LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

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-BF060716.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	1.678	7	8	17	rVV	254372	406890	12.56%	1.517%
2	1.804	17	19	63	rVB	1472330	3239765	100.00%	12.078%
3	4.890	286	289	300	rVB	96122	145870	4.50%	0.544%
4	5.313	323	326	328	rBV	2061117	2171911	67.04%	8.097%
5	6.365	415	418	421	rBV	1842829	2051299	63.32%	7.647%
6	6.490	426	429	431	rBV	2189603	2407936	74.32%	8.977%
7	6.719	447	449	451	rBV	822240	718618	22.18%	2.679%
8	6.879	460	463	465	rVB	1599710	1919727	59.26%	7.157%
9	7.290	496	499	501	rBV	1573372	1647312	50.85%	6.141%
10	7.999	559	561	564	rBV	855435	939736	29.01%	3.503%
11	9.085	653	656	658	rBV	2676102	2561585	79.07%	9.550%
12	9.473	688	690	692	rVB	400997	512617	15.82%	1.911%
13	9.748	712	714	717	rVB	776516	1043496	32.21%	3.890%
14	10.194	752	753	755	rVB	94098	67567	2.09%	0.252%
15	10.411	769	772	775	rBV	30428	46347	1.43%	0.173%
16	10.536	781	783	786	rBV2	1210613	1390932	42.93%	5.185%
17	10.662	792	794	799	rVB	108742	116629	3.60%	0.435%
18	11.108	831	833	835	rBV	57267	51639	1.59%	0.193%
19	11.234	842	844	846	rBV	1110618	1006456	31.07%	3.752%
20	11.771	889	891	895	rBV	48574	84355	2.60%	0.314%
21	12.434	948	949	952	rBV3	32432	32868	1.01%	0.123%
22	12.651	966	968	971	rBV2	148591	198201	6.12%	0.739%
23	12.719	973	974	976	rVB	41944	37871	1.17%	0.141%
24	12.811	980	982	985	rVB	1426976	1811540	55.92%	6.754%
25	13.348	1027	1029	1031	rBV	106761	97064	3.00%	0.362%
26	13.714	1059	1061	1068	rBV	135730	199635	6.16%	0.744%
27	13.862	1071	1074	1076	rBV	780829	791091	24.42%	2.949%
28	14.342	1113	1116	1121	rBV3	28472	62054	1.92%	0.231%
29	14.617	1138	1140	1144	rBV3	47886	82480	2.55%	0.307%
30	14.868	1159	1162	1166	rBV	43035	89624	2.77%	0.334%
31	14.960	1166	1170	1172	rBV2	22051	49557	1.53%	0.185%
32	15.131	1184	1185	1189	rVB	26020	35875	1.11%	0.134%
33	15.200	1189	1191	1193	rBV	33169	50137	1.55%	0.187%
34	15.245	1193	1195	1198	rBV	566175	712161	21.98%	2.655%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.571	1308	1311	1314	rBV	22259	42708	1.32%	0.159%

