LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)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	1.632	3	4	6	rVB	4643332	5906609	100.00%	16.836%
2	1.735	6	13	16	rVB	256898	832333	14.09%	2.373%
3	2.021	35	38	41	rBV	62763	79640	1.35%	0.227%
4	4.970	293	296	301	rBB	142467	218444	3.70%	0.623%
5	5.393	329	333	335	rBV	2575398	3193143	54.06%	9.102%
6	6.433	420	424	426	rBV	2619096	3381234	57.24%	9.638%
7	6.559	432	435	437	rBV	3022365	3086112	52.25%	8.797%
8	6.787	453	455	457	rBV	850654	687178	11.63%	1.959%
9	6.947	466	469	471	rVB	2685759	2511542	42.52%	7.159%
10	7.359	501	505	507	rBV	1451013	2076830	35.16%	5.920%
11	8.067	565	567	570	rBV	758902	820515	13.89%	2.339%
12	9.153	659	662	664	rBV	3185031	3289115	55.69%	9.375%
13	9.542	694	696	698	rBV	542903	438479	7.42%	1.250%
14	9.816	718	720	722	rBV2	726334	801878	13.58%	2.286%
15	10.605	787	789	792	rBV	1553703	1481616	25.08%	4.223%
16	10.730	799	800	804	rBV	74150	89301	1.51%	0.255%
17	11.176	838	839	845	rVB	43830	75562	1.28%	0.215%
18	11.302	847	850	853	rVB	581101	829256	14.04%	2.364%
19	11.828	894	896	898	rVB	64037	63604	1.08%	0.181%
20	11.908	901	903	907	rVB2	84871	122951	2.08%	0.350%
21	12.091	917	919	924	rVB2	37568	64275	1.09%	0.183%
22	12.342	939	941	943	rBV	50812	61995	1.05%	0.177%
23	12.502	953	955	958	rVB	373046	310829	5.26%	0.886%
24	12.731	972	975	977	rBV	386010	455960	7.72%	1.300%
25	12.879	986	988	991	rVB	1887198	1909177	32.32%	5.442%
26	13.062	998	1004	1005	rVB	44227	106067	1.80%	0.302%
27	13.817	1067	1070	1075	rBV4	40553	100333	1.70%	0.286%
28	13.919	1076	1079	1085	rVB2	665295	992896	16.81%	2.830%
29	14.925	1164	1167	1172	rBV	131520	249119	4.22%	0.710%
30	15.200	1189	1191	1194	rBV	75075	92684	1.57%	0.264%
31	15.257	1194	1196	1199	rVB	101689	111943	1.90%	0.319%
32	15.314	1199	1201	1204	rBV	323907	494147	8.37%	1.409%
33	16.651	1315	1318	1322	rBV2	39375	80272	1.36%	0.229%
34	17.051	1350	1353	1358	rVB	30811	67317	1.14%	0.192%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)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: 35082356

