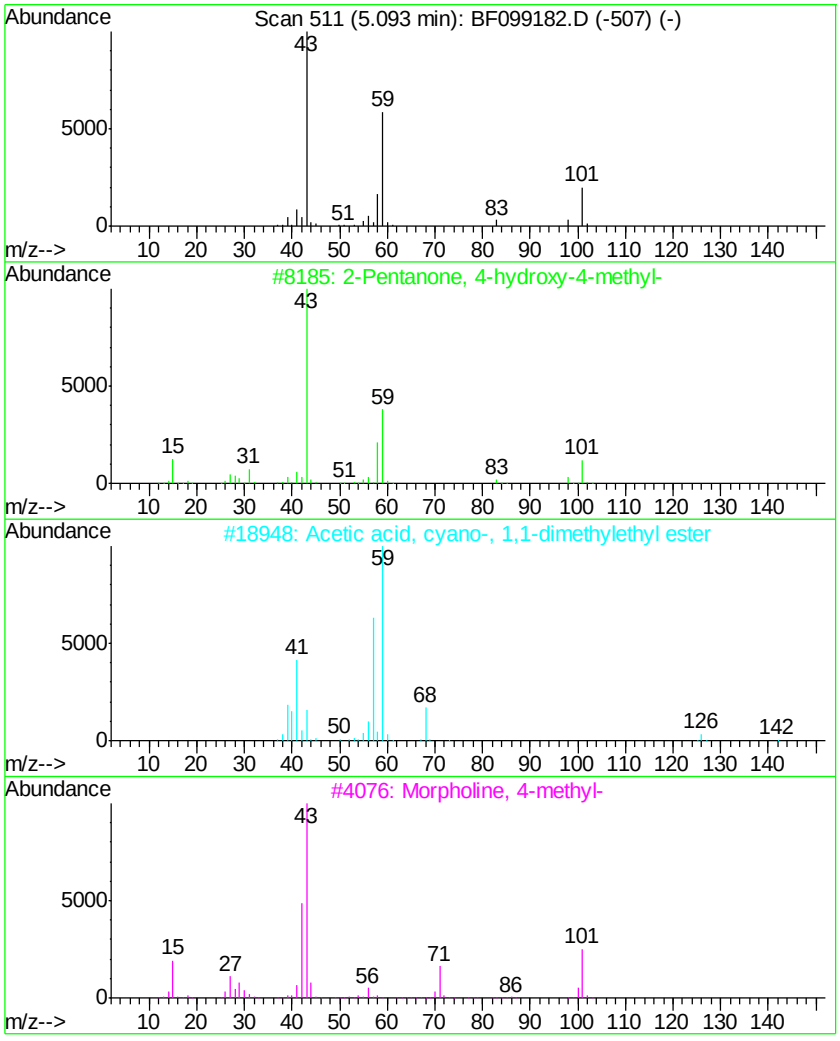
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

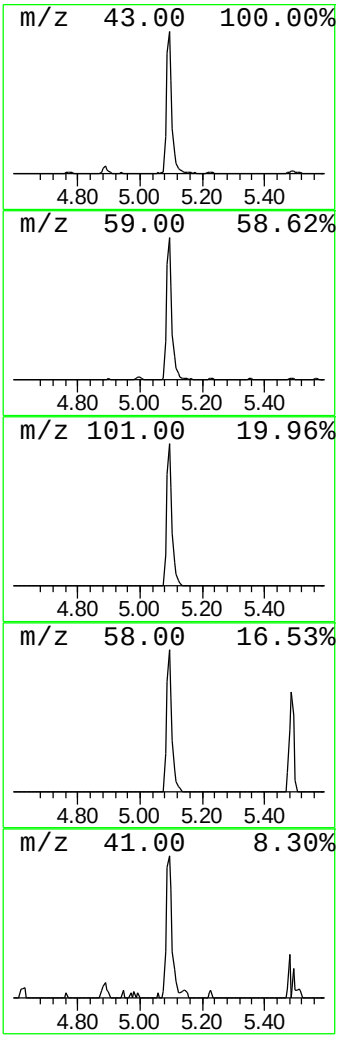
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	7.82 ng	297857	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099182.D
Acq On : 7 Oct 2017 7:58
Operator : SJ/JU
Sample : I5675-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RI-MW-2-GW