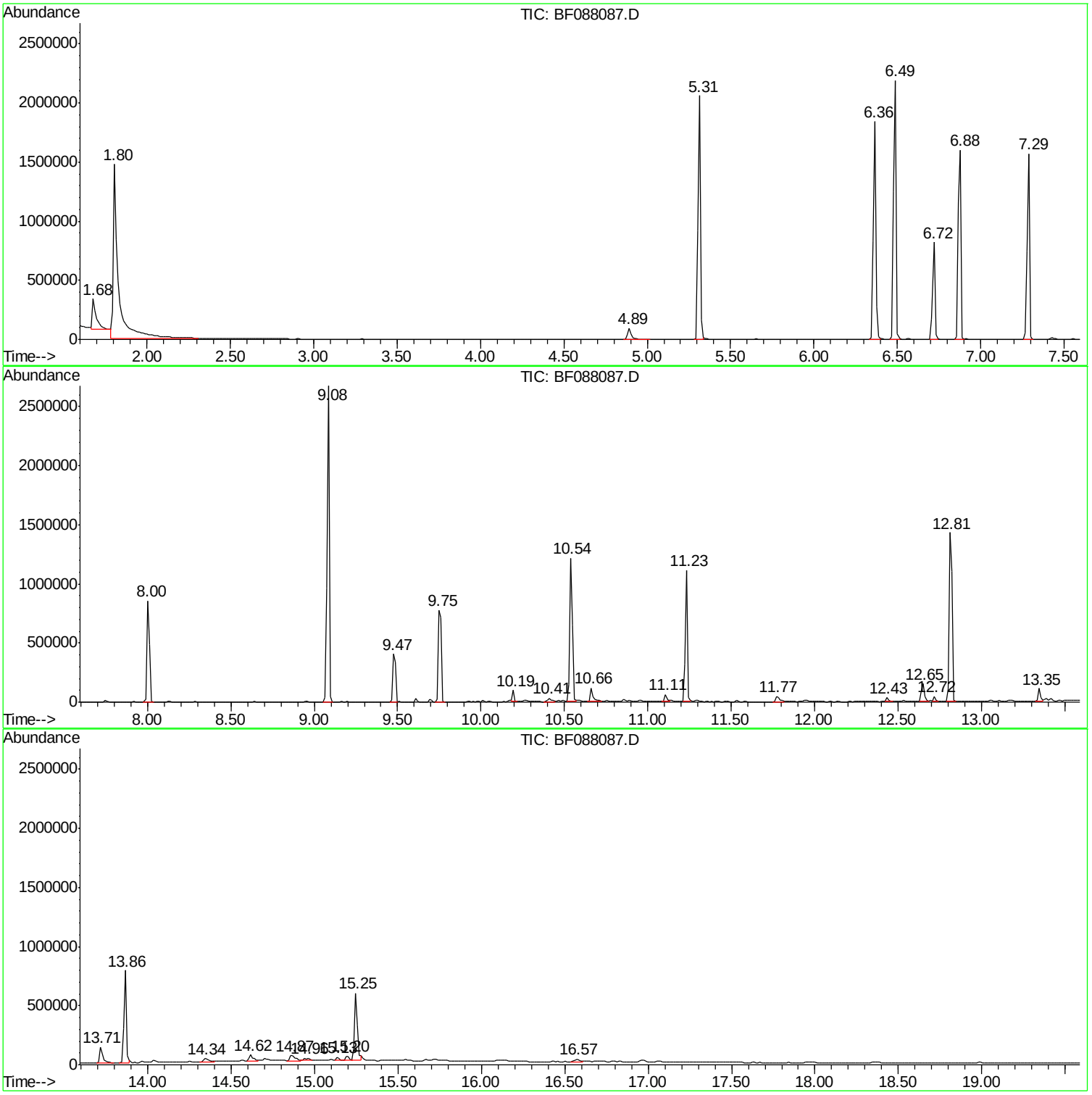
Sum of corrected areas: 26823553

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

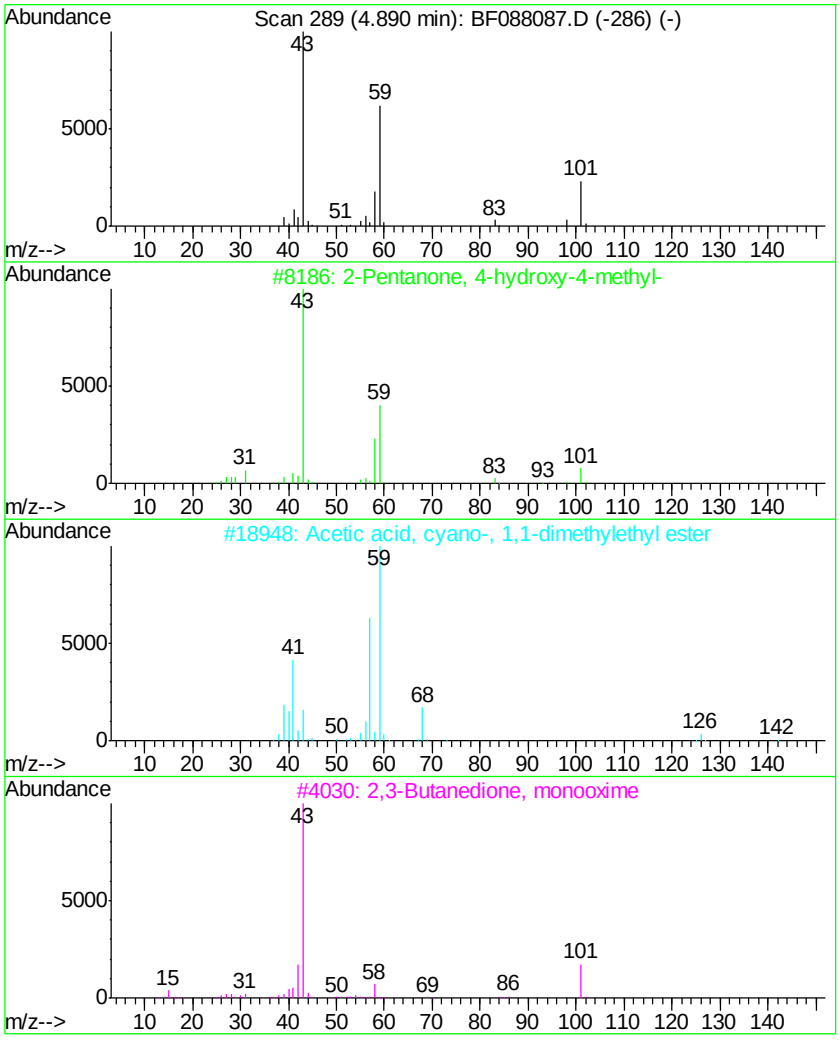
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

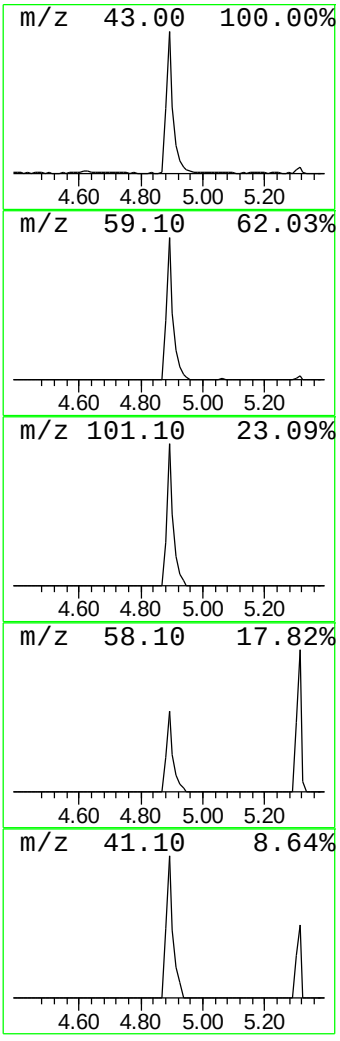
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	4.06 ng	145870	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