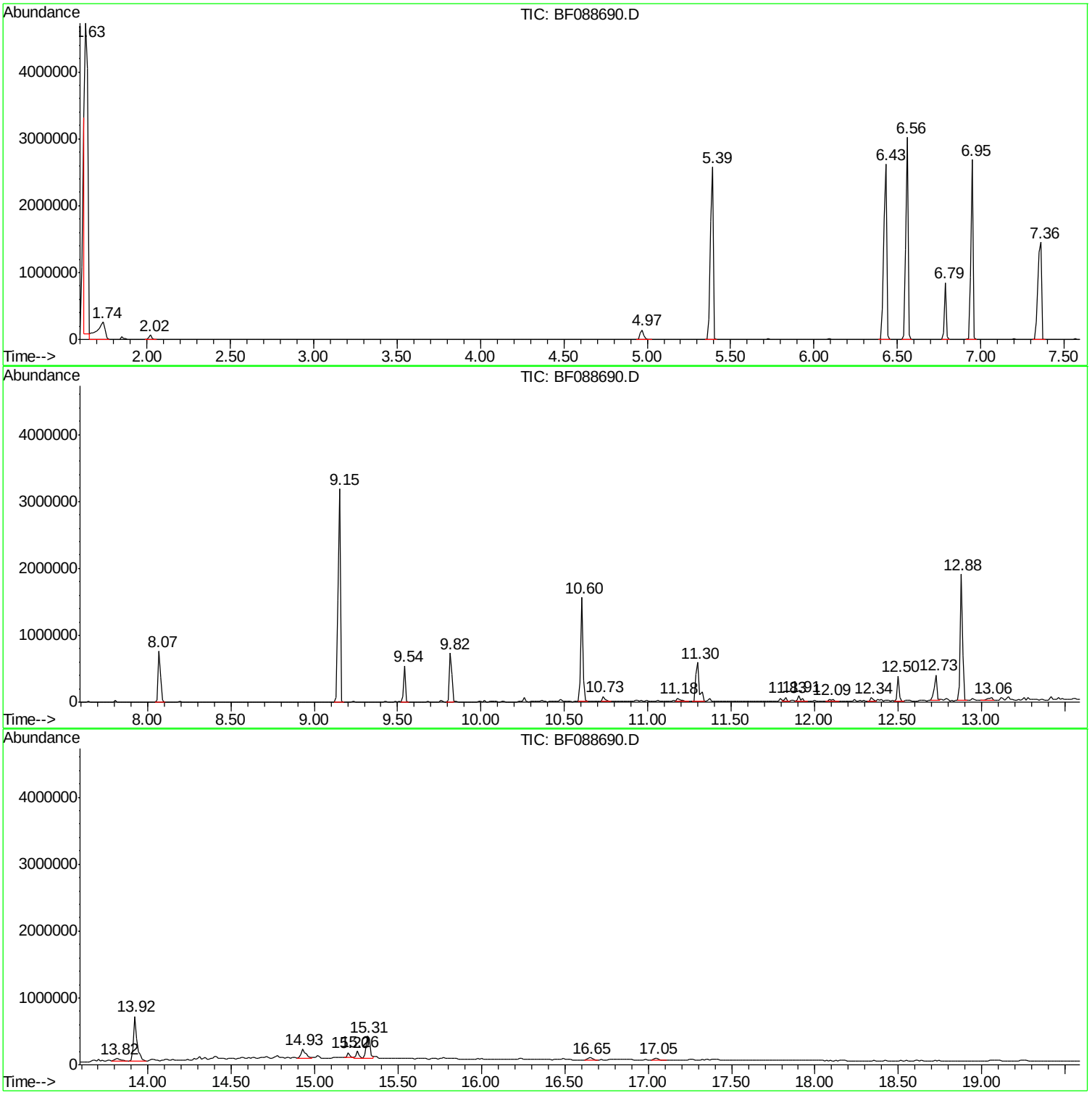
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)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\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)C

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

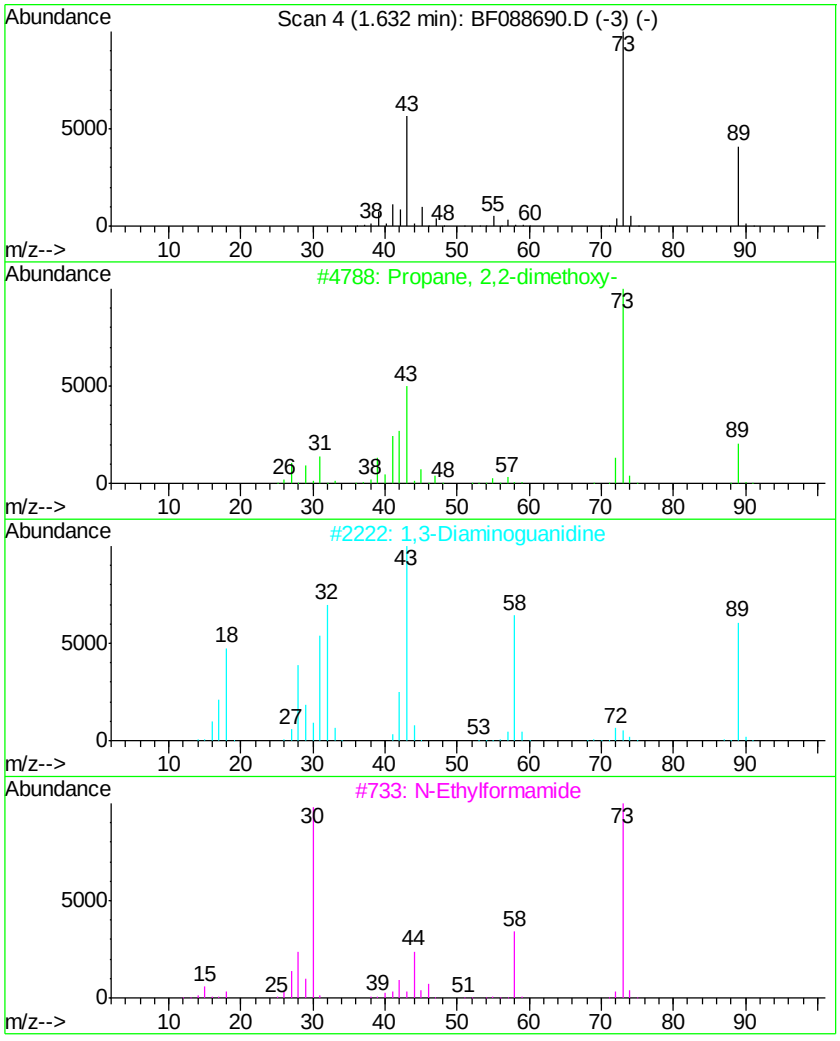
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

