LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-15(6-12FTBGS)

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-BF042716.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	4.967	249	252	260	rBV	80190	118302	3.10%	0.330%
2	5.390	286	289	291	rBV	2572071	3647529	95.57%	10.167%
3	6.430	377	380	382	rBV	3493314	3801930	99.62%	10.598%
4	6.556	388	391	394	rBV	3681426	3596032	94.22%	10.024%
5	6.625	395	397	400	rVB	65422	63769	1.67%	0.178%
6	6.785	409	411	414	rBV	931550	963597	25.25%	2.686%
7	6.945	422	425	427	rBV	3107298	2808489	73.59%	7.829%
8	7.356	458	461	463	rBV	2360594	2429363	63.65%	6.772%
9	7.459	467	470	477	rVB	74474	143611	3.76%	0.400%
10	8.076	521	524	526	rBV	1465704	1300711	34.08%	3.626%
11	9.150	616	618	621	rBV	2807750	3816475	100.00%	10.638%
12	9.550	651	653	655	rBV	649475	559590	14.66%	1.560%
13	9.733	664	669	671	rBV	49283	101811	2.67%	0.284%
14	9.768	671	672	675	rVB	87214	60116	1.58%	0.168%
15	9.825	675	677	680	rBV	1215127	1262633	33.08%	3.520%
16	10.236	711	713	714	rBV	50113	65341	1.71%	0.182%
17	10.271	714	716	717	rVB	133248	130761	3.43%	0.364%
18	10.488	732	735	736	rBV	59840	80636	2.11%	0.225%
19	10.613	744	746	749	rBV	1889412	1933768	50.67%	5.390%
20	10.739	755	757	762	rVB	205914	234473	6.14%	0.654%
21	10.934	772	774	776	rBV	29703	39883	1.05%	0.111%
22	11.185	795	796	798	rBV	122710	100727	2.64%	0.281%
23	11.311	805	807	808	rBV	1106918	1041315	27.28%	2.903%
24	11.379	811	813	819	rVB2	40558	81156	2.13%	0.226%
25	11.539	825	827	832	rBV	177788	222896	5.84%	0.621%
26	11.608	832	833	840	rVB	66320	90808	2.38%	0.253%
27	11.916	858	860	865	rVB3	25625	48953	1.28%	0.136%
28	12.019	867	869	870	rVV	56517	49106	1.29%	0.137%
29	12.099	874	876	881	rBV4	16252	38464	1.01%	0.107%
30	12.408	900	903	905	rBV	41481	40002	1.05%	0.112%
31	12.511	910	912	915	rBV	112029	173178	4.54%	0.483%
32	12.739	928	932	934	rBV	133085	232009	6.08%	0.647%
33	12.899	943	946	948	rBV	2317812	2765422	72.46%	7.708%
34	13.128	964	966	968	rVB2	35141	45541	1.19%	0.127%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-15(6-12FTBGS)

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-BF042716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.368	986	987	991	rVB	51350	52680	1.38%	0.147%
36	13.471	994	996	1000	rVV	56195	81186	2.13%	0.226%
37	13.802	1022	1025	1029	rVB	162246	268664	7.04%	0.749%
38	13.940	1034	1037	1044	rVV	822761	1147010	30.05%	3.197%
39	14.042	1044	1046	1051	rVV3	30342	54106	1.42%	0.151%
40	14.122	1051	1053	1055	rVV	75877	95358	2.50%	0.266%
41	14.328	1069	1071	1075	rVB2	23327	44153	1.16%	0.123%
42	14.420	1077	1079	1081	rBV	90092	103591	2.71%	0.289%
43	14.694	1101	1103	1108	rBV2	222773	330788	8.67%	0.922%
44	14.945	1123	1125	1130	rVB	76662	155030	4.06%	0.432%
45	15.037	1130	1133	1136	rBV2	38093	80557	2.11%	0.225%
46	15.231	1147	1150	1152	rBV	38774	64385	1.69%	0.179%
47	15.288	1152	1155	1157	rVV	39212	71525	1.87%	0.199%
48	15.345	1157	1160	1167	rVB	576311	836186	21.91%	2.331%
49	15.791	1196	1199	1201	rBV	40827	69969	1.83%	0.195%
50	16.740	1279	1282	1286	rVB2	181990	331498	8.69%	0.924%