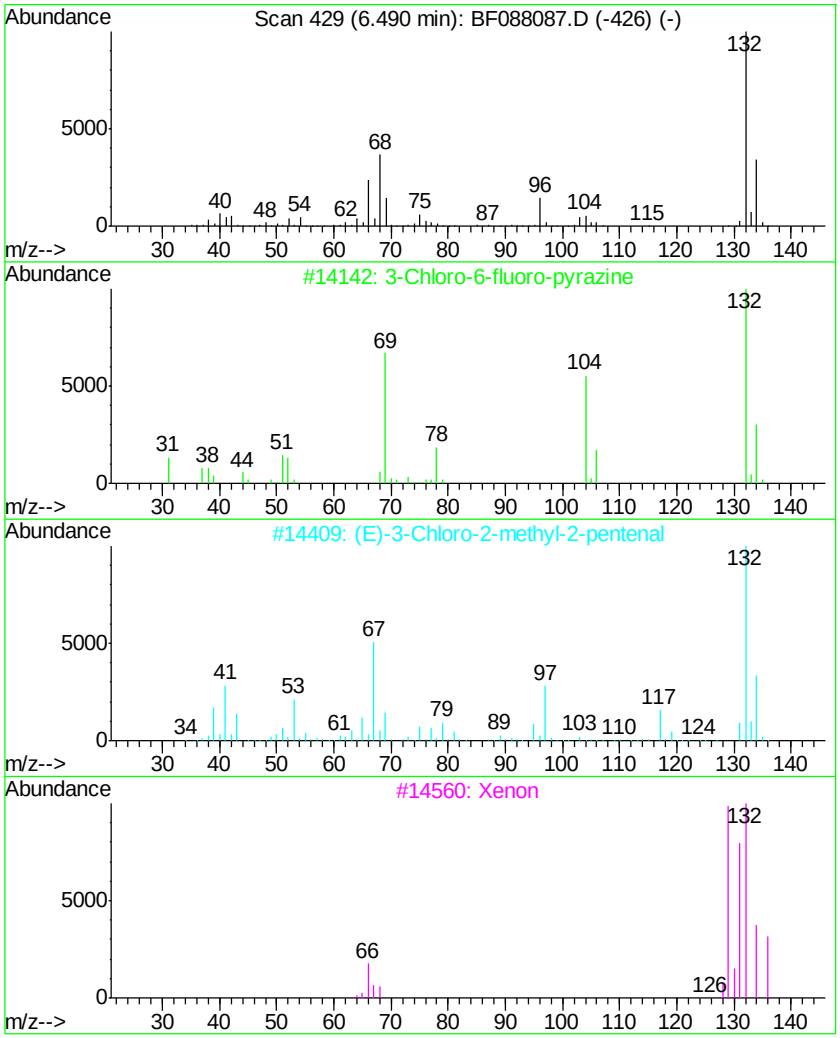
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

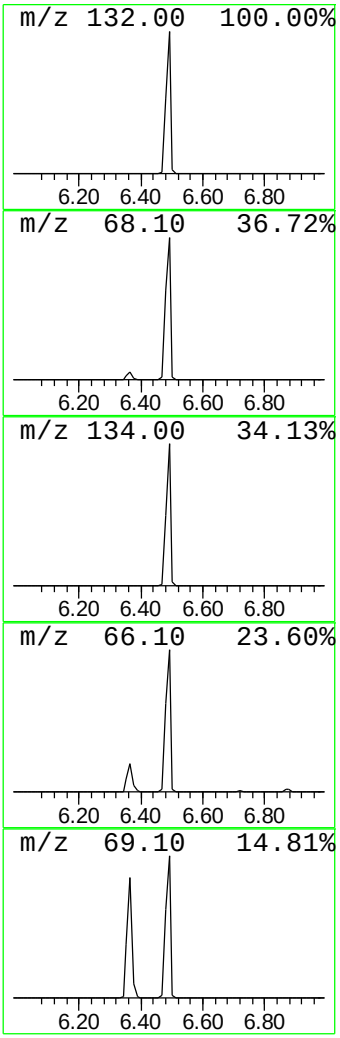
****

Peak Number 4 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	67.02 ng	2407940	1,4-Dichlorobenzene-d4	6.72

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	17
3	Xenon	132	Xe	007440-63-3	9
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

