LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071816\
Data File : BF089095.D
Acq On : 18 Jul 2016 21:41
Operator : UM/SJ
Sample : H4044-17
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M9-B5(0-6)C

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-BF063016.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	1.633	3	4	13	rVB	158448	244306	11.09%	1.767%
2	1.747	13	14	50	rVB	1162750	2202754	100.00%	15.929%
3	4.787	277	280	285	rBB	51045	85060	3.86%	0.615%
4	5.233	317	319	322	rBV	1269348	1247998	56.66%	9.025%
5	6.296	409	412	415	rBV	1055193	1207883	54.84%	8.735%
6	6.410	420	422	425	rBV	1313752	1244616	56.50%	9.000%
7	6.479	426	428	430	rBV	73894	58628	2.66%	0.424%
8	6.639	440	442	444	rBB	382839	312284	14.18%	2.258%
9	6.799	453	456	458	rBV	1157136	1035559	47.01%	7.488%
10	7.210	489	492	494	rBV	839526	811439	36.84%	5.868%
11	7.930	552	555	557	rBV	390642	396366	17.99%	2.866%
12	9.005	646	649	651	rBV	1378024	1180797	53.61%	8.539%
13	9.405	681	684	686	rVB	214591	194127	8.81%	1.404%
14	9.679	705	708	709	rBV	291534	352837	16.02%	2.551%
15	10.456	774	776	779	rBV	565808	544326	24.71%	3.936%
16	10.594	786	788	792	rVB	31299	41902	1.90%	0.303%
17	11.039	825	827	828	rBV	26309	22696	1.03%	0.164%
18	11.154	834	837	840	rVB	227166	340660	15.47%	2.463%
19	12.354	940	942	944	rVB	138971	117431	5.33%	0.849%
20	12.582	959	962	963	rBV	86111	118269	5.37%	0.855%
21	12.731	973	975	978	rVB	799283	723372	32.84%	5.231%
22	12.914	987	991	993	rBV2	19043	33634	1.53%	0.243%
23	12.971	993	996	998	rBV3	18656	23547	1.07%	0.170%
24	13.005	998	999	1006	rBV6	11908	34977	1.59%	0.253%
25	13.520	1042	1044	1045	rBV	19309	24644	1.12%	0.178%
26	13.645	1052	1055	1058	rBV2	46812	68262	3.10%	0.494%
27	13.771	1063	1066	1071	rVV2	374949	501467	22.77%	3.626%
28	13.874	1073	1075	1077	rBV2	24521	34449	1.56%	0.249%
29	14.765	1151	1153	1157	rBV	78026	135698	6.16%	0.981%
30	15.017	1173	1175	1178	rBV	34425	53703	2.44%	0.388%
31	15.074	1178	1180	1183	rVV	58294	82360	3.74%	0.596%
32	15.131	1183	1185	1194	rVB	188254	267683	12.15%	1.936%
33	16.388	1293	1295	1300	rVB2	23222	39584	1.80%	0.286%
34	16.754	1325	1327	1335	rVB2	18110	45397	2.06%	0.328%

LSC Area Percent Report

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Acq On : 18 Jul 2016 21:41
Operator : UM/SJ
Sample : H4044-17
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M9-B5(0-6)C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