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

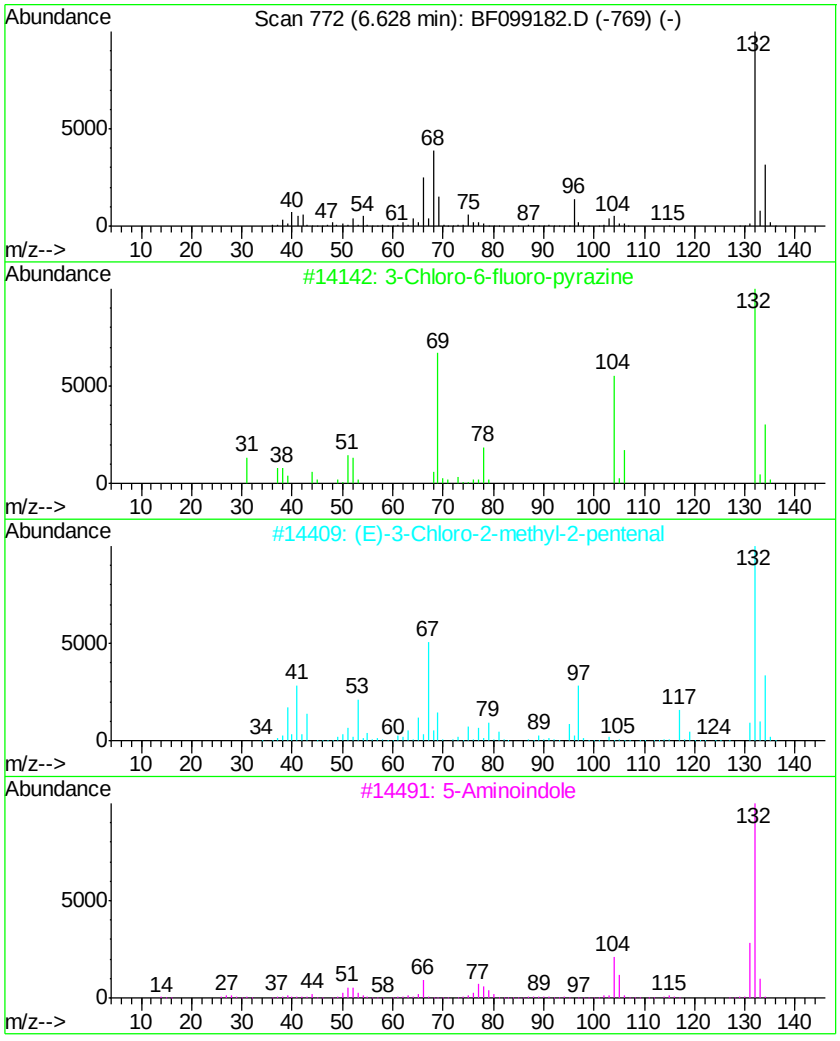
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