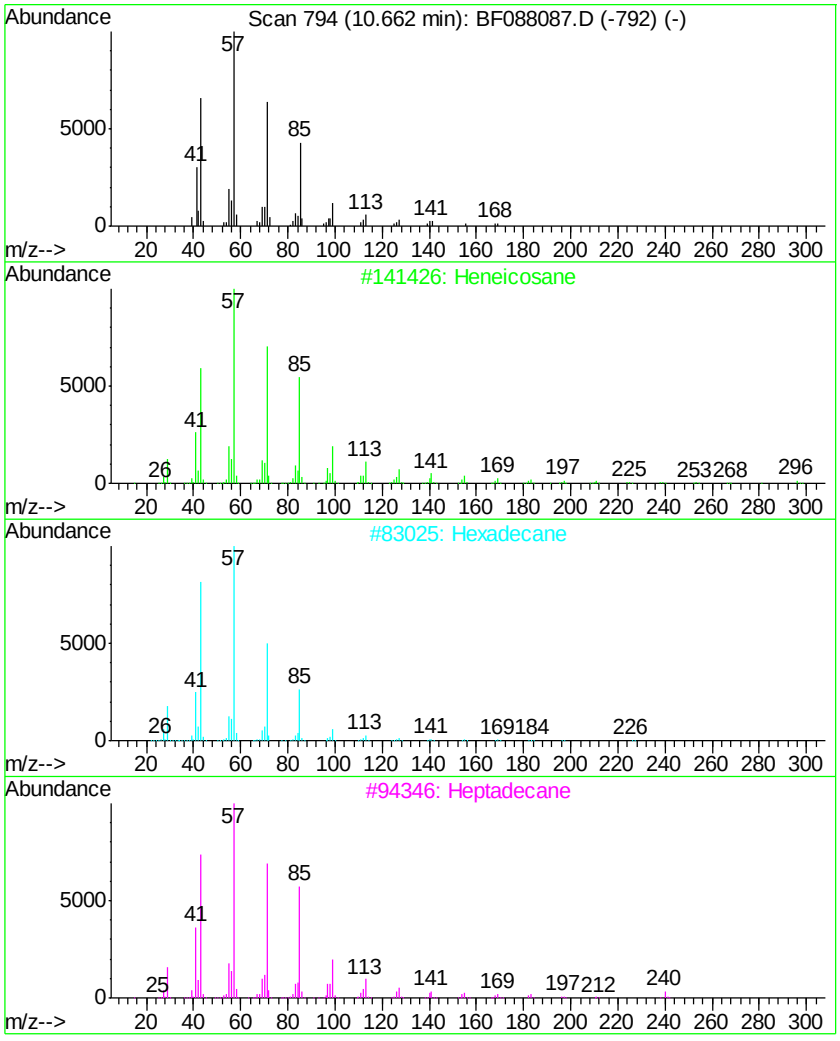
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

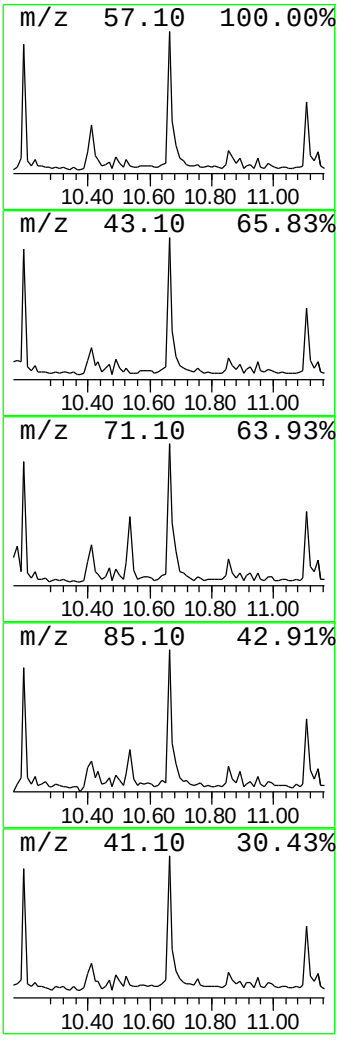
****

Peak Number 6 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.32 ng	116629	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptadecane	240	C17H36	000629-78-7	87
4	Tetradecane	198	C14H30	000629-59-4	87
5	Eicosane	282	C20H42	000112-95-8	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