Sum of corrected areas: 35875083

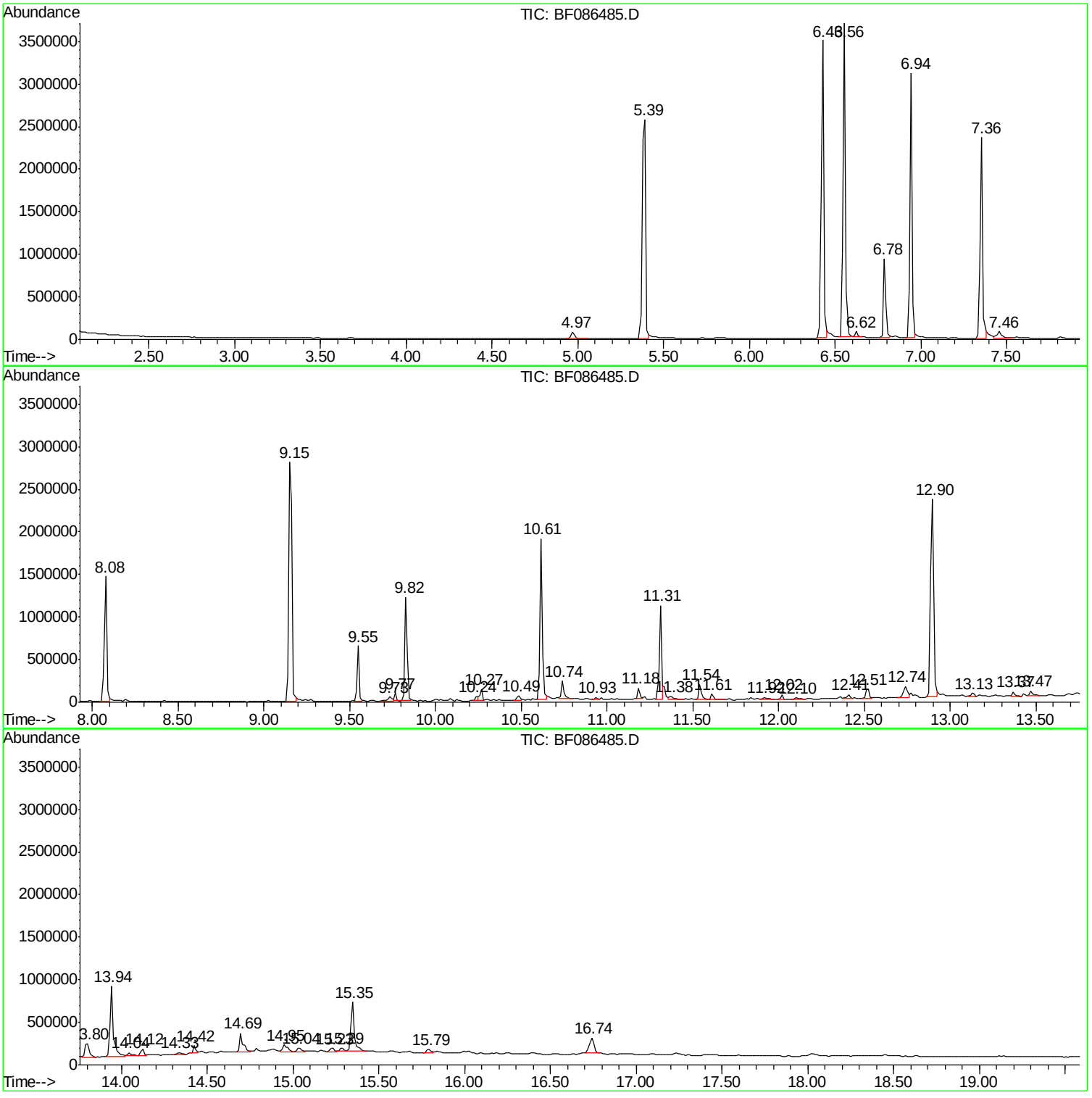
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

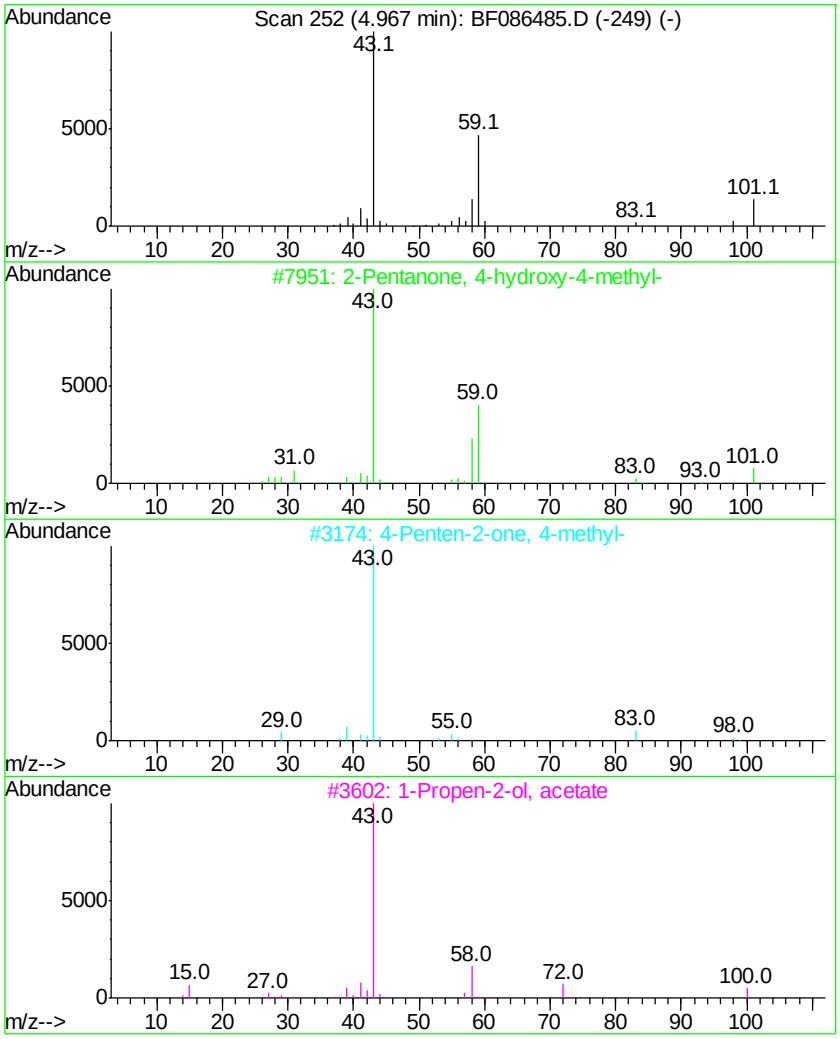
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

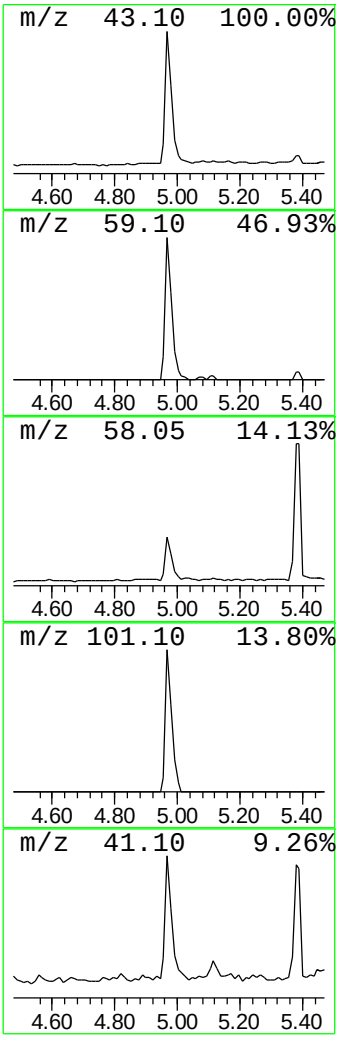
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	2.46 ng	118302	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane	58	C4H10	000106-97-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

