LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085696.D
Acq On : 23 Mar 2016 9:55
Operator : UM/SJ
Sample : H1857-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(13-15)

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-BF031816.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	5.018	237	239	251	rBV	286468	443195	13.07%	1.509%
2	5.441	272	276	278	rBV	2361618	3348513	98.71%	11.400%
3	5.841	309	311	313	rVB	26207	36174	1.07%	0.123%
4	6.470	363	366	369	rBV	2625544	3022211	89.09%	10.289%
5	6.596	375	377	380	rBV	2449648	3392135	100.00%	11.548%
6	6.836	395	398	400	rBV	556956	714689	21.07%	2.433%
7	6.984	409	411	414	rBV	2294300	2294718	67.65%	7.812%
8	7.247	429	434	441	rBV	41260	64862	1.91%	0.221%
9	7.396	444	447	450	rVV	1904221	2071867	61.08%	7.053%
10	7.864	485	488	489	rBV	25097	36576	1.08%	0.125%
11	8.116	507	510	512	rBV	1176505	1018676	30.03%	3.468%
12	9.190	601	604	607	rBV	2805548	3015020	88.88%	10.264%
13	9.590	636	639	641	rBV	677969	627912	18.51%	2.138%
14	9.808	654	658	659	rBV	62197	76142	2.24%	0.259%
15	9.865	661	663	666	rVB	955819	1068153	31.49%	3.636%
16	10.036	674	678	681	rBV2	16713	40051	1.18%	0.136%
17	10.299	699	701	703	rVB	116227	111491	3.29%	0.380%
18	10.516	717	720	724	rBV	36447	75089	2.21%	0.256%
19	10.653	729	732	735	rBV2	1553118	2221535	65.49%	7.563%
20	10.779	741	743	749	rVB	92412	170754	5.03%	0.581%
21	10.962	757	759	764	rBV	18777	38979	1.15%	0.133%
22	11.225	780	782	783	rBV	46521	55862	1.65%	0.190%
23	11.351	791	793	795	rBV	1247616	1041994	30.72%	3.547%
24	11.876	838	839	850	rVB	77430	110510	3.26%	0.376%
25	12.756	914	916	918	rVB	51252	40918	1.21%	0.139%
26	12.939	929	932	934	rBV	2089750	2565986	75.65%	8.736%
27	13.831	1008	1010	1019	rBV	182968	294134	8.67%	1.001%
28	13.979	1021	1023	1026	rVB	725980	647218	19.08%	2.203%
29	14.448	1062	1064	1071	rBV2	19649	53312	1.57%	0.181%
30	15.397	1145	1147	1150	rBV	460724	593986	17.51%	2.022%
31	17.648	1341	1344	1349	rBV7	11021	35954	1.06%	0.122%
32	18.288	1395	1400	1405	rBV6	13041	45475	1.34%	0.155%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085696.D
Acq On : 23 Mar 2016 9:55
Operator : UM/SJ
Sample : H1857-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02(13-15)

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-BF031816.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