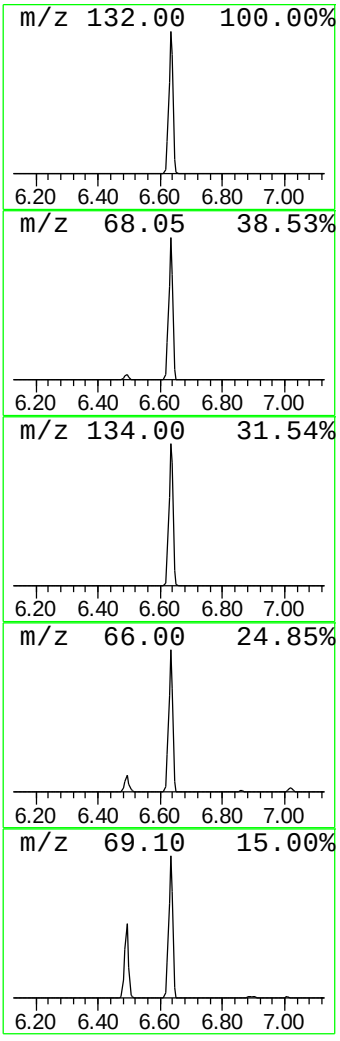
****

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	78.47 ng	2989780	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
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	12
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
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Operator : SJ/JU
Sample : I5675-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RI-MW-2-GW

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

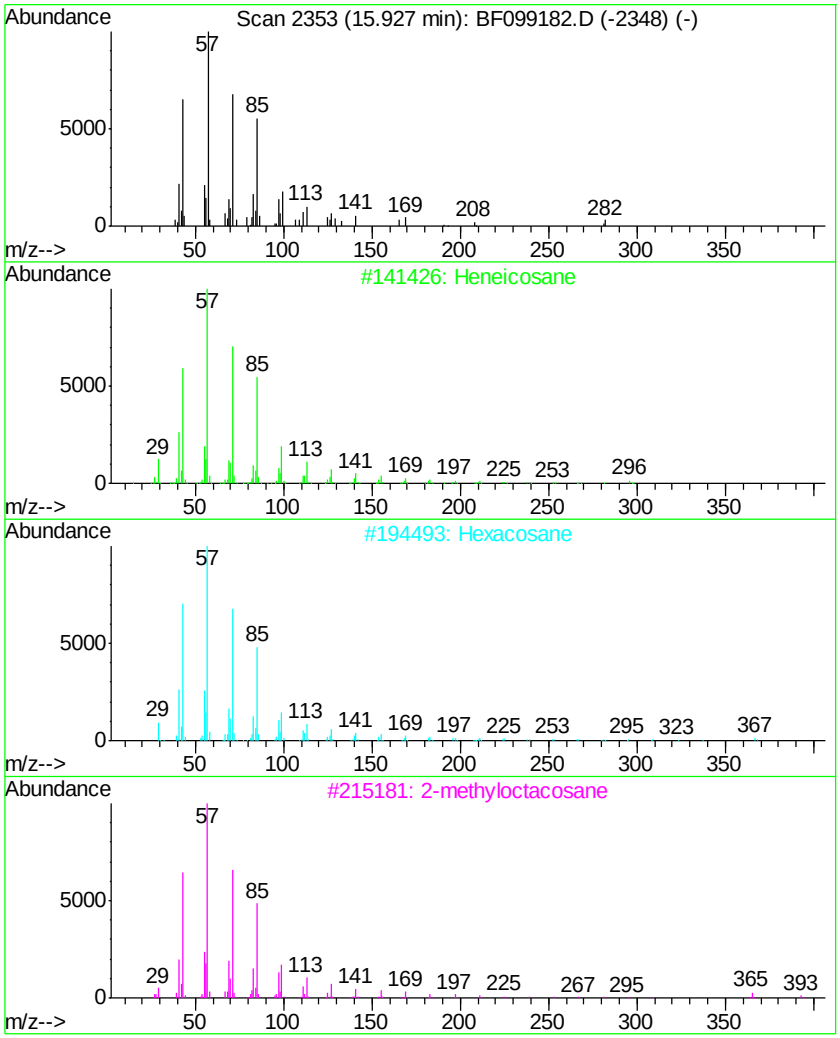
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