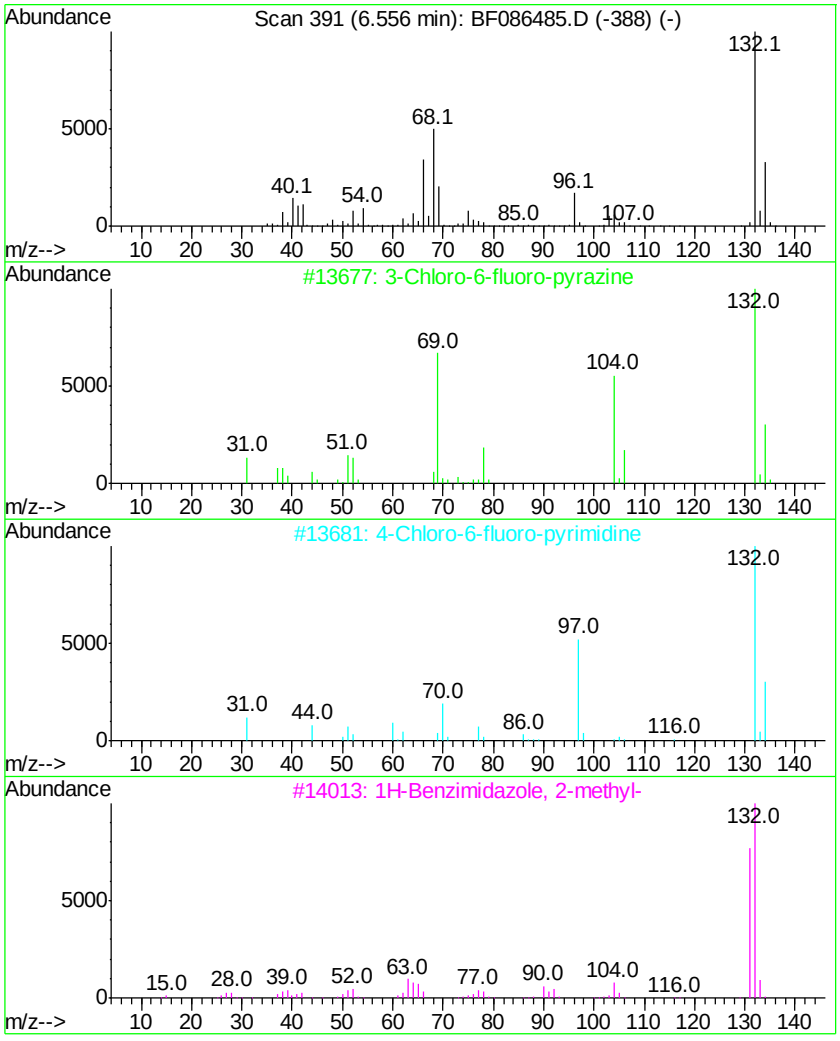
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

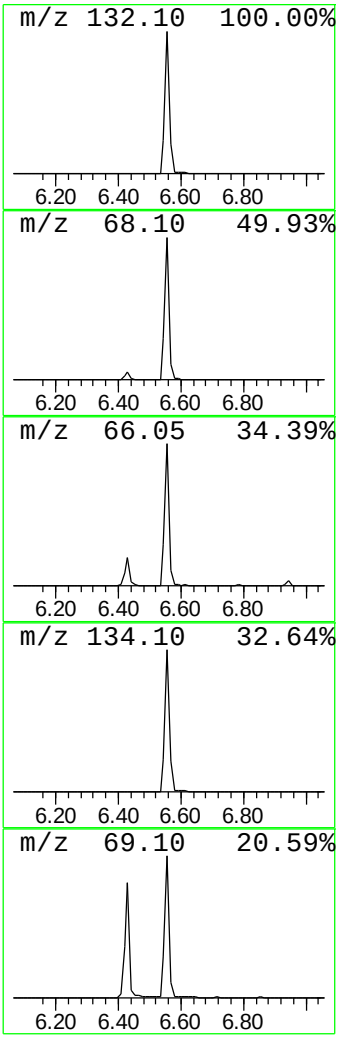
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	74.64 ng	3596030	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

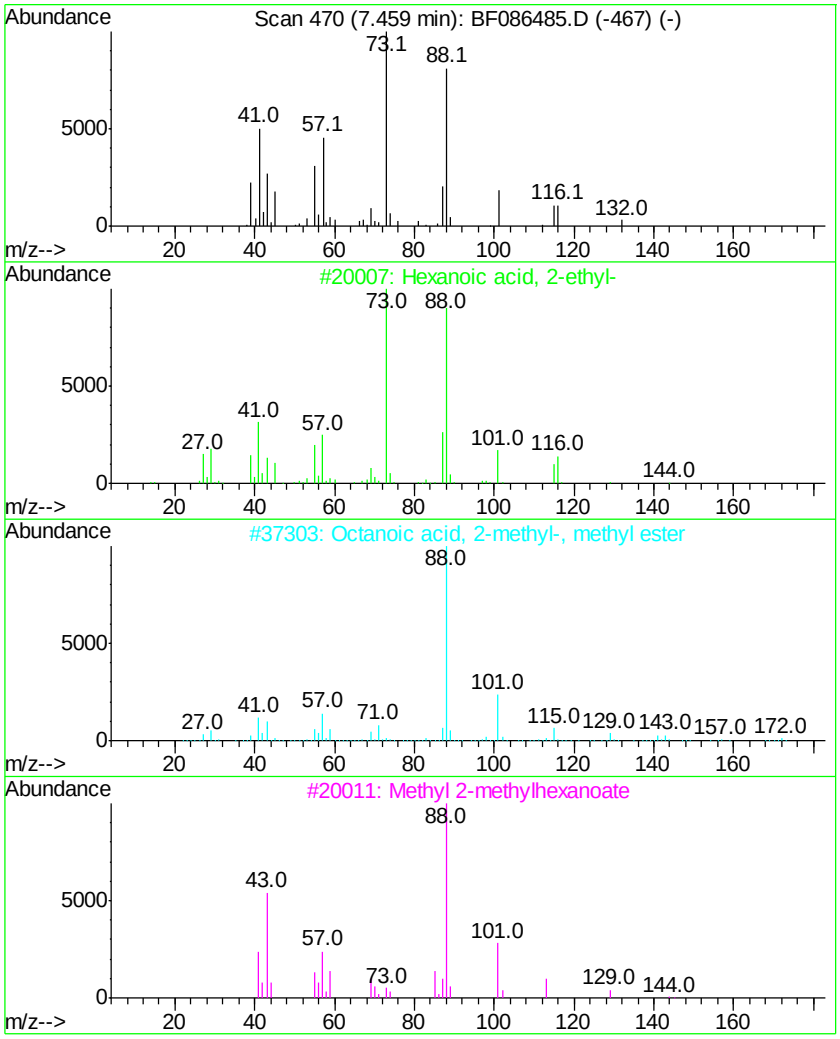
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