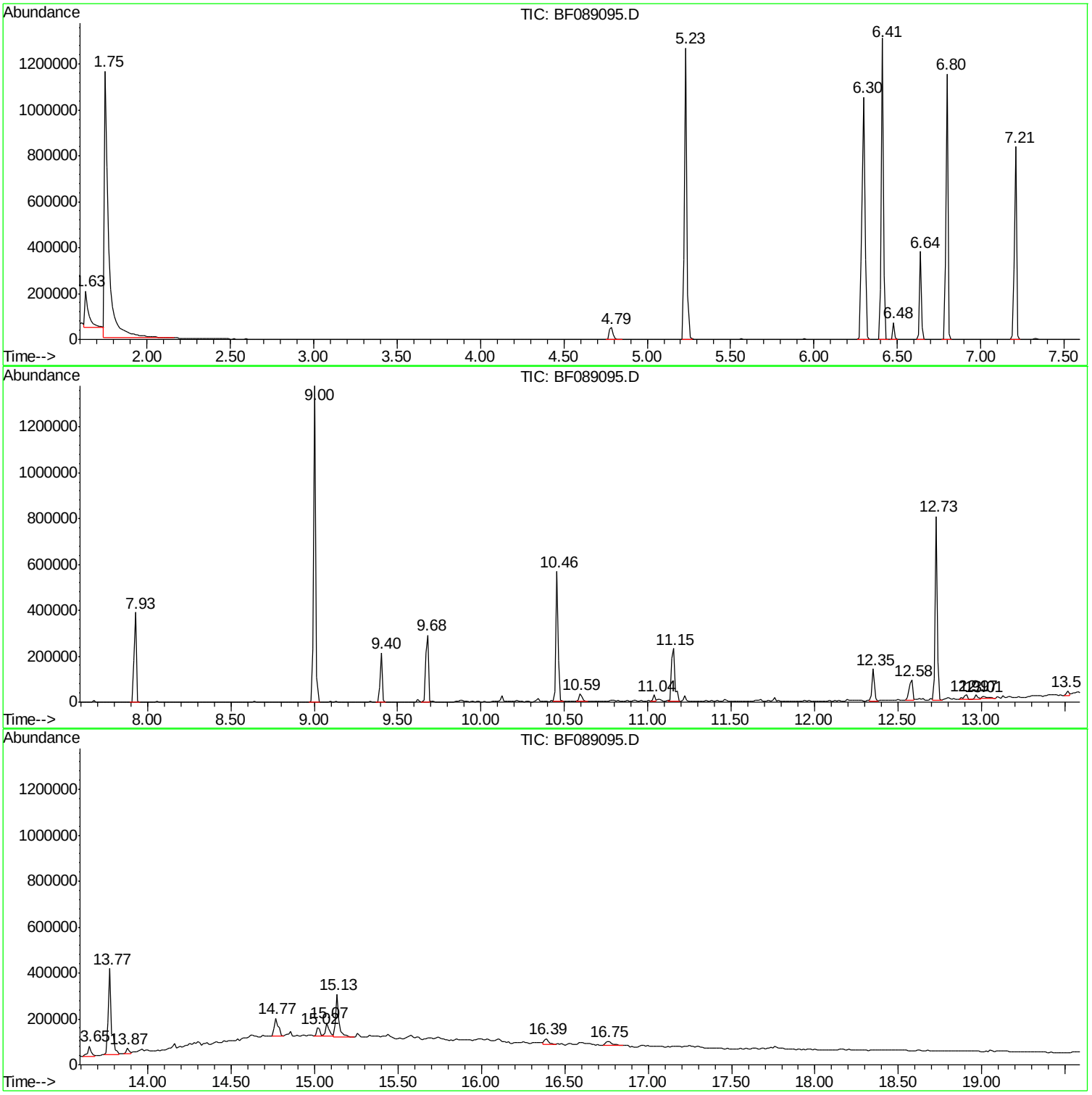
Sum of corrected areas: 13828715

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071816\
Data File : BF089095.D
Acq On : 18 Jul 2016 21:41
Operator : UM/SJ
Sample : H4044-17
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
M9-B5(0-6)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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\BF071816\
Data File : BF089095.D
Acq On : 18 Jul 2016 21:41
Operator : UM/SJ
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Instrument : BNA_F
ClientSampleId : M9-B5(0-6)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