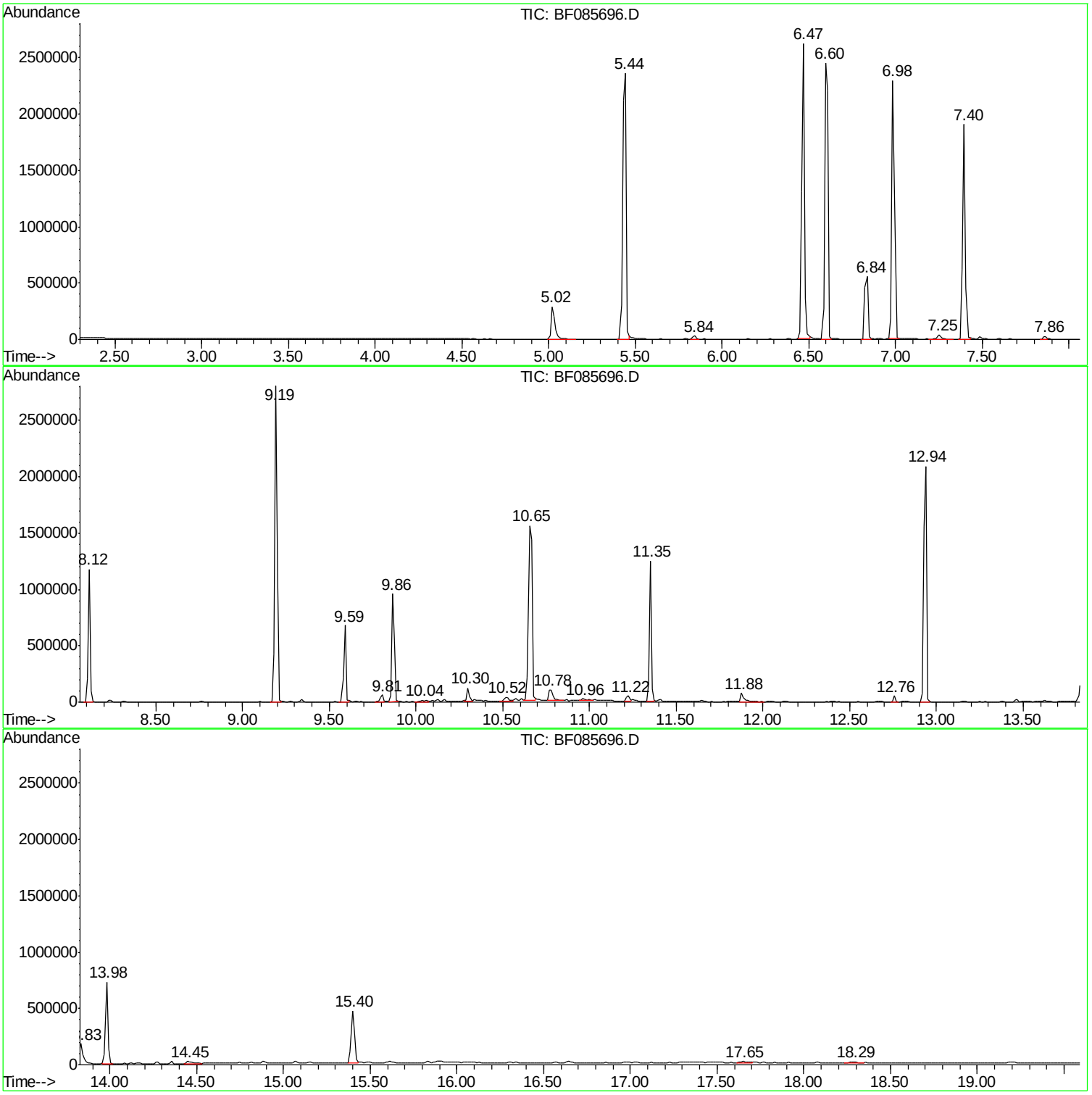
Sum of corrected areas: 29374091

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085696.D
Acq On : 23 Mar 2016 9:55
Operator : UM/SJ
Sample : H1857-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085696.D
Acq On : 23 Mar 2016 9:55
Operator : UM/SJ
Sample : H1857-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