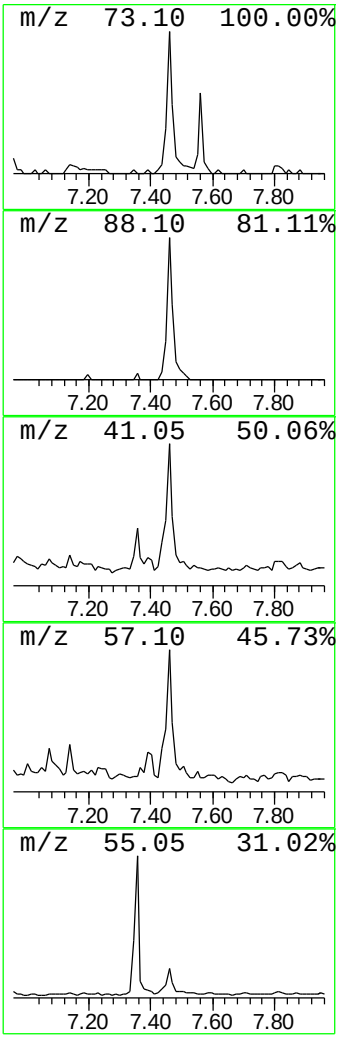
****

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	2.21 ng	143611	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	36
3	Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	33
4	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	33
5	Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	33





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

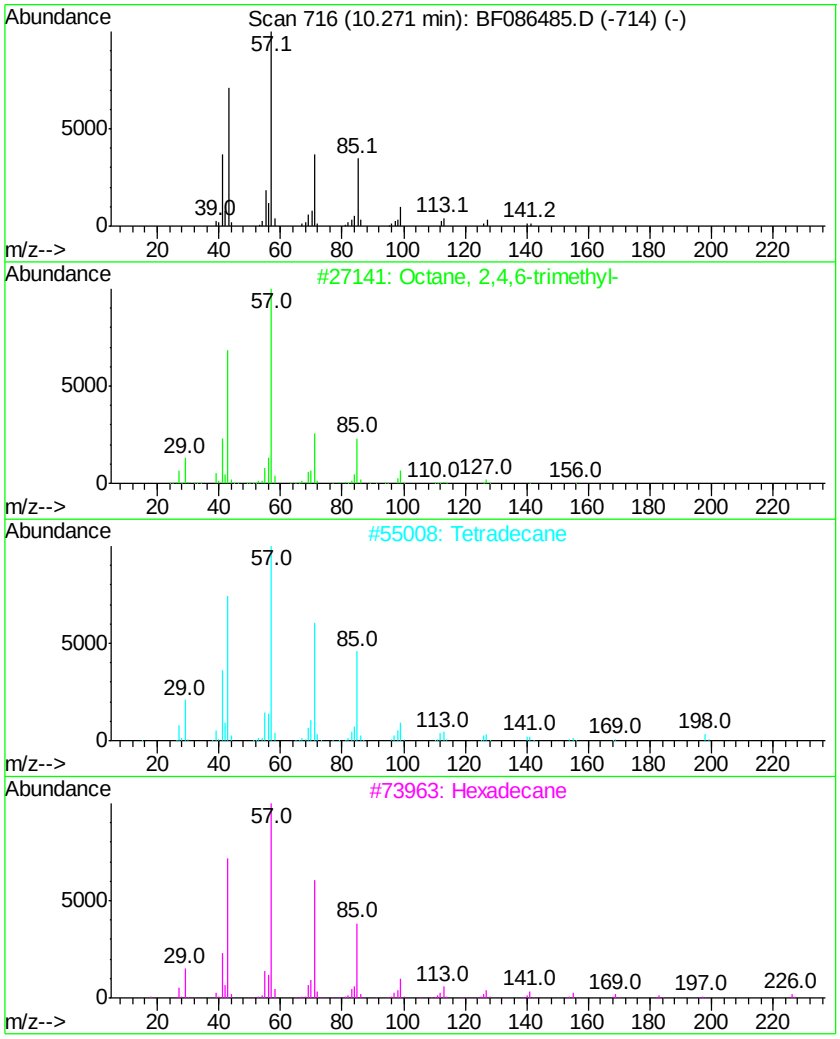
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