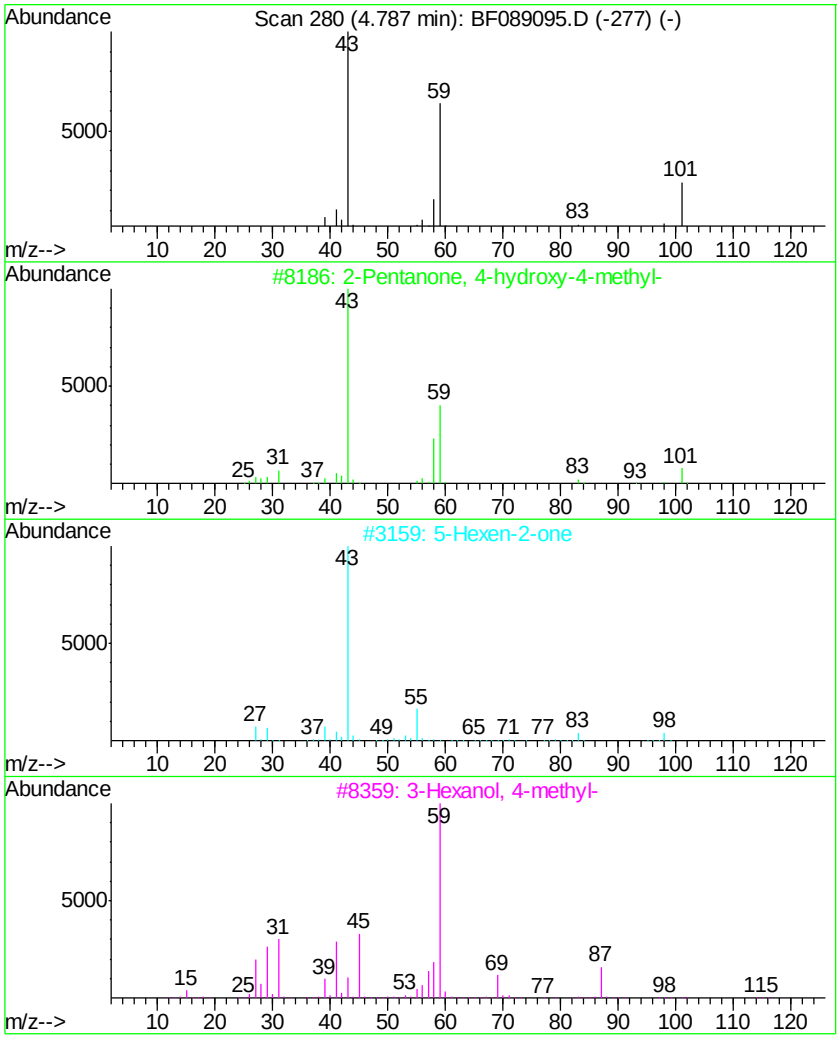
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

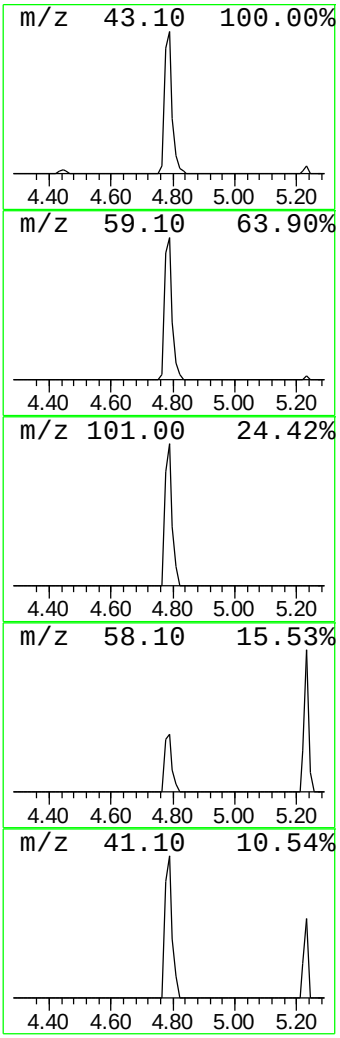
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	5.45 ng	85060	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
4	3-Pentanol	88	C5H12O	000584-02-1	9
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071816\
Data File : BF089095.D
Acq On : 18 Jul 2016 21:41
Operator : UM/SJ
Sample : H4044-17
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M9-B5(0-6)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