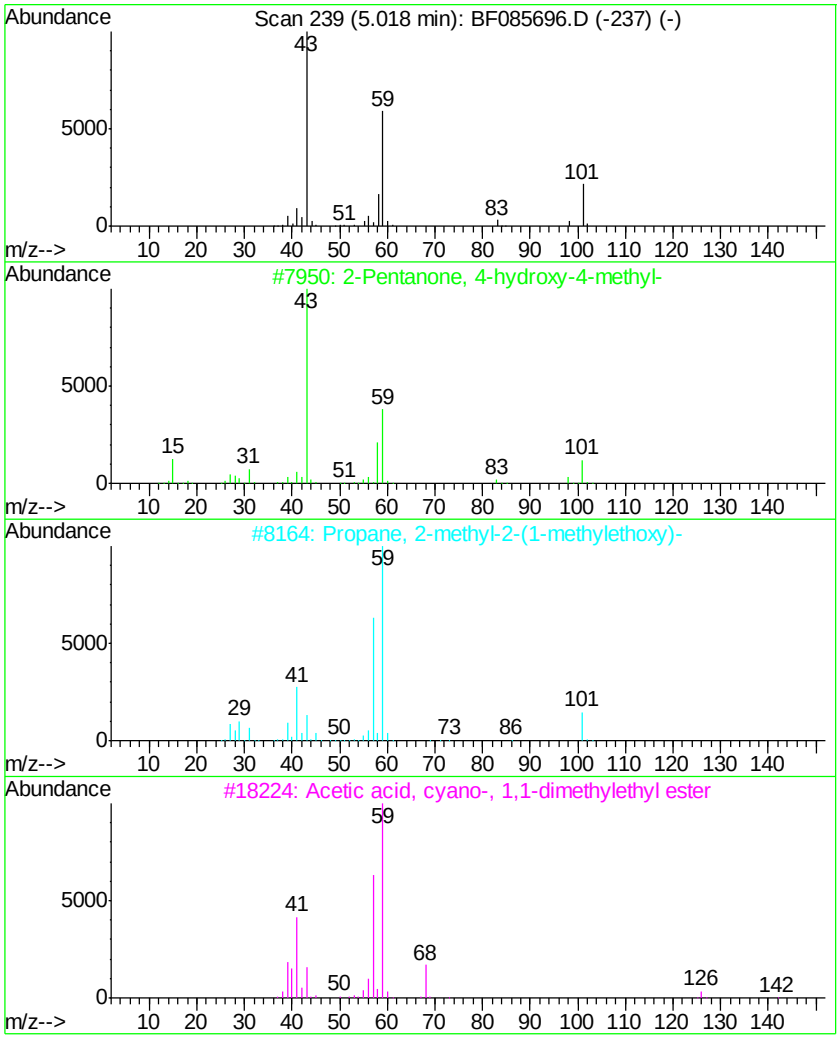
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

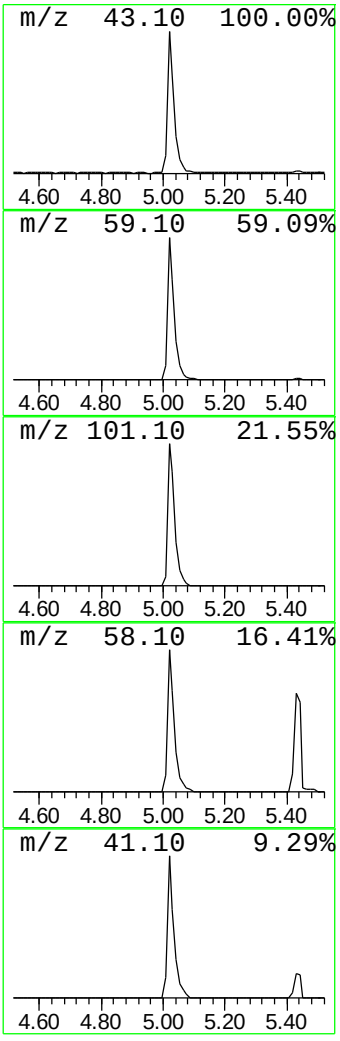
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	12.40 ng	443195	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085696.D
Acq On : 23 Mar 2016 9:55
Operator : UM/SJ
Sample : H1857-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