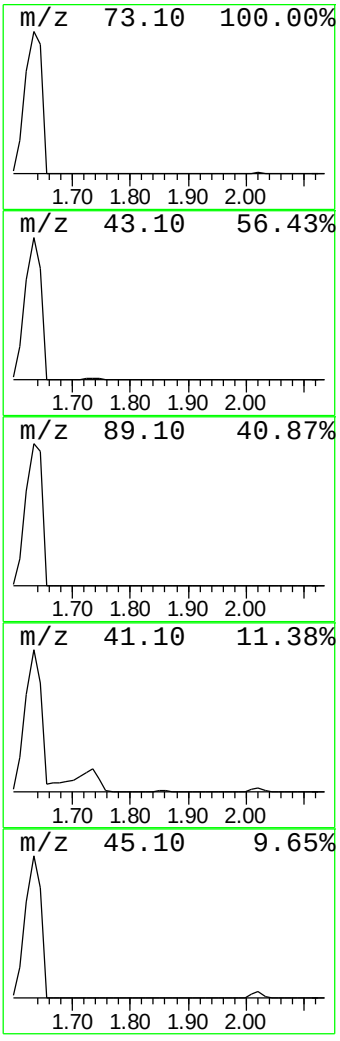
****

Peak Number 1 unknown1.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.63	171.91 ng	5906610	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	42
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)C

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

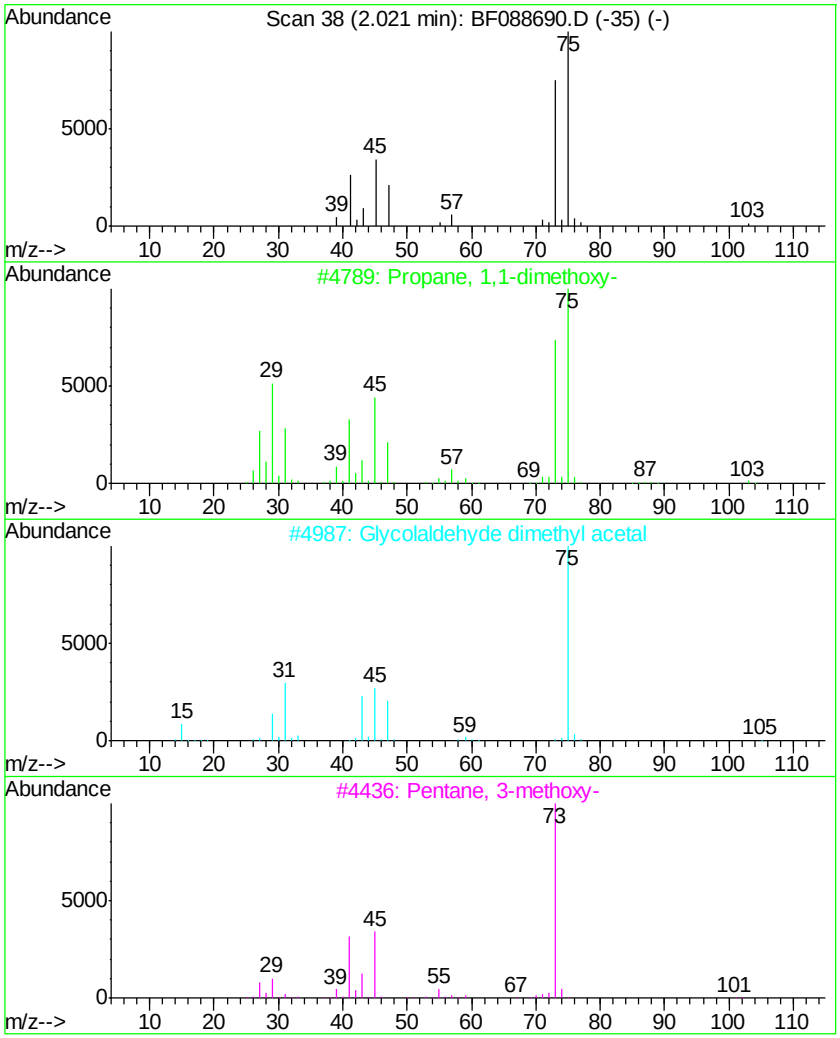
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