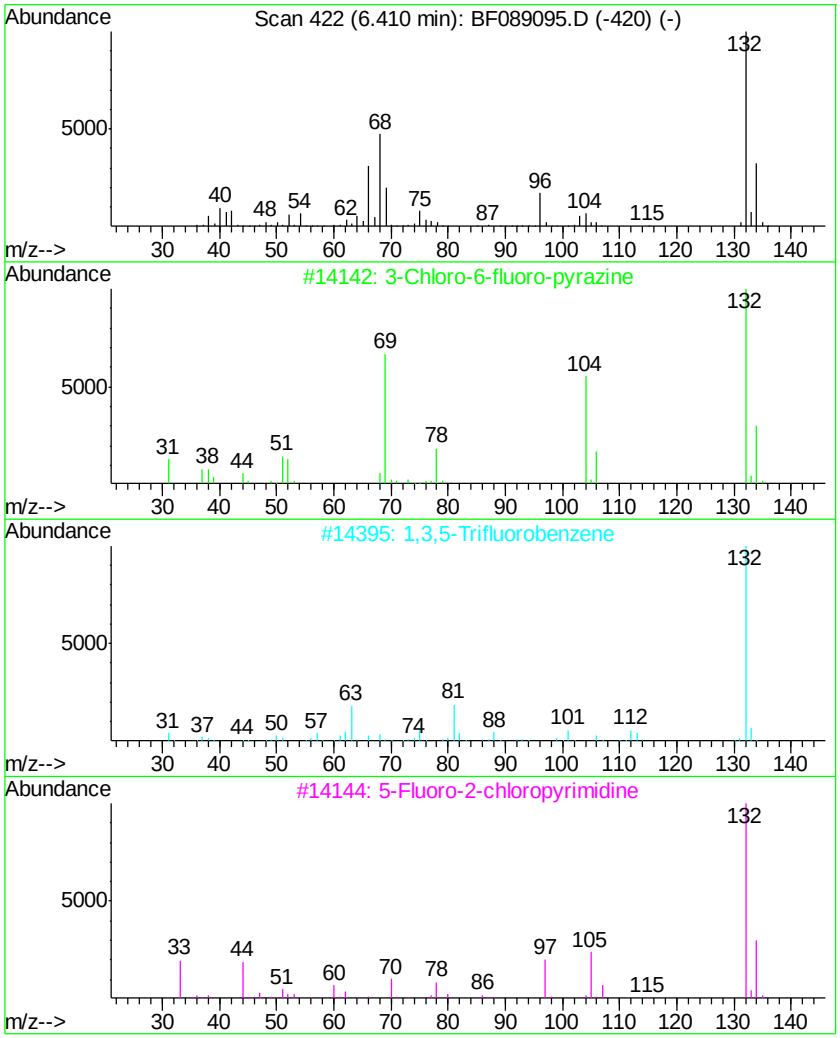
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

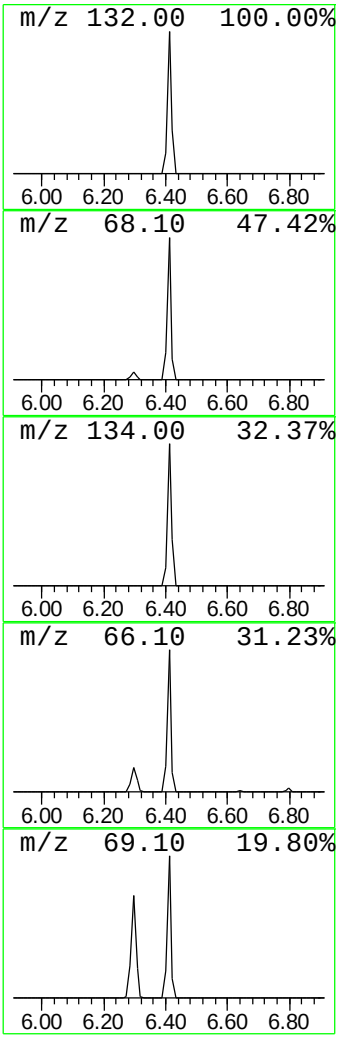
****

Peak Number 4 unknown6.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	79.71 ng	1244620	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





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Data File : BF089095.D
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Operator : UM/SJ
Sample : H4044-17
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M9-B5(0-6)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