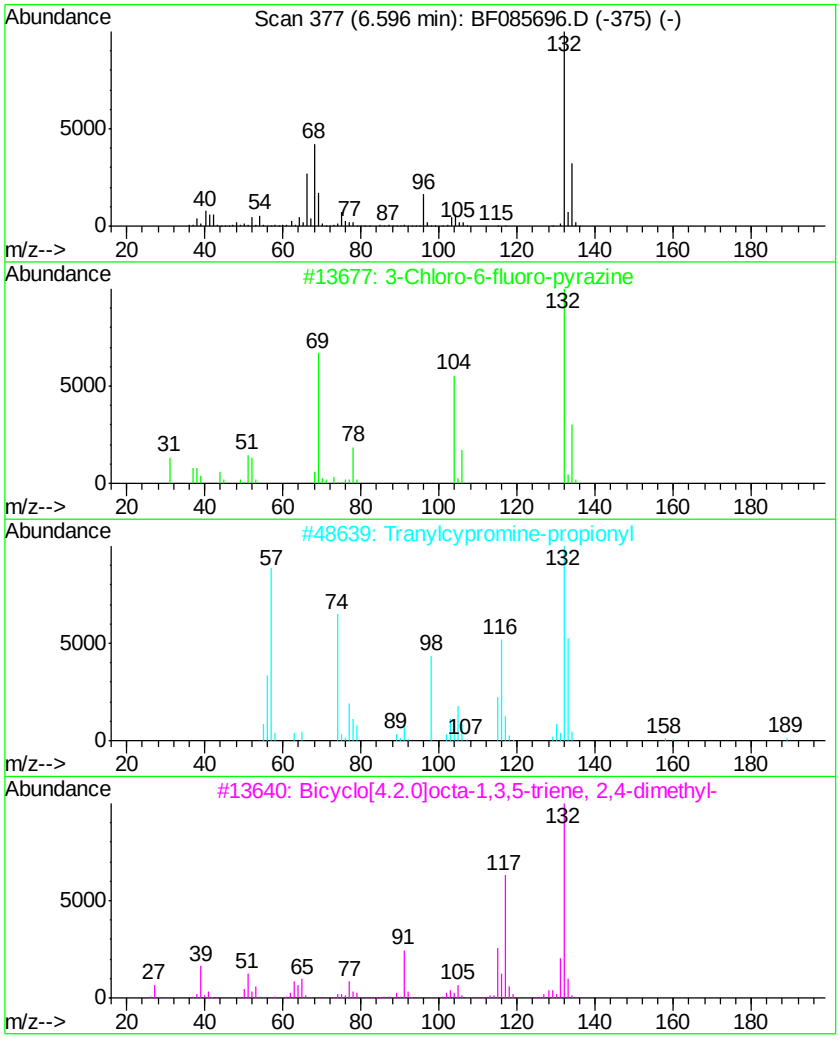
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

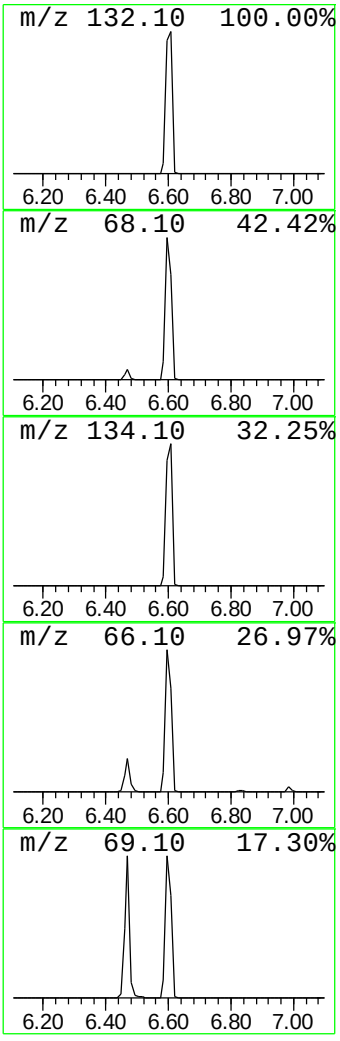
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	94.93 ng	3392140	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085696.D
Acq On : 23 Mar 2016 9:55
Operator : UM/SJ
Sample : H1857-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