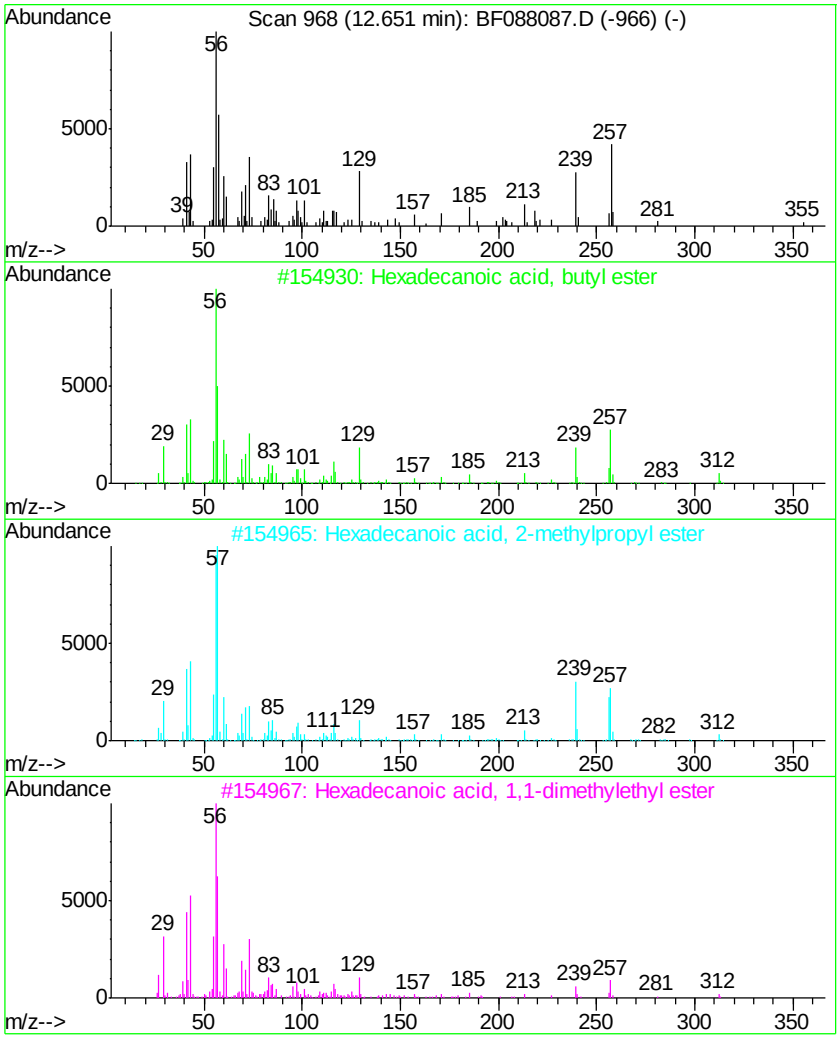
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

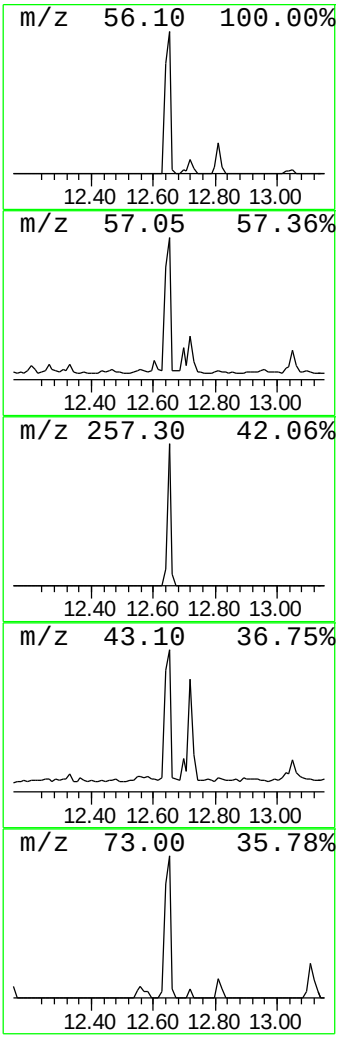
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	5.01 ng	198201	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	53
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
4	Nipecotic acid	129	C6H11NO2	000498-95-3	38
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

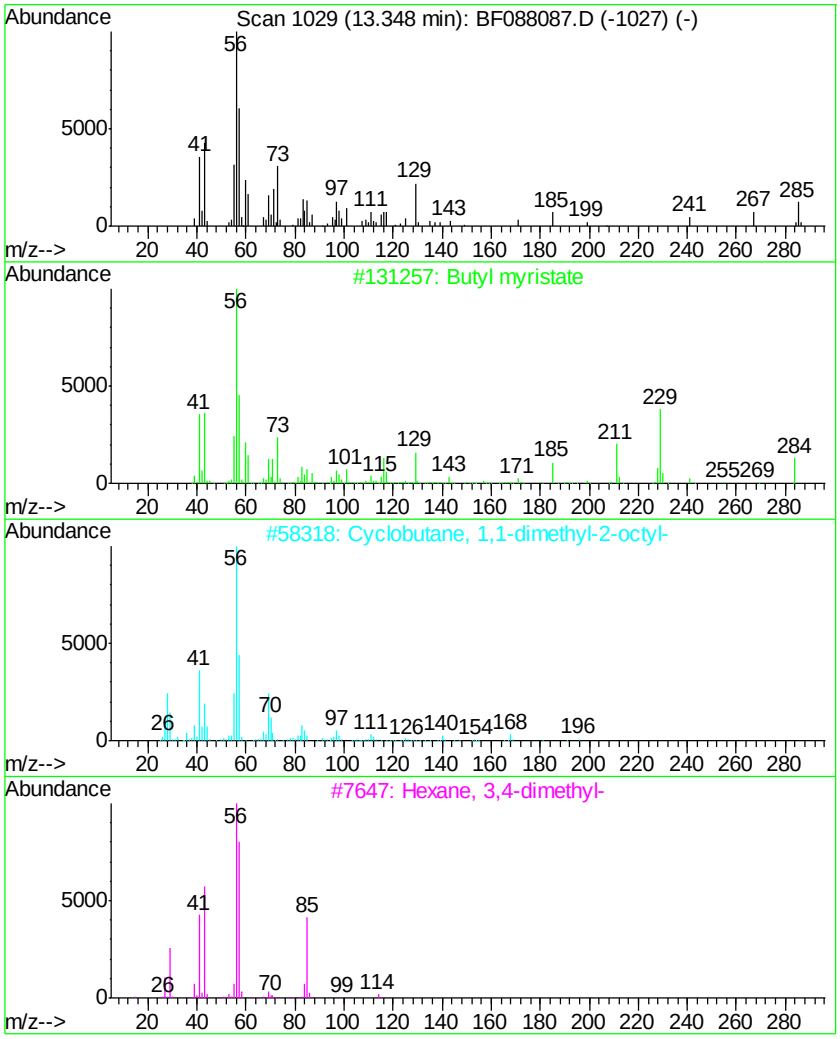
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