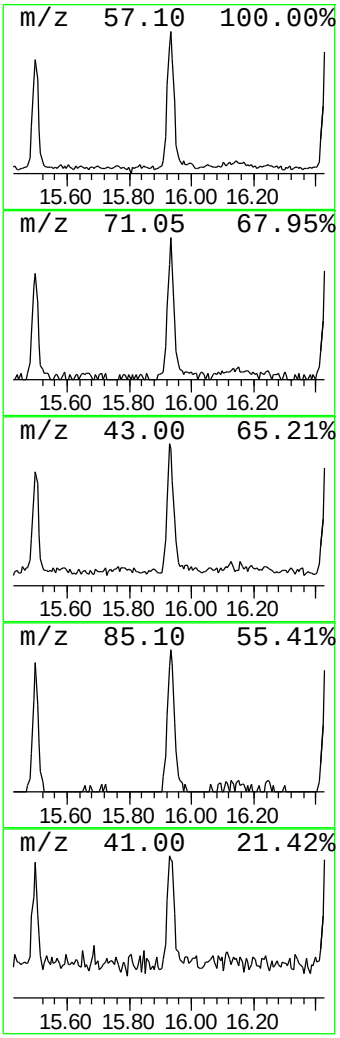
****

Peak Number 5 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.97 ng	104175	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Octacosane	394	C28H58	000630-02-4	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099182.D
Acq On : 7 Oct 2017 7:58
Operator : SJ/JU
Sample : I5675-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RI-MW-2-GW

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

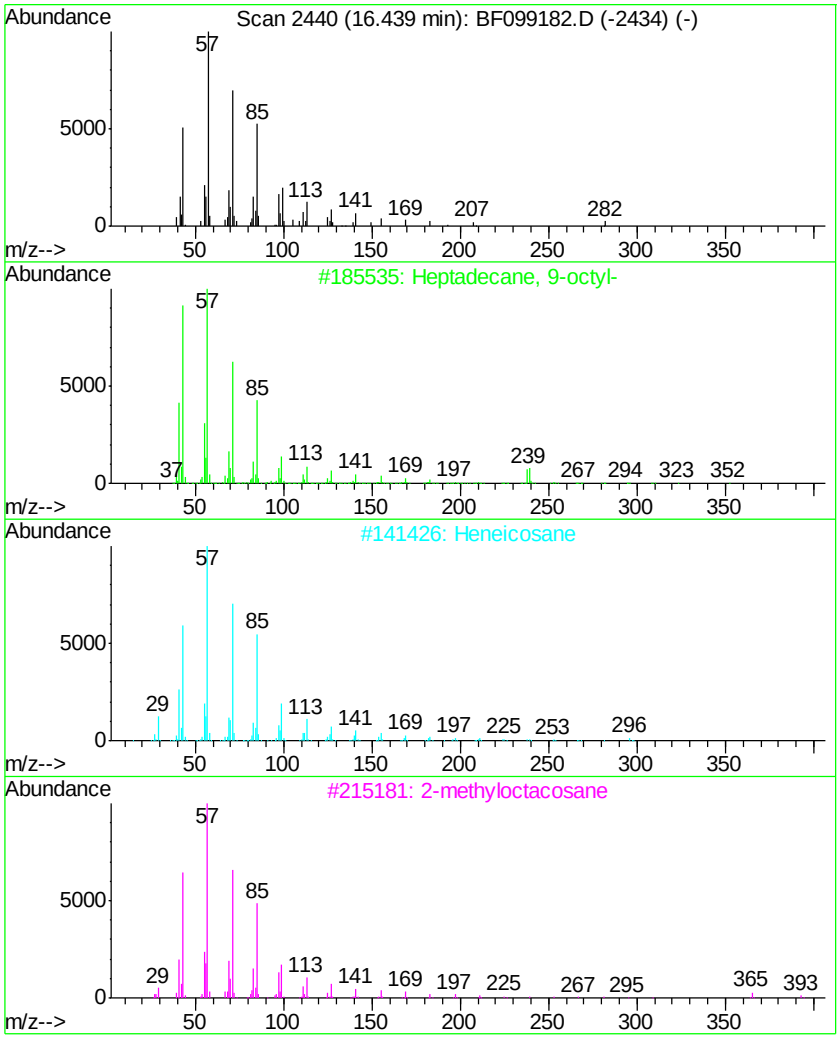
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