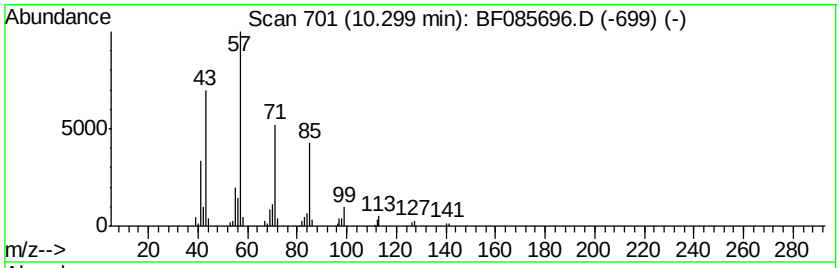
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

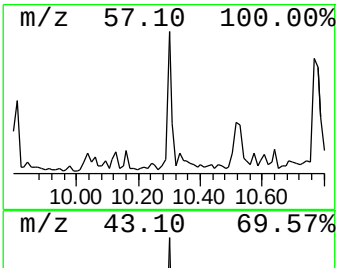
****

Peak Number 4 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.30	2.09 ng	111491	Acenaphthene-d10	9.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Eicosane	282	C20H42	000112-95-8	86
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
4	Tridecane	184	C13H28	000629-50-5	78
5	Pentadecane	212	C15H32	000629-62-9	78





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085696.D
Acq On : 23 Mar 2016 9:55
Operator : UM/SJ
Sample : H1857-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

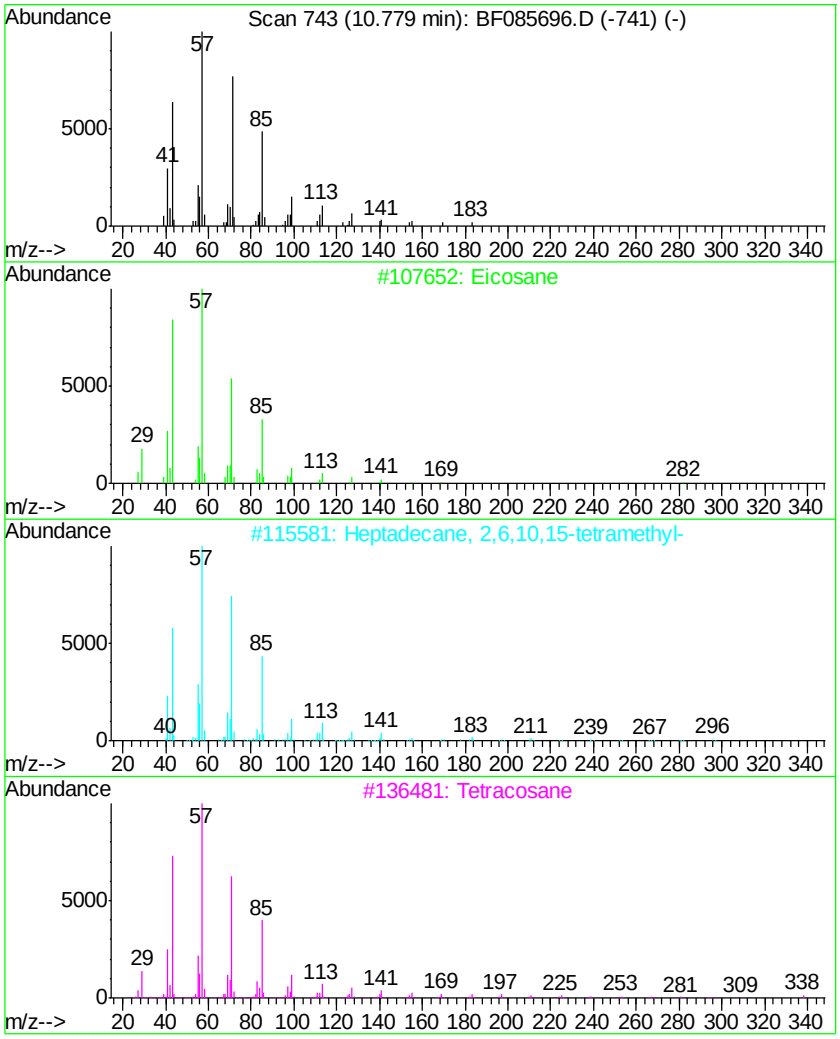
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