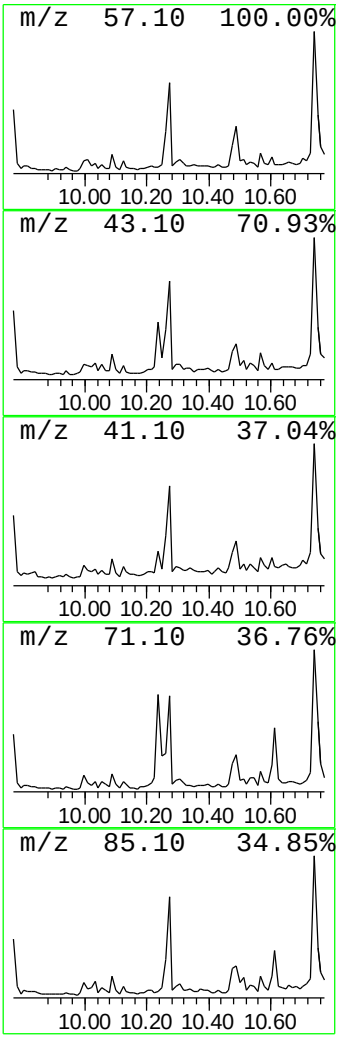
****

Peak Number 5 Octane, 2,4,6-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.07 ng	130761	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Hexadecane	226	C16H34	000544-76-3	83
4	Pentadecane	212	C15H32	000629-62-9	78
5	Tridecane	184	C13H28	000629-50-5	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

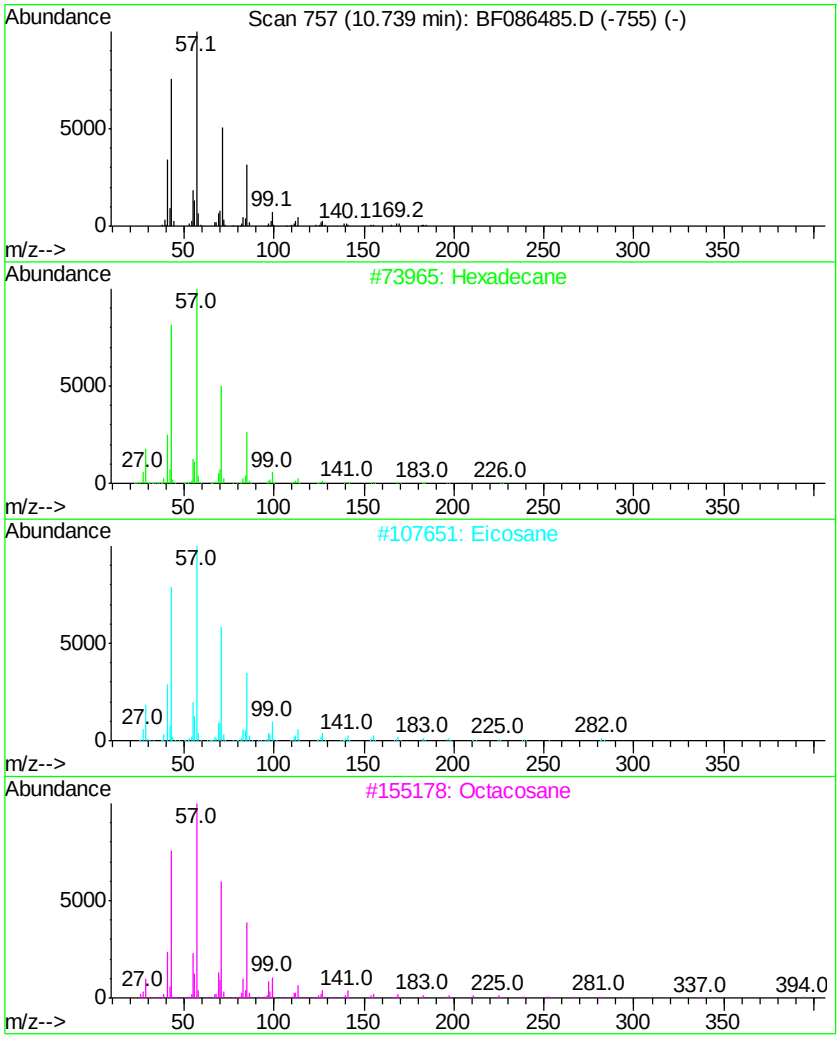
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

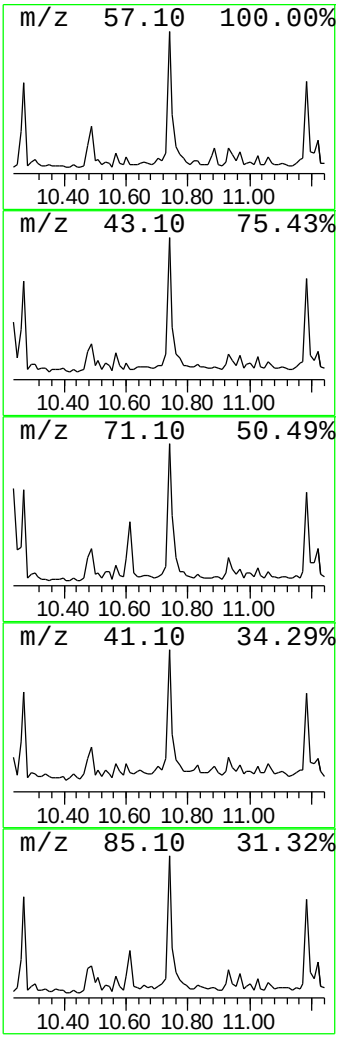
****

Peak Number 6 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	4.50 ng	234473	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	86
3	Octacosane	394	C28H58	000630-02-4	78
4	Tridecane	184	C13H28	000629-50-5	78
5	Tetradecane	198	C14H30	000629-59-4	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