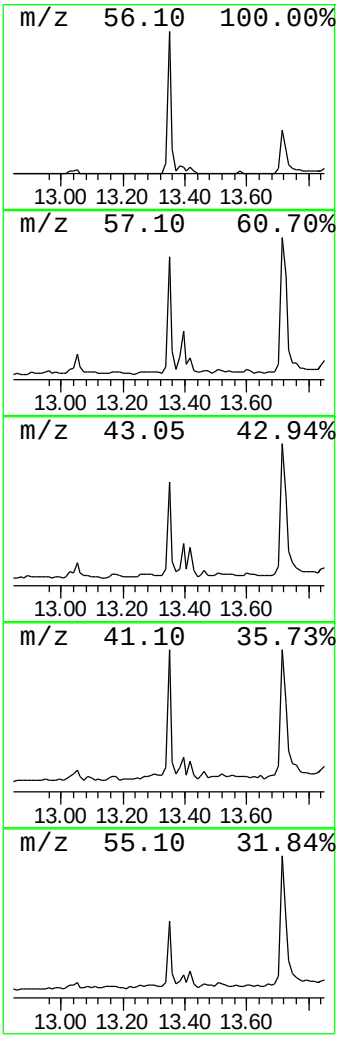
****

Peak Number 8 Butyl myristate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	2.45 ng	97064	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	72
2	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
3	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	35
4	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	30
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

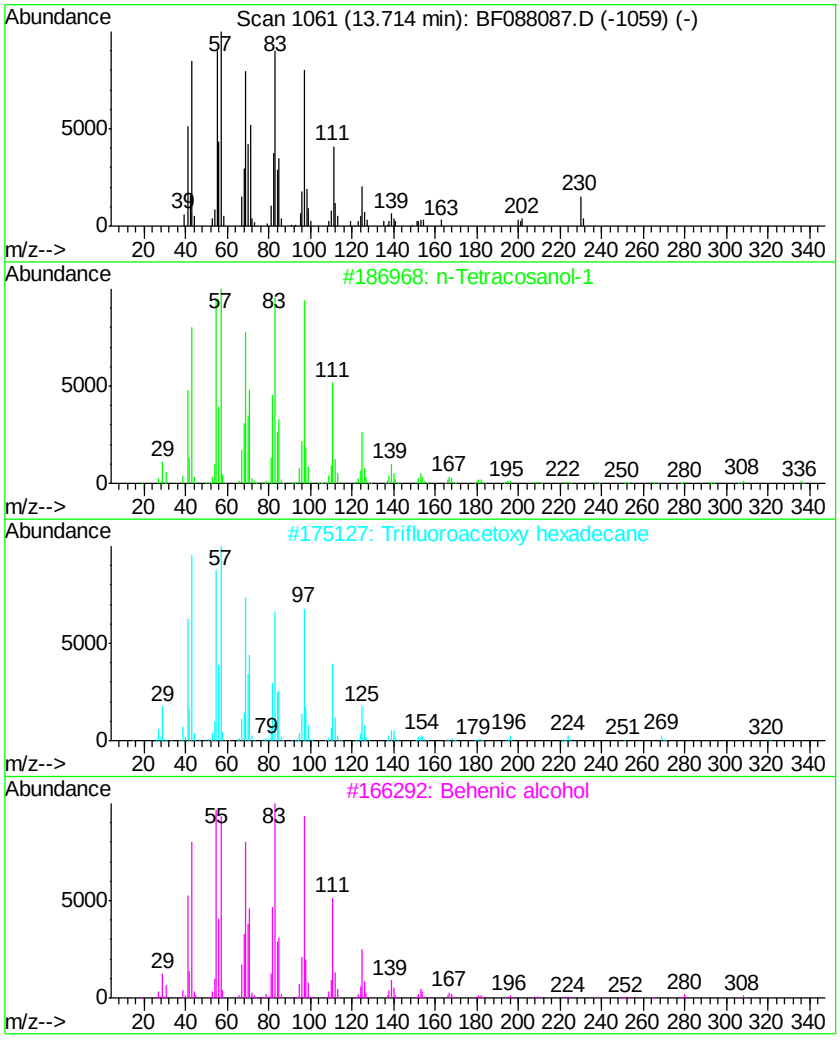
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