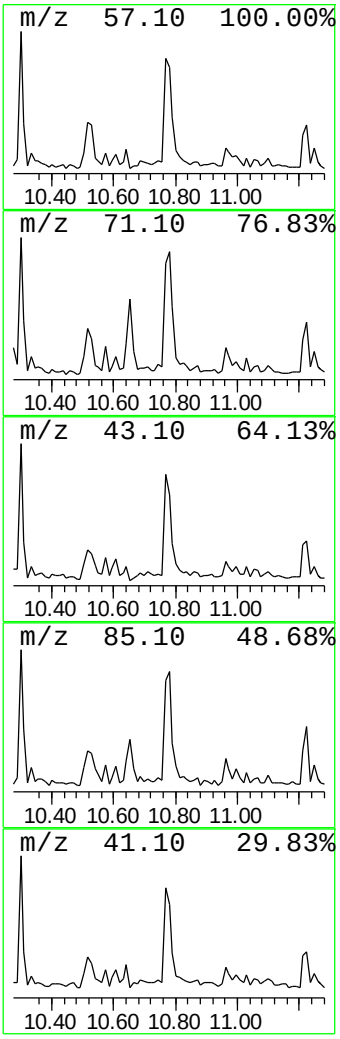
****

Peak Number 5 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	3.28 ng	170754	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Pentadecane	212	C15H32	000629-62-9	91
5	Hexadecane	226	C16H34	000544-76-3	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085696.D
Acq On : 23 Mar 2016 9:55
Operator : UM/SJ
Sample : H1857-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

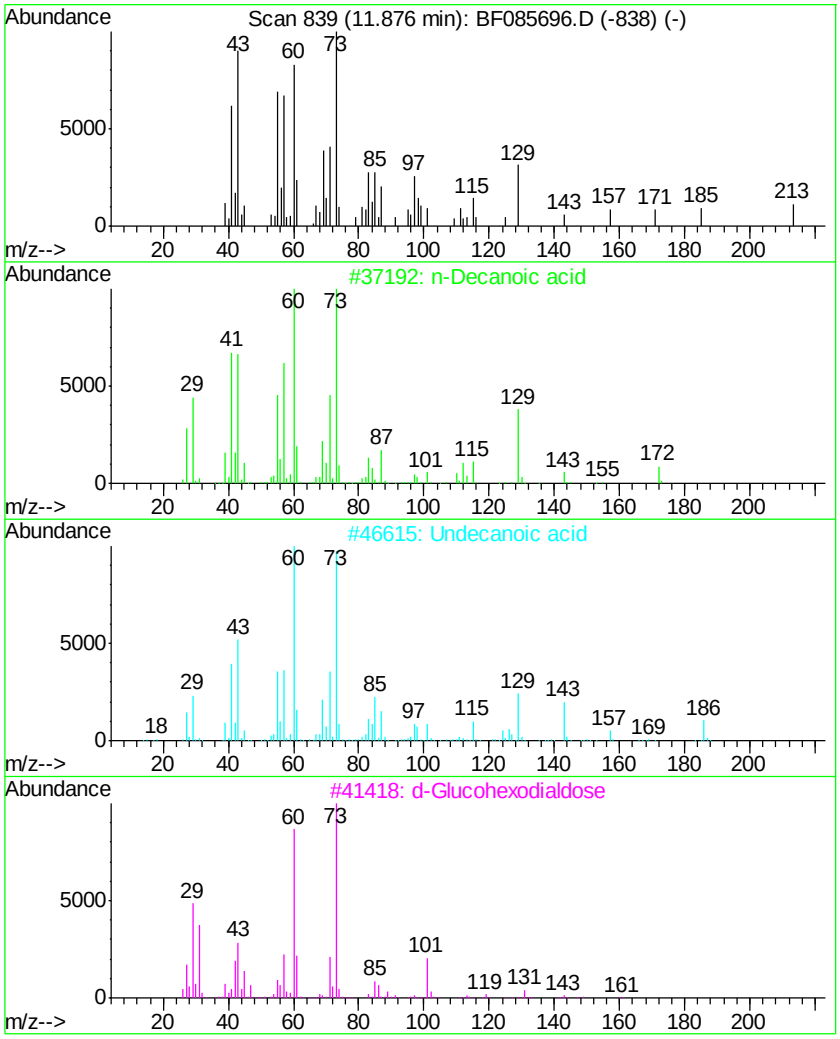
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