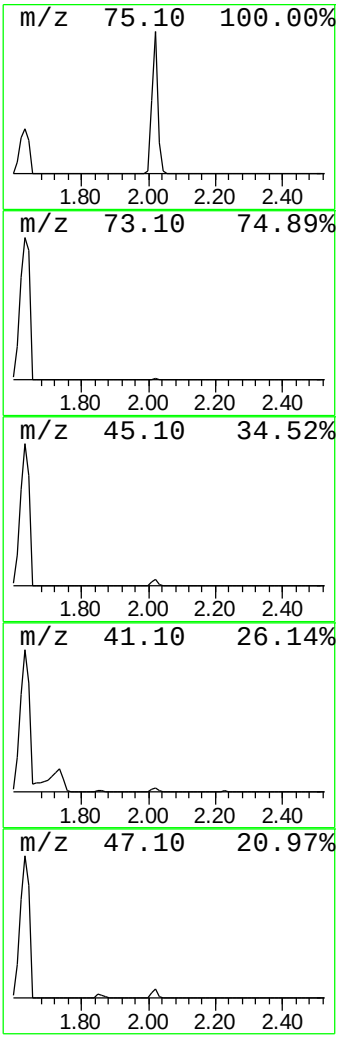
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	2.32 ng	79640	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	14
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)C

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

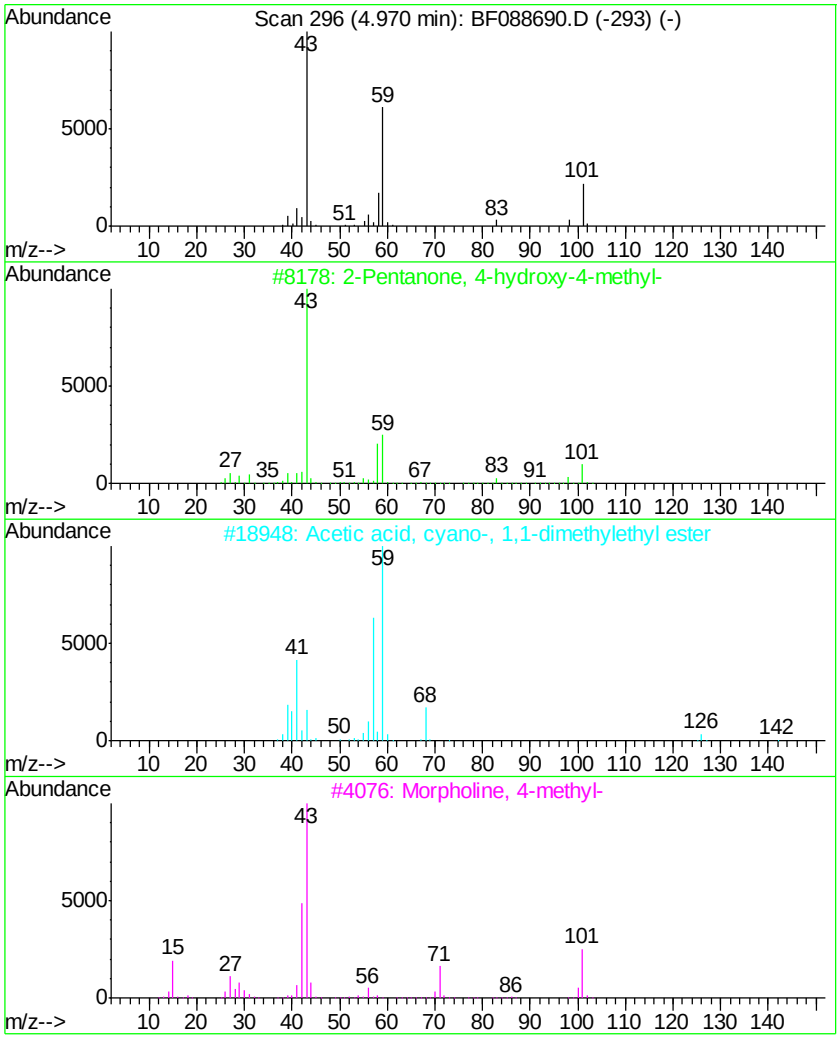
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