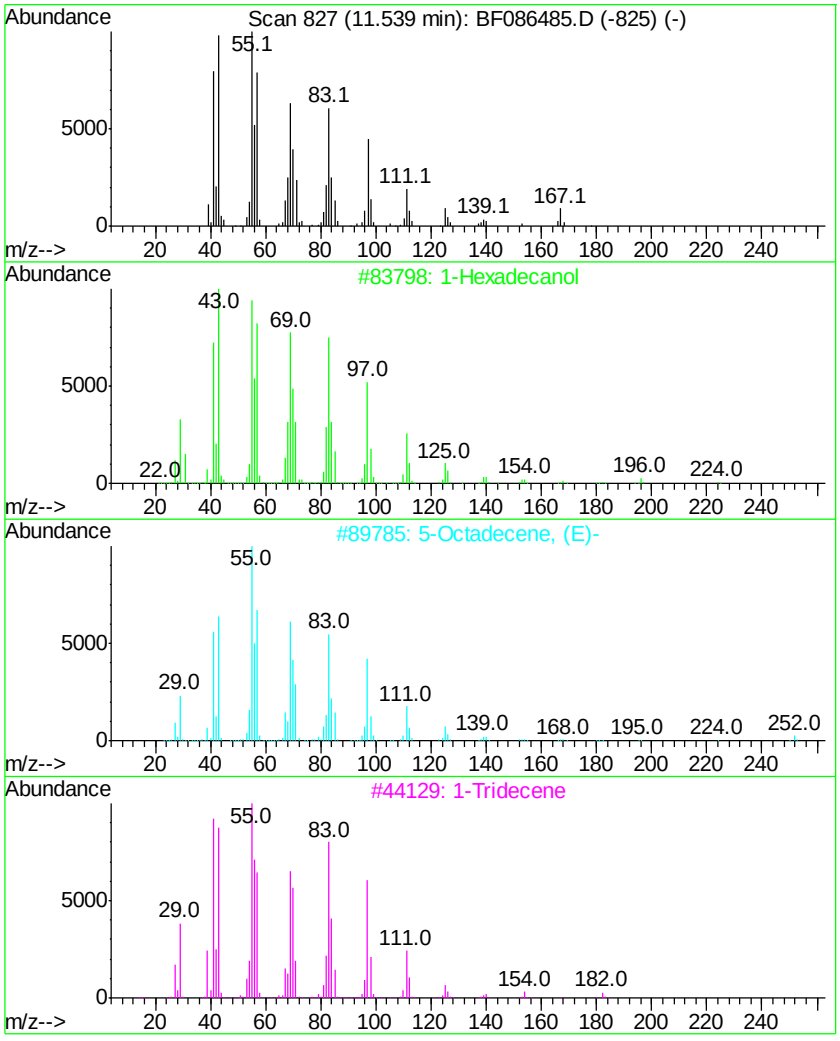
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

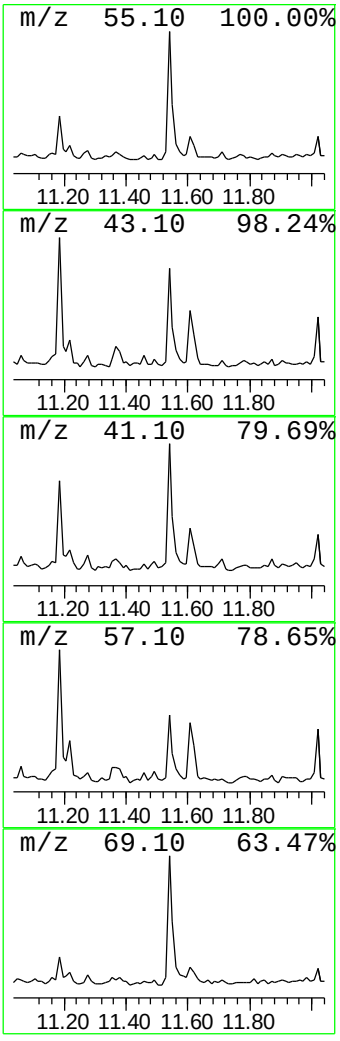
****

Peak Number 7 1-Hexadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	4.28 ng	222896	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	95
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
3	1-Tridecene	182	C13H26	002437-56-1	87
4	1-Dodecene	168	C12H24	000112-41-4	87
5	1-Hexadecene	224	C16H32	000629-73-2	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

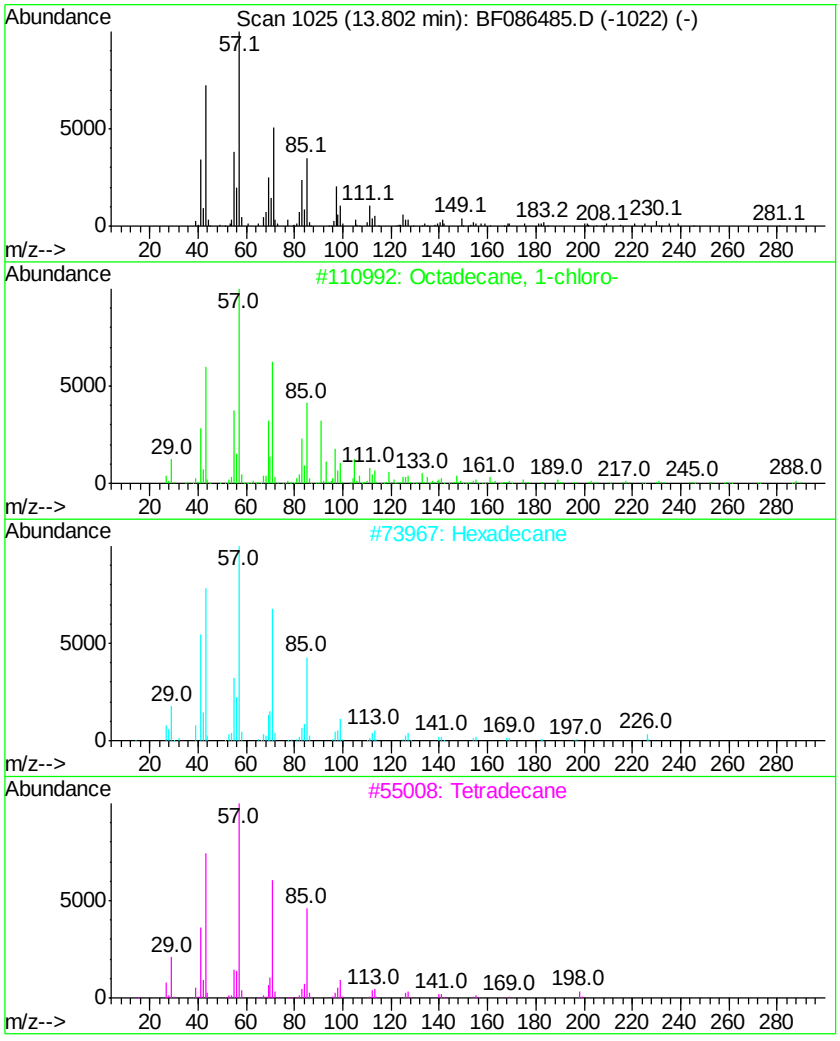
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