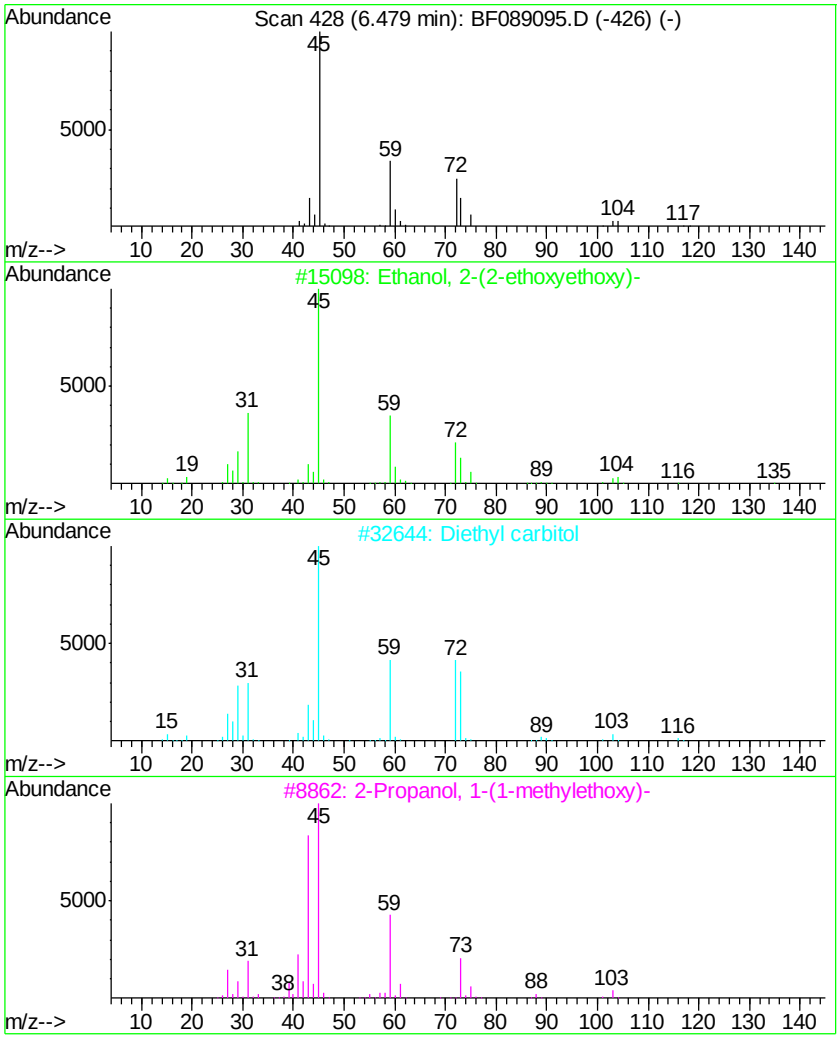
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

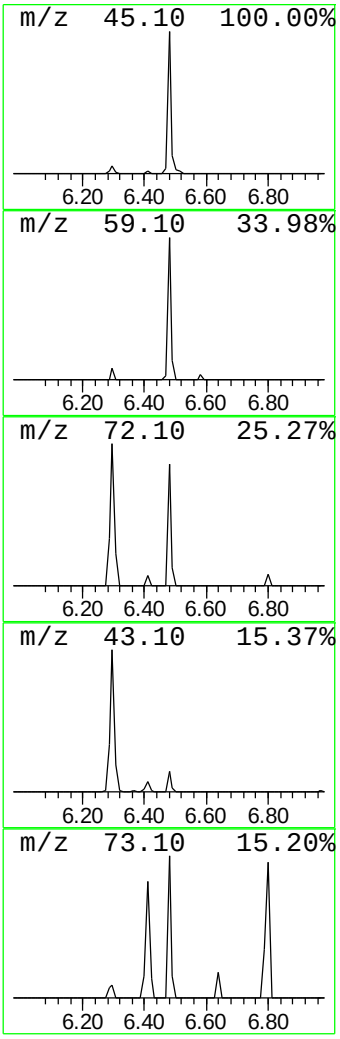
****

Peak Number 5 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	3.75 ng	58628	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	40