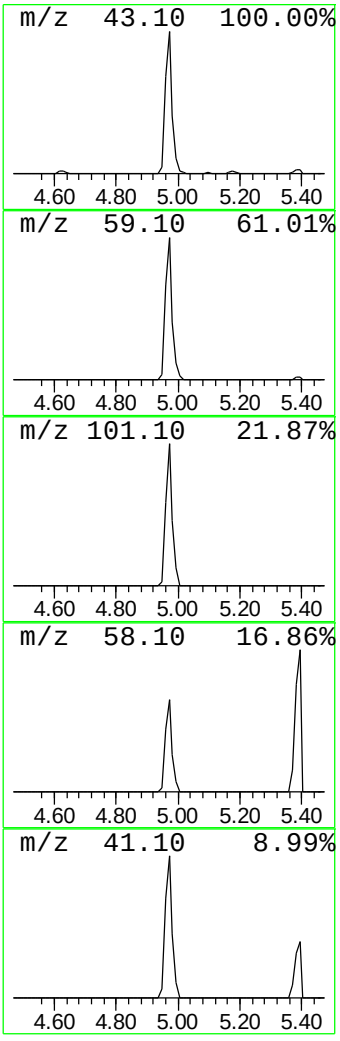
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	6.36 ng	218444	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)C

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

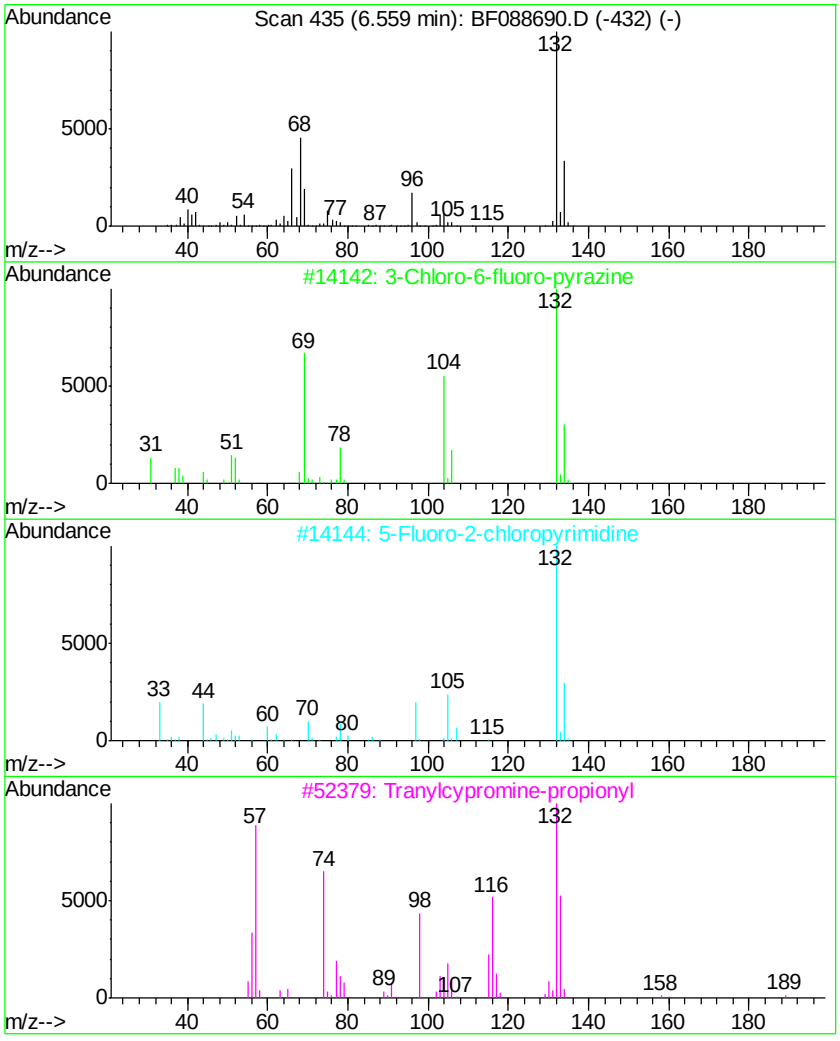
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