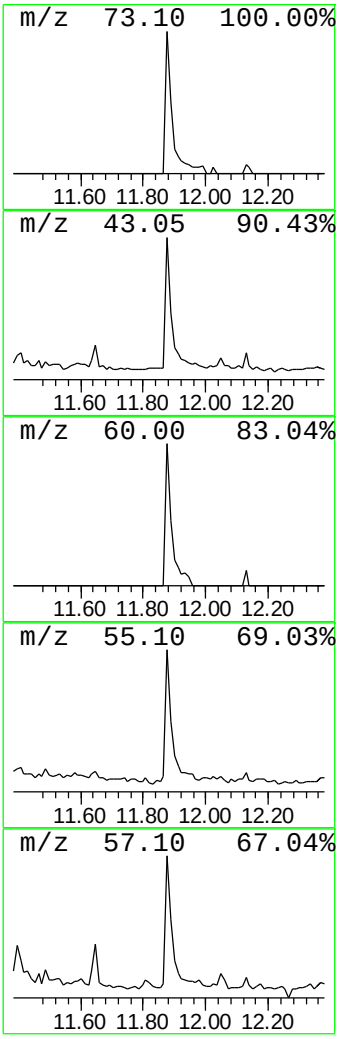
****

Peak Number 6 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	2.12 ng	110510	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	59
2	Undecanoic acid	186	C11H22O2	000112-37-8	43
3	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38
4	Sedoheptulosan	192	C7H12O6	000469-90-9	27
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	14





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085696.D
Acq On : 23 Mar 2016 9:55
Operator : UM/SJ
Sample : H1857-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