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071816\
Data File : BF089095.D
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Operator : UM/SJ
Sample : H4044-17
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M9-B5(0-6)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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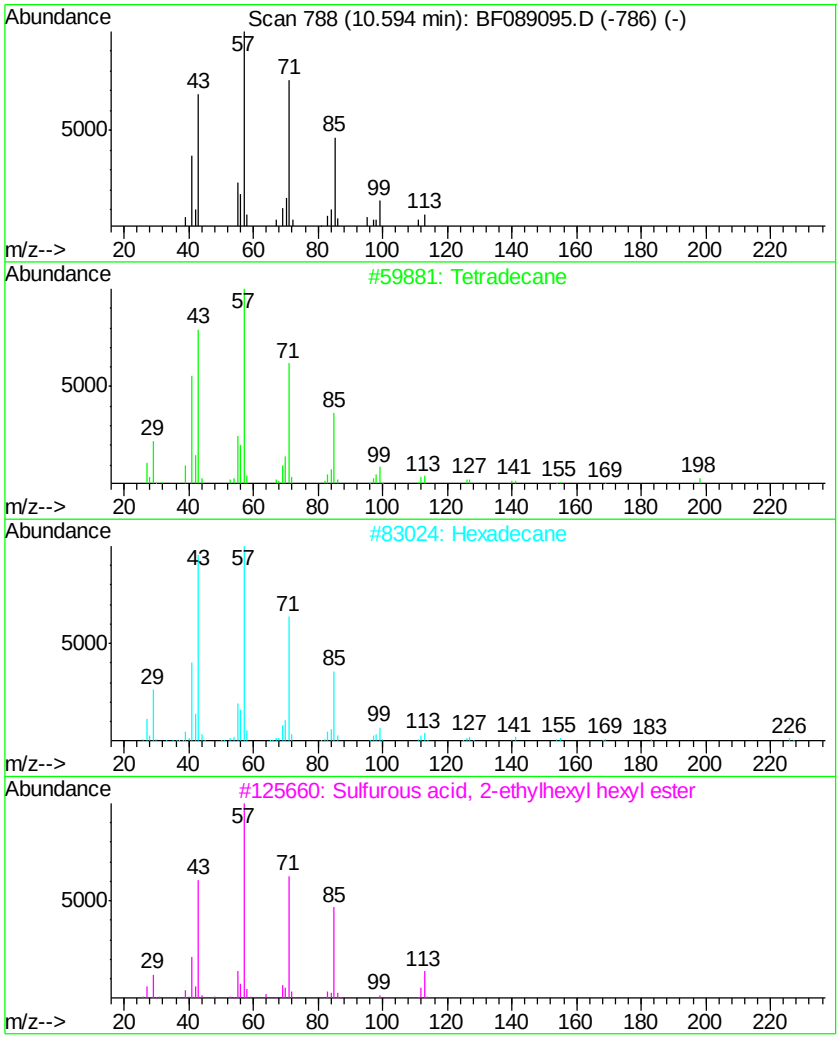
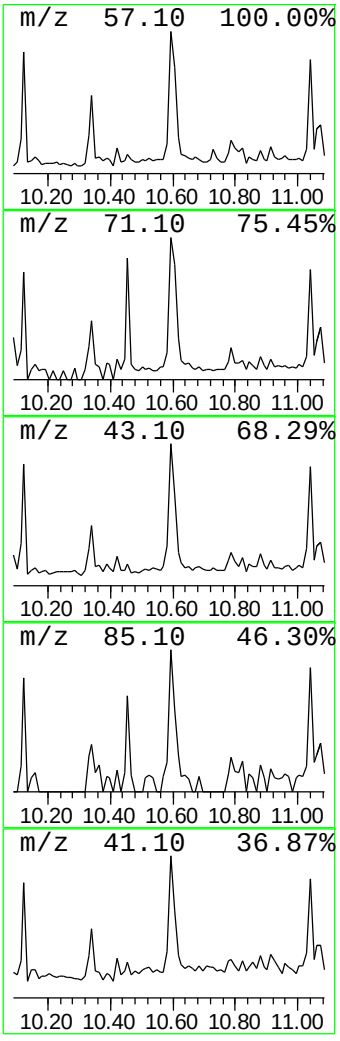
Peak Number 7 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	2.46 ng	41902	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	86
2	Hexadecane	226	C16H34	000544-76-3	78
3	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64
4	3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	64
5	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	59





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Misc :
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Instrument : BNA_F
ClientSampleId : M9-B5(0-6)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