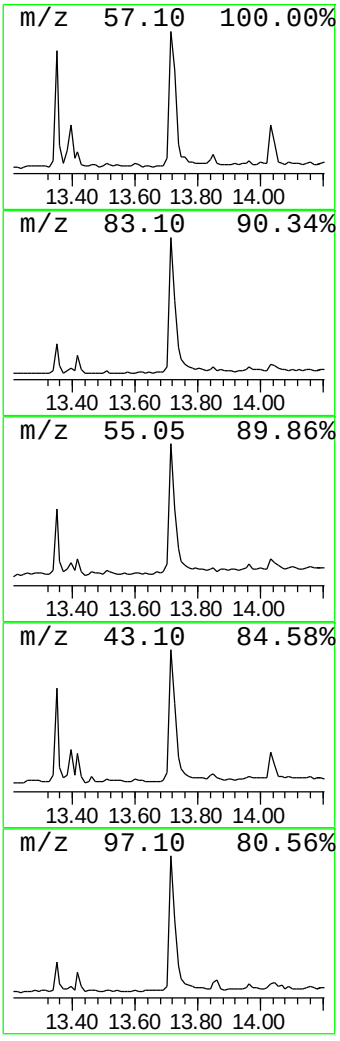
****

Peak Number 9 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	5.05 ng	199635	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

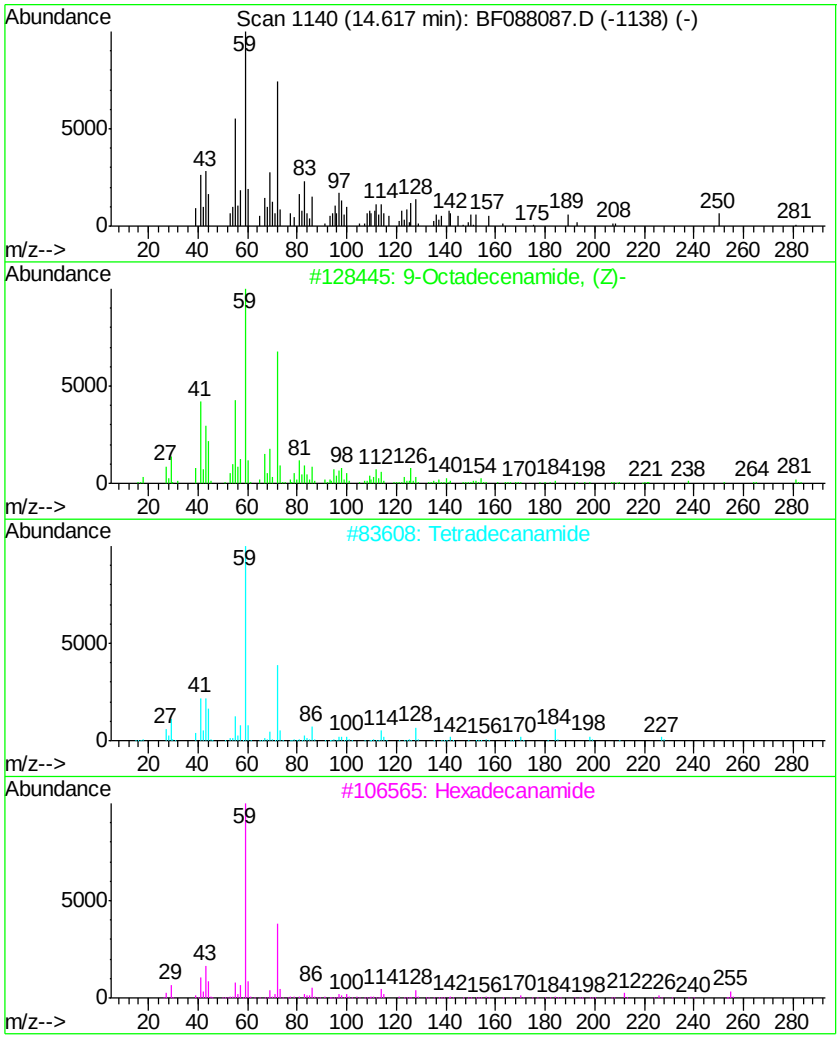
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

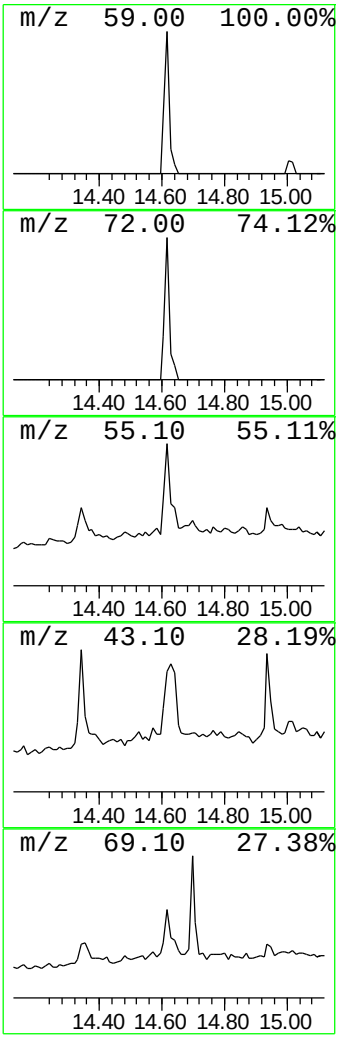
****

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.32 ng	82480	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	Tetradecanamide	227	C14H29NO	000638-58-4	64
3	Hexadecanamide	255	C16H33NO	000629-54-9	59
4	Decanamide-	171	C10H21NO	002319-29-1	47
5	2,2,2-Trichloro-N,N-dimethylacet...	189	C4H6Cl3NO	007291-33-0	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