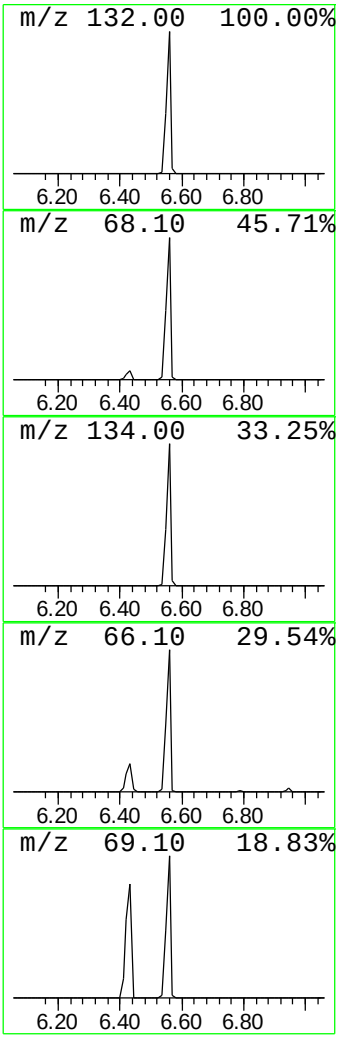
****

Peak Number 5 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	89.82 ng	3086110	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)C

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

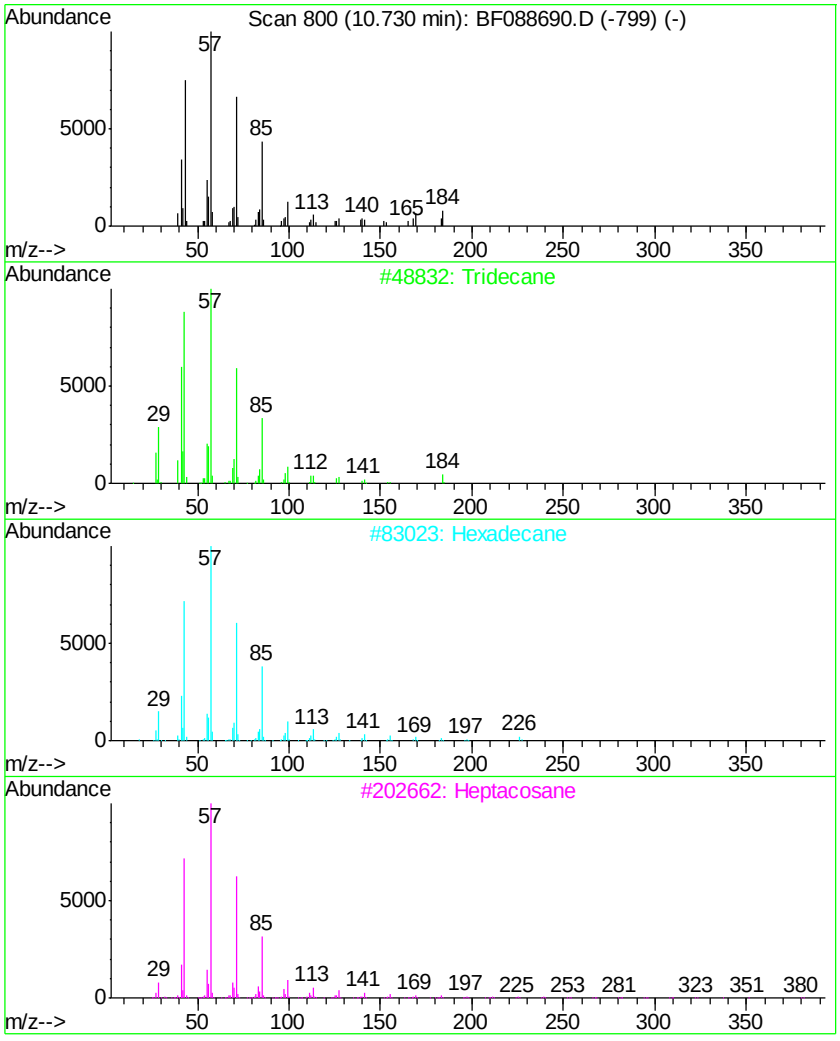
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

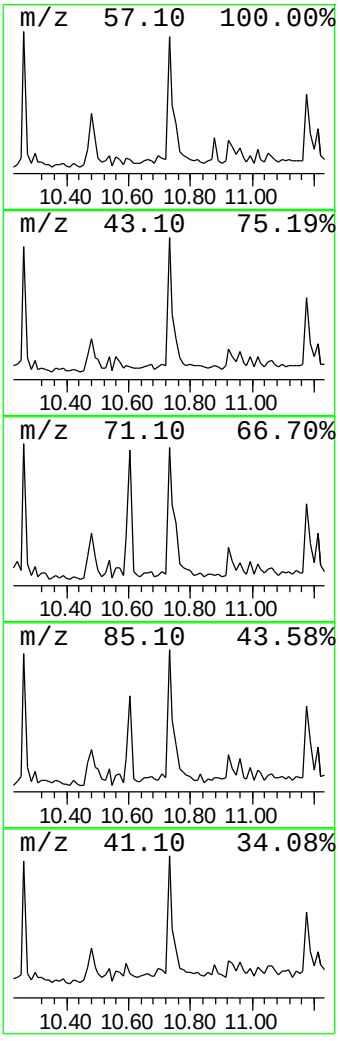
****

Peak Number 7 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.15 ng	89301	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	86
2	Hexadecane	226	C16H34	000544-76-3	80
3	Heptacosane	380	C27H56	000593-49-7	80
4	Pentadecane	212	C15H32	000629-62-9	80
5	Eicosane	282	C20H42	000112-95-8	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)C