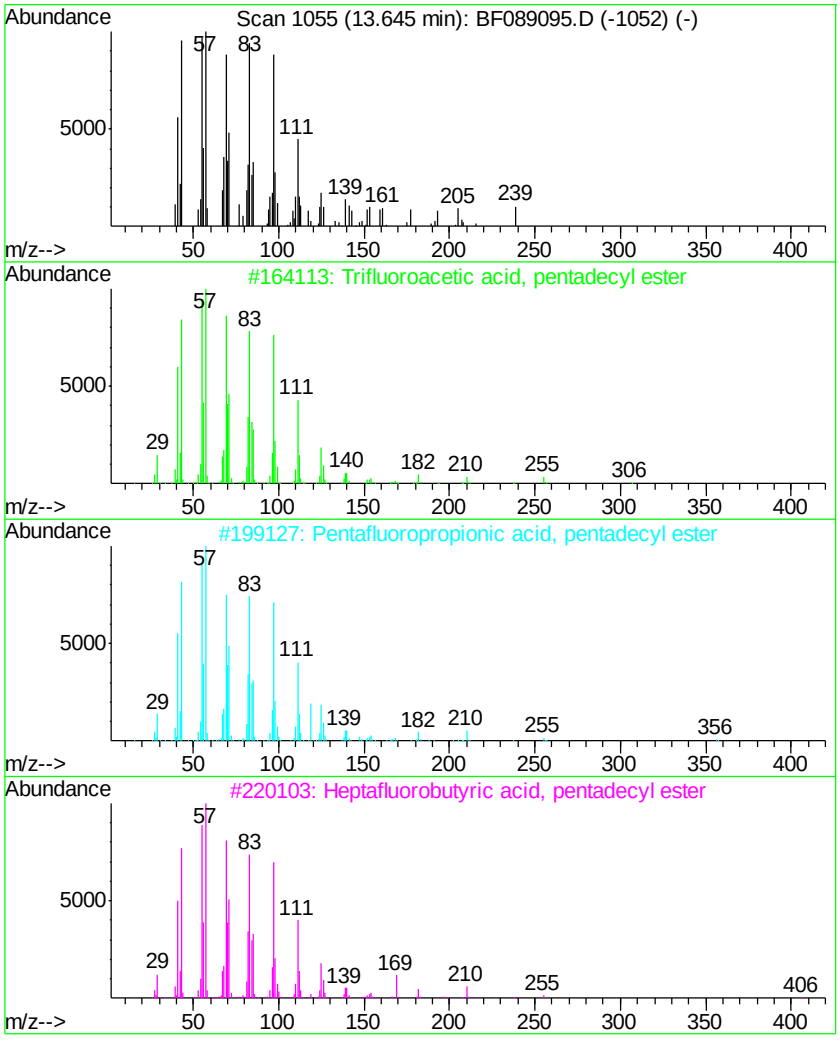
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

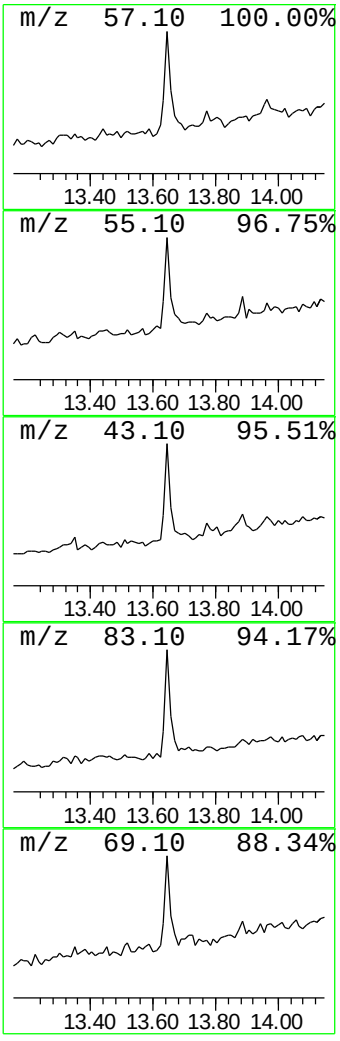
****

Peak Number 8 Trifluoroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	2.72 ng	68262	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





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Sample : H4044-17
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M9-B5(0-6)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