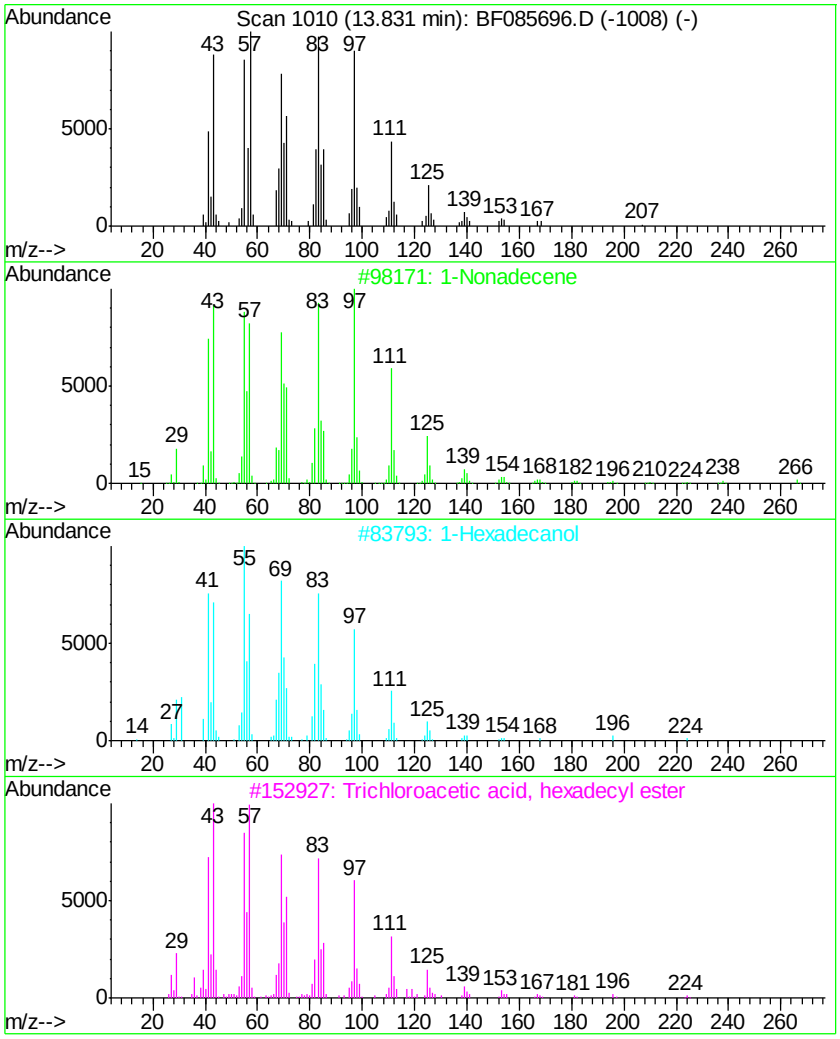
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

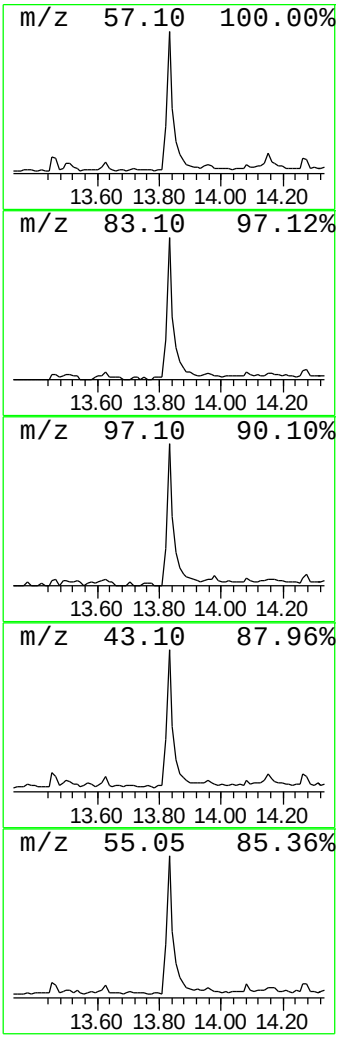
****

Peak Number 7 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	9.09 ng	294134	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	87
2	1-Hexadecanol	242	C16H34O	036653-82-4	87
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4	1-Heptadecanol	256	C17H36O	001454-85-9	87
5	1-Tetracosanol	354	C24H50O	000506-51-4	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085696.D
Acq On : 23 Mar 2016 9:55
Operator : UM/SJ
Sample : H1857-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	12.4	ng	443195	1	6.84	714689	20.0
unknown6.60	6.60	94.9	ng	3392140	1	6.84	714689	20.0
Heptadecane	10.30	2.1	ng	111491	3	9.86	1068150	20.0
Eicosane	10.78	3.3	ng	170754	4	11.35	1041990	20.0
n-Decanoic acid	11.88	2.1	ng	110510	4	11.35	1041990	20.0
1-Nonadecene	13.83	9.1	ng	294134	5	13.98	647218	20.0