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

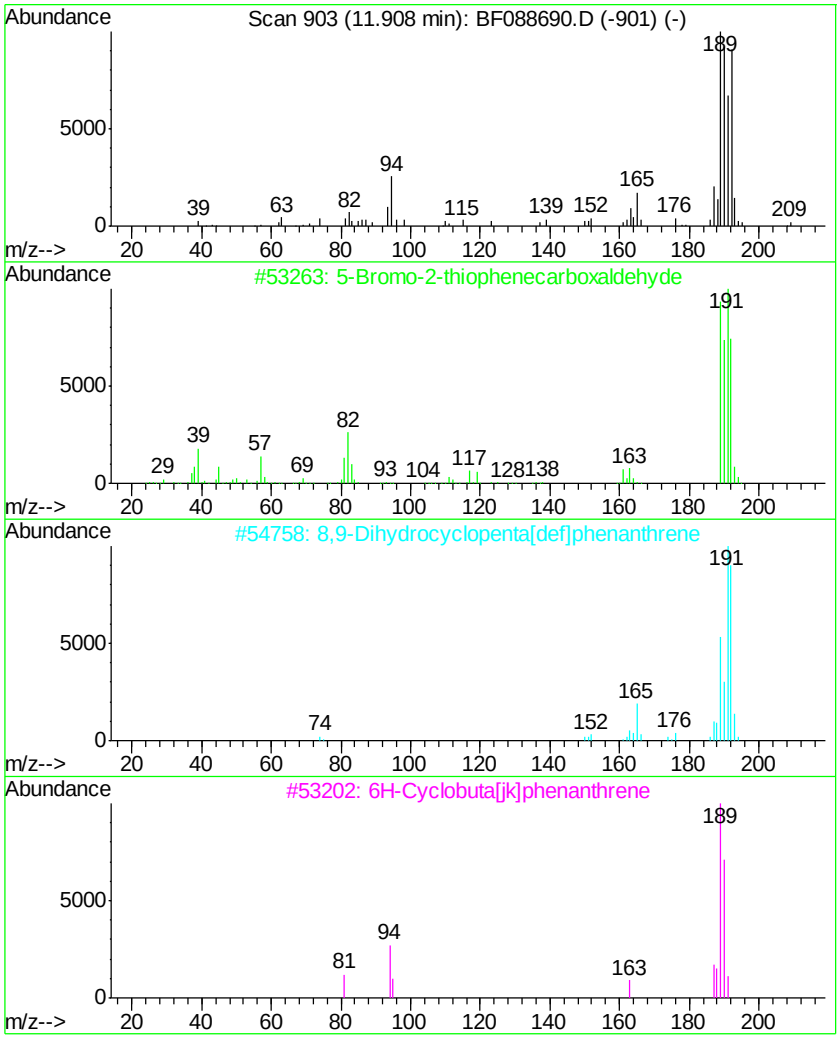
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

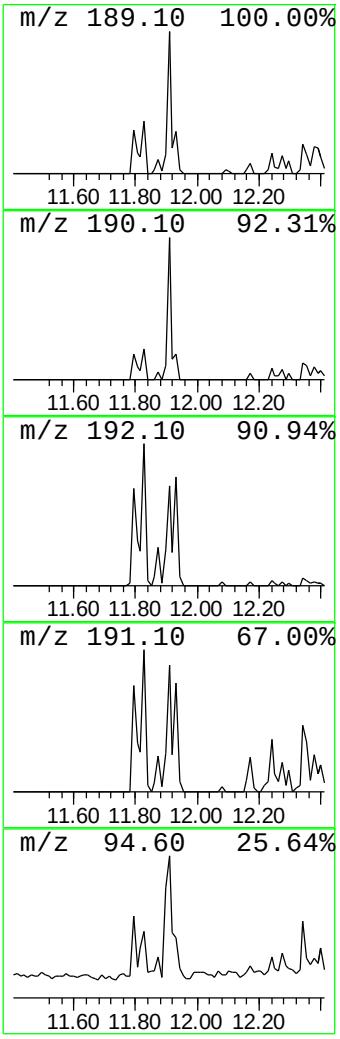
****

Peak Number 8 5-Bromo-2-thiophenecarboxal... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.97 ng	122951	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	58
2	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	50
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
4	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	46
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	46