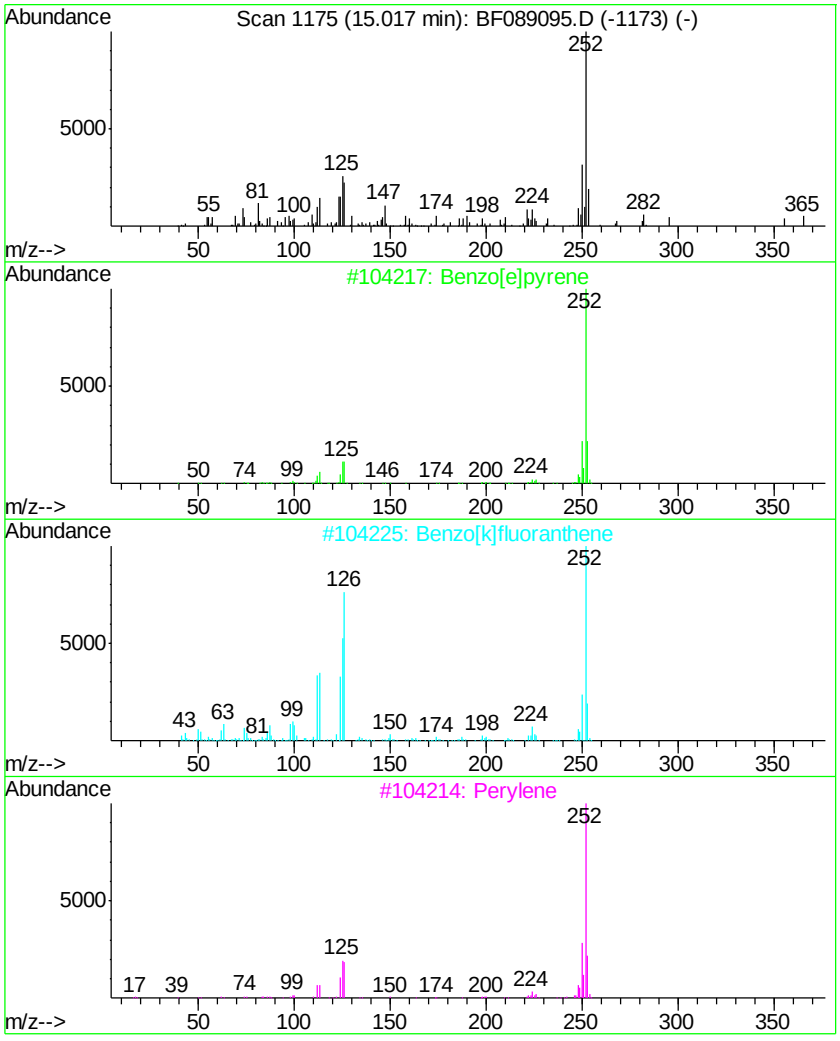
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

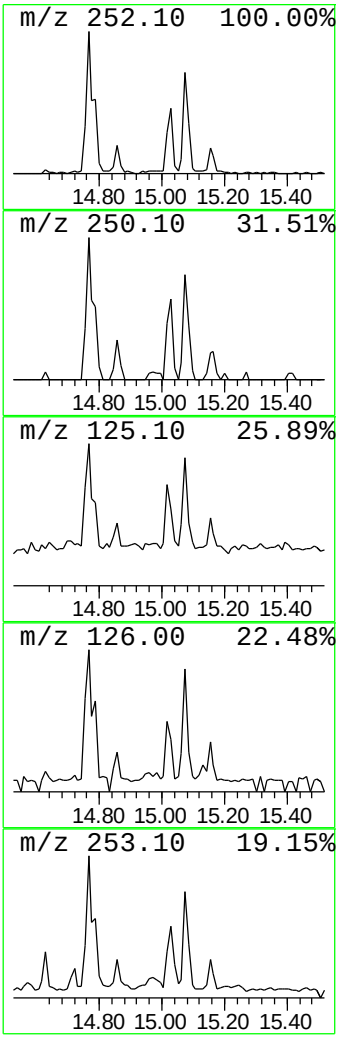
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	4.01 ng	53703	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
3	Perylene	252	C20H12	000198-55-0	89
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	83
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	76





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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...	4.79	5.5	ng	85060	1	6.64	312284	20.0
unknown6.41	6.41	79.7	ng	1244620	1	6.64	312284	20.0
Ethanol, 2-(2-eth...	6.48	3.8	ng	58628	1	6.64	312284	20.0
Tetradecane	10.59	2.5	ng	41902	4	11.15	340660	20.0
Trifluoroacetic a...	13.65	2.7	ng	68262	5	13.77	501467	20.0
Benzo[e]pyrene	15.02	4.0	ng	53703	6	15.13	267683	20.0