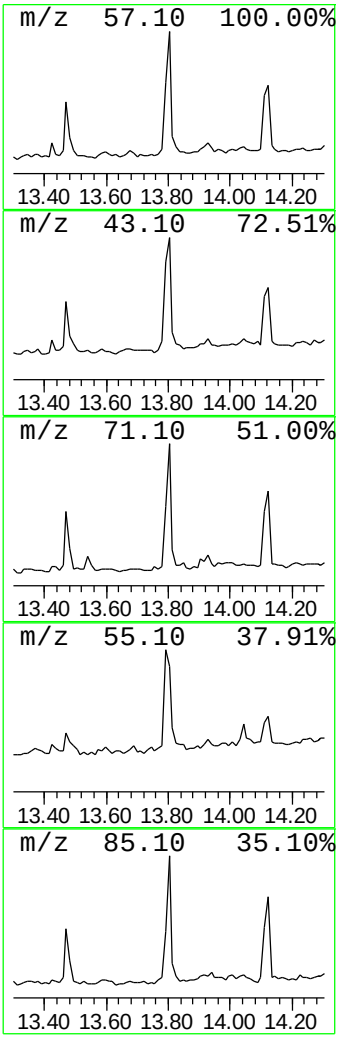
****

Peak Number 8 Octadecane, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	4.68 ng	268664	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	80
2	Hexadecane	226	C16H34	000544-76-3	53
3	Tetradecane	198	C14H30	000629-59-4	53
4	Nonadecane	268	C19H40	000629-92-5	52
5	Tridecane	184	C13H28	000629-50-5	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

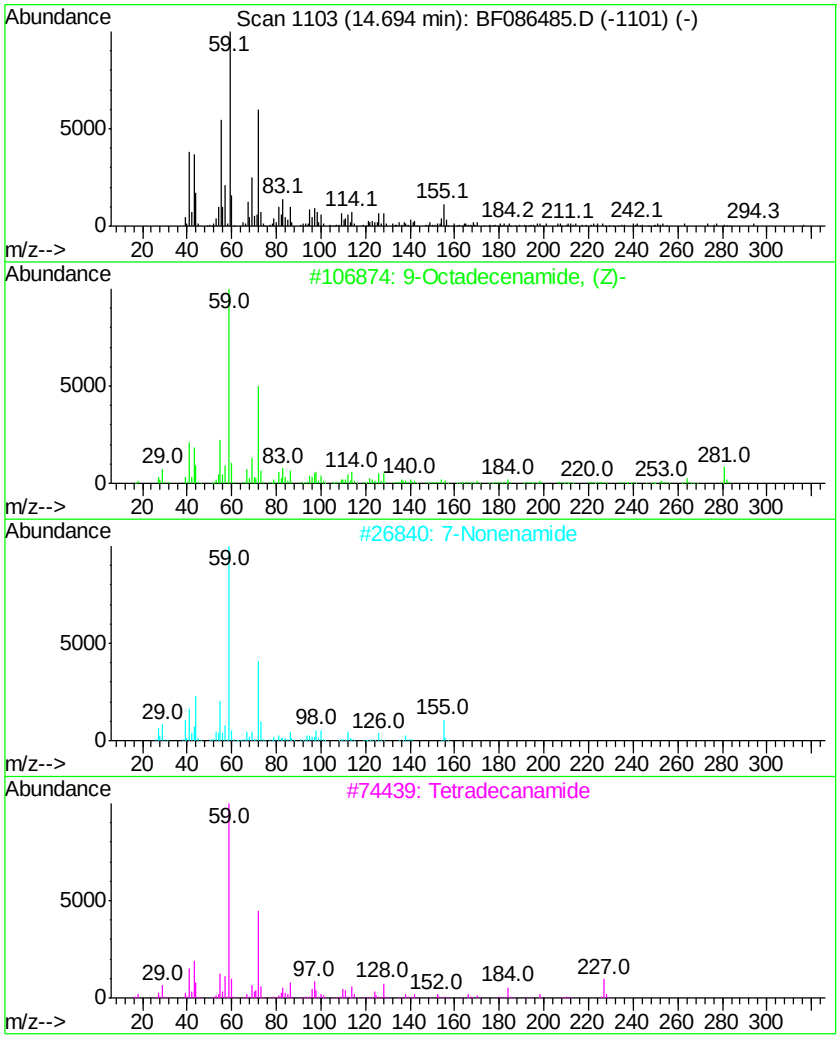
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

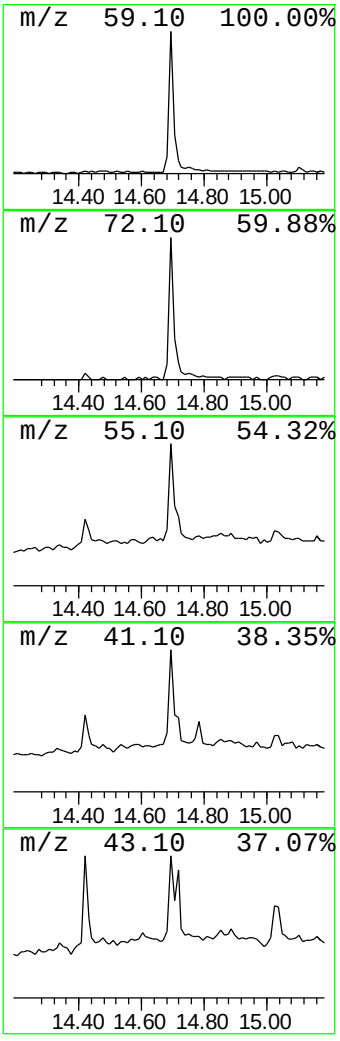
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	7.91 ng	330788	Perylene-d12	15.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	7-Nonenamide	155	C9H17NO	090949-53-4	81
3	Tetradecanamide	227	C14H29NO	000638-58-4	78
4	Hexadecanamide	255	C16H33NO	000629-54-9	72
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