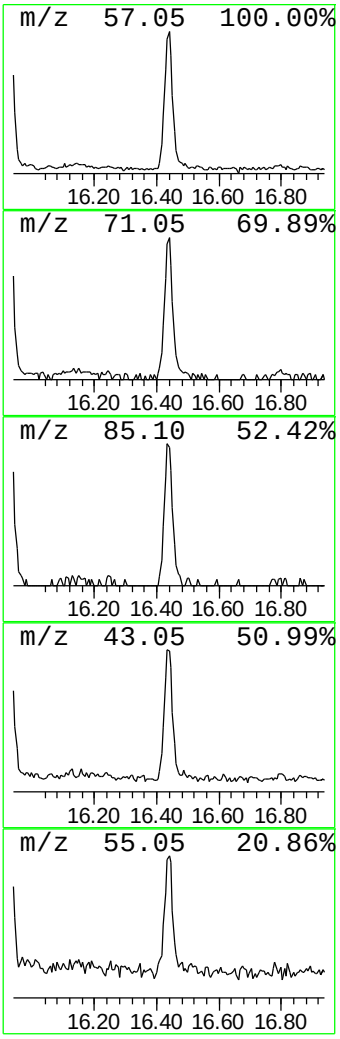
****

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	3.65 ng	127873	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Triacontane	422	C30H62	000638-68-6	90





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Operator : SJ/JU