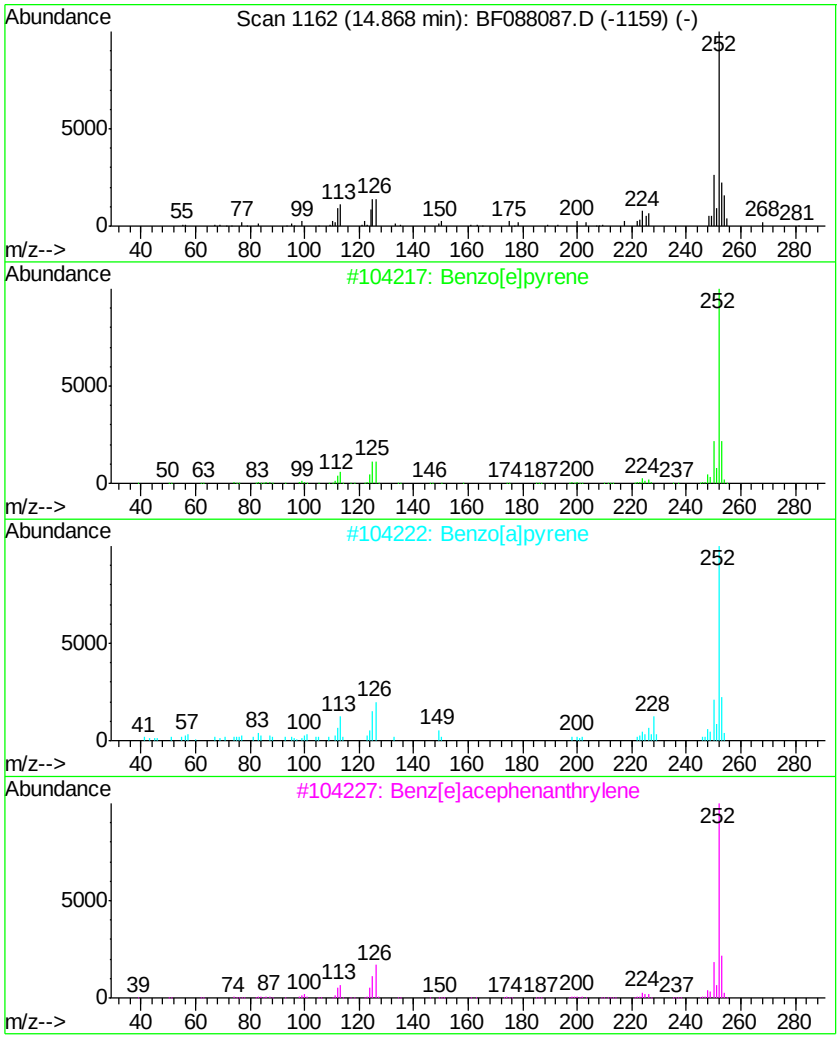
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

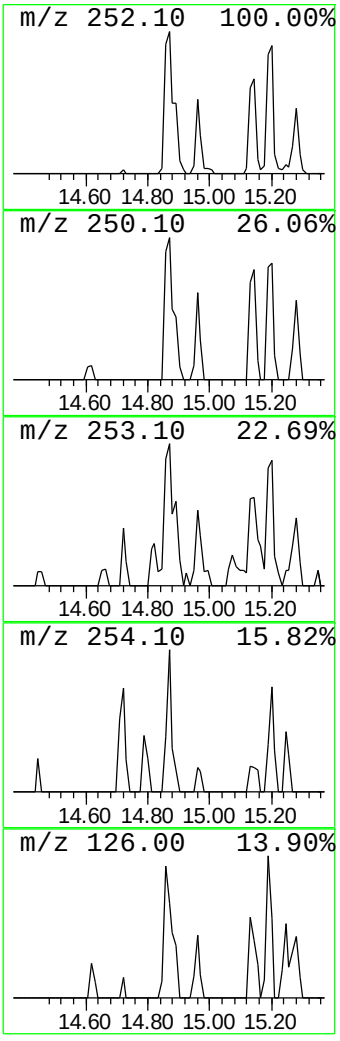
****

Peak Number 11 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.52 ng	89624	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benzo[a]pyrene	252	C20H12	000050-32-8	89
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
4	Perylene	252	C20H12	000198-55-0	81
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061616\
Data File : BF088087.D
Acq On : 16 Jun 2016 20:47
Operator : UM/SJ
Sample : H3571-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-30-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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
2-Pentanone, 4-hy...	4.89	4.1	ng	145870	1	6.72	718618	20.0
unknown6.49	6.49	67.0	ng	2407940	1	6.72	718618	20.0
Heneicosane	10.66	2.3	ng	116629	4	11.23	1006460	20.0
Hexadecanoic acid...	12.65	5.0	ng	198201	5	13.86	791091	20.0
Butyl myristate	13.35	2.5	ng	97064	5	13.86	791091	20.0
n-Tetracosanol-1	13.71	5.0	ng	199635	5	13.86	791091	20.0
9-Octadecenamide,...	14.62	2.3	ng	82480	6	15.25	712161	20.0
Benzo[e]pyrene	14.87	2.5	ng	89624	6	15.25	712161	20.0