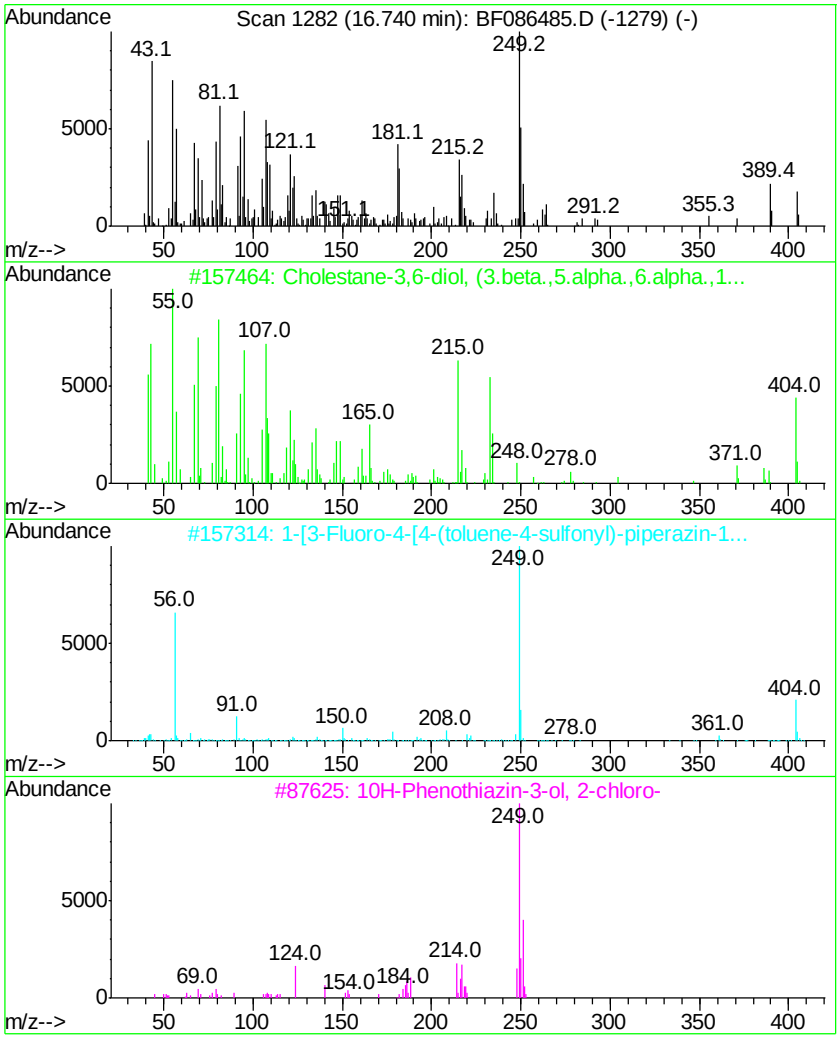
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

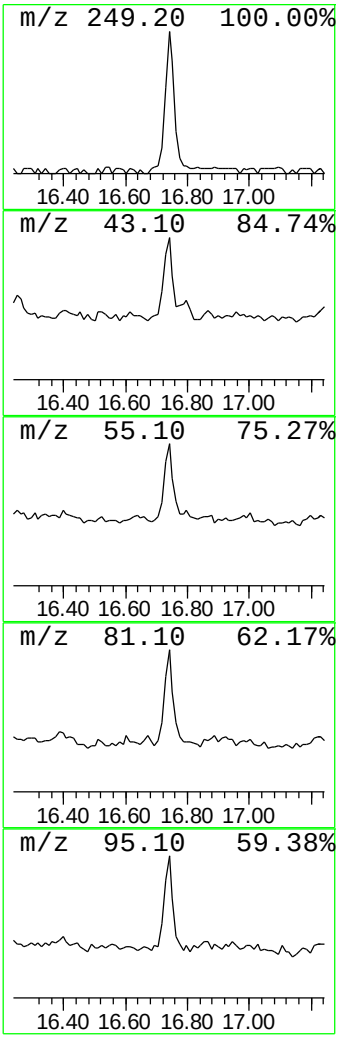
****

Peak Number 10 Cholestane-3,6-diol, (3.bet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	7.93 ng	331498	Perylene-d12	15.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestane-3,6-diol, (3.beta.,5....	404	C27H48O2	041083-77-6	62
2	1-[3-Fluoro-4-[4-(toluene-4-sulf...	404	C21H25FN2O3S	333751-65-8	22
3	10H-Phenothiazin-3-ol, 2-chloro-	249	C12H8ClNOS	016770-99-3	18
4	5-Methylsulfonyl-6-phenyl-pyrid-...	249	C12H11NO3S	034502-64-2	14
5	10H-Phenothiazin-3-ol, 8-chloro-	249	C12H8ClNOS	002002-32-6	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042816\
Data File : BF086485.D
Acq On : 29 Apr 2016 2:24
Operator : UM/SJ
Sample : H2654-14
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-15(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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...	4.97	2.5	ng	118302	1	6.78	963597	20.0
unknown6.56	6.56	74.6	ng	3596030	1	6.78	963597	20.0
Hexanoic acid, 2-...	7.46	2.2	ng	143611	2	8.08	1300710	20.0
Octane, 2,4,6-tri...	10.27	2.1	ng	130761	3	9.82	1262630	20.0
Hexadecane	10.74	4.5	ng	234473	4	11.31	1041320	20.0
1-Hexadecanol	11.54	4.3	ng	222896	4	11.31	1041320	20.0
Octadecane, 1-chl...	13.80	4.7	ng	268664	5	13.94	1147010	20.0
9-Octadecenamide,...	14.69	7.9	ng	330788	6	15.35	836186	20.0
Cholestane-3,6-di...	16.74	7.9	ng	331498	6	15.35	836186	20.0