Sample : I5675-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RI-MW-2-GW

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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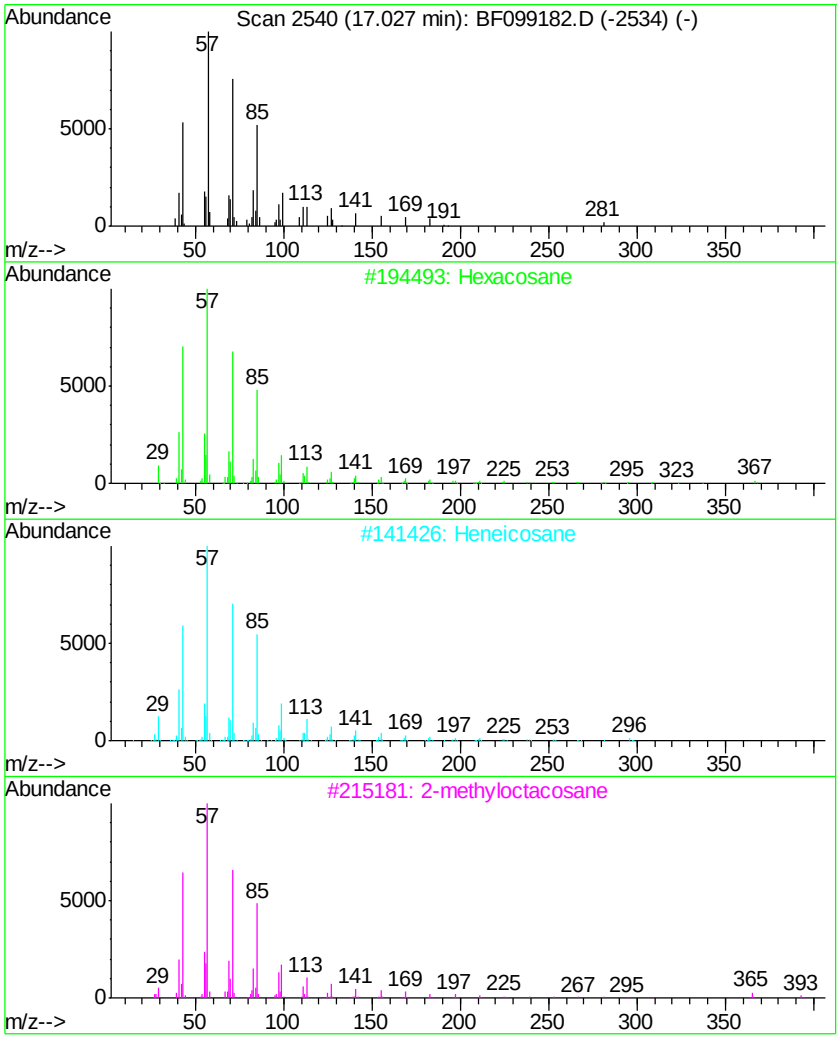
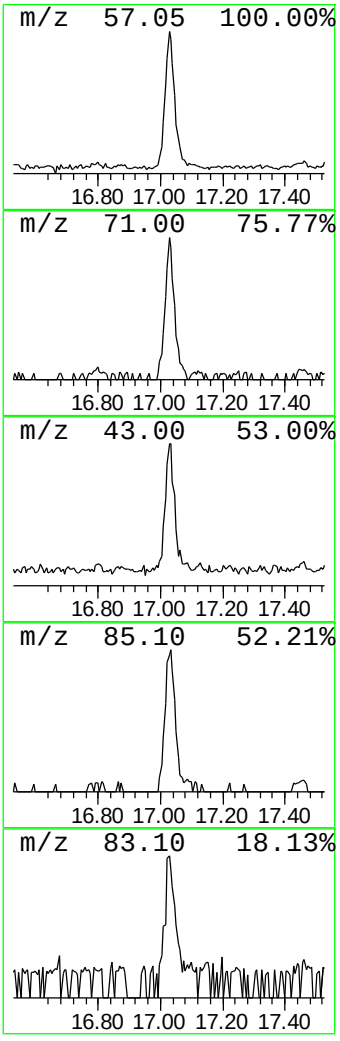
Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.03	3.07 ng	107538	Perylene-d12	15.50

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	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	90





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ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RI-MW-2-GW

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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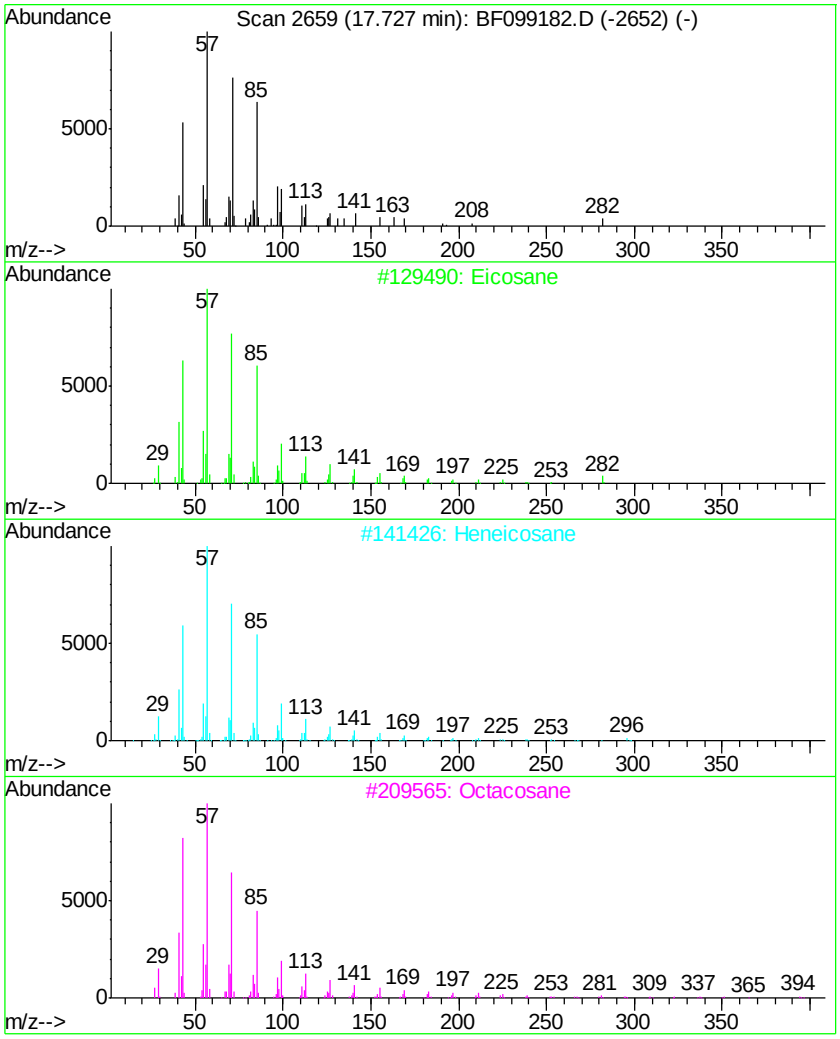
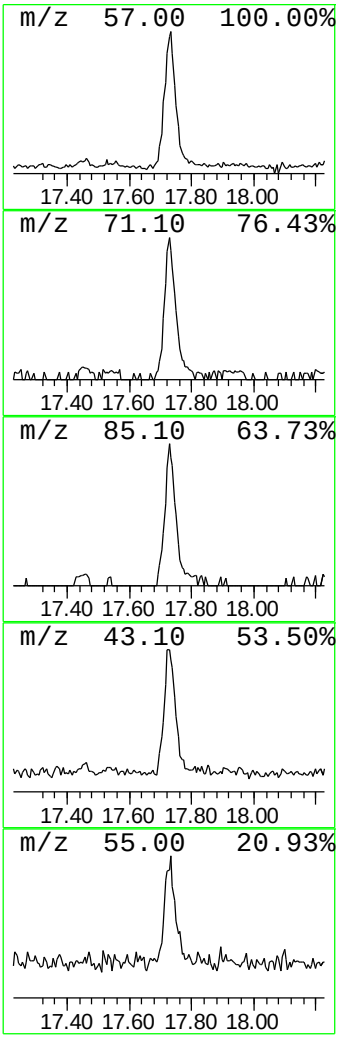
Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.73	3.42 ng	119655	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Heneicosane	296	C21H44	000629-94-7	87
3	Octacosane	394	C28H58	000630-02-4	87
4	10-Methylnonadecane	282	C20H42	056862-62-5	86
5	Hexacosane	366	C26H54	000630-01-3	83





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Sample : I5675-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RI-MW-2-GW

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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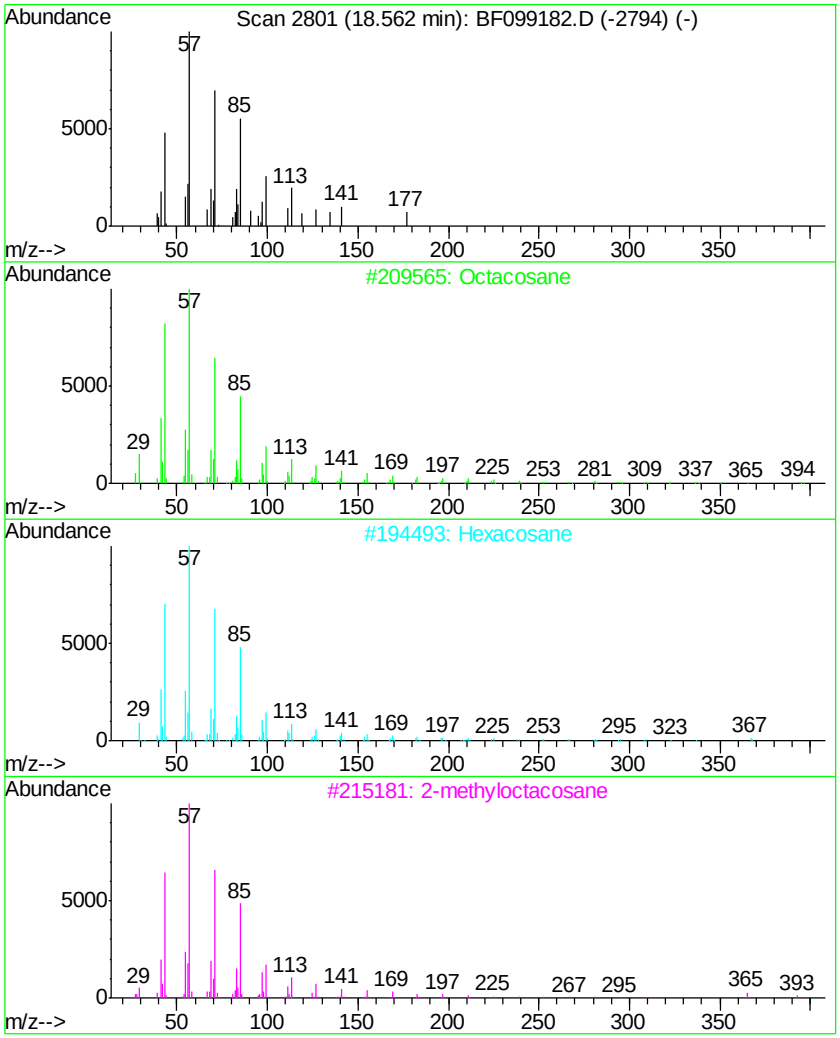
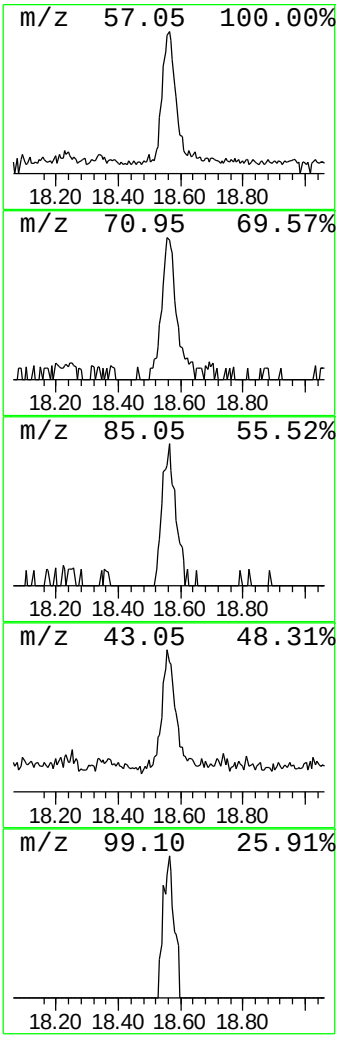
Peak Number 9 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.56	2.04 ng	71425	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	80
2	Hexacosane	366	C26H54	000630-01-3	80
3	2-methyloctacosane	408	C29H60	1000376-72-8	72
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	72
5	Heptacosane	380	C27H56	000593-49-7	72





Tentatively Identified Compound (LSC) summary

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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.17	19.6	ng	746708	1	6.86	762042	20.0
2-Pentanone, 4-hy...	5.09	7.8	ng	297857	1	6.86	762042	20.0
unknown6.63	6.63	78.5	ng	2989780	1	6.86	762042	20.0
Heneicosane	15.93	3.0	ng	104175	6	15.50	700415	20.0
Heptadecane, 9-oc...	16.44	3.6	ng	127873	6	15.50	700415	20.0
Hexacosane	17.03	3.1	ng	107538	6	15.50	700415	20.0
Eicosane	17.73	3.4	ng	119655	6	15.50	700415	20.0
Octacosane	18.56	2.0	ng	71425	6	15.50	700415	20.0