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)C

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

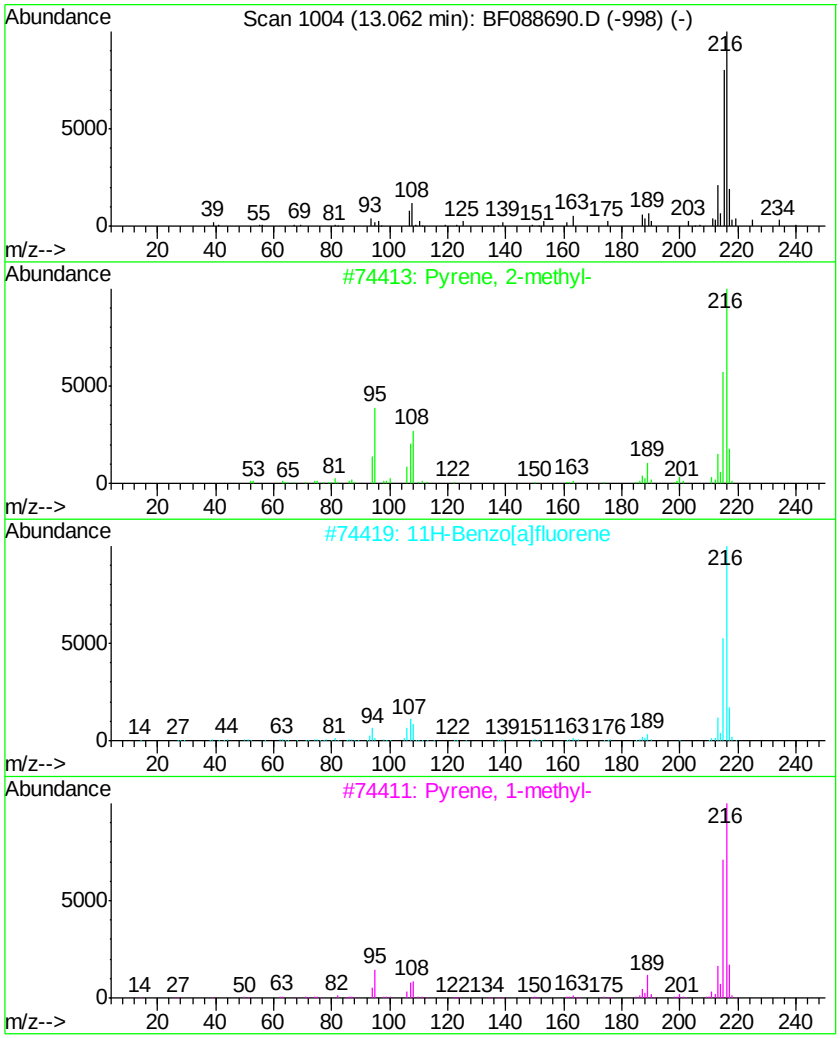
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

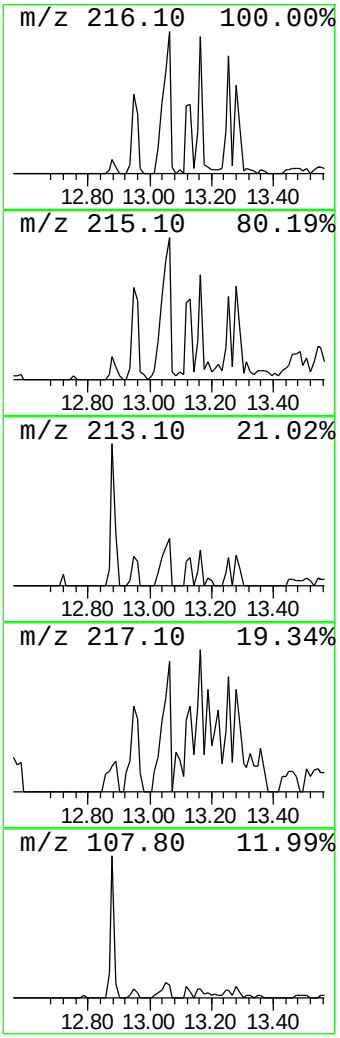
****

Peak Number 9 Pyrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.06	2.14 ng	106067	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	91
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
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Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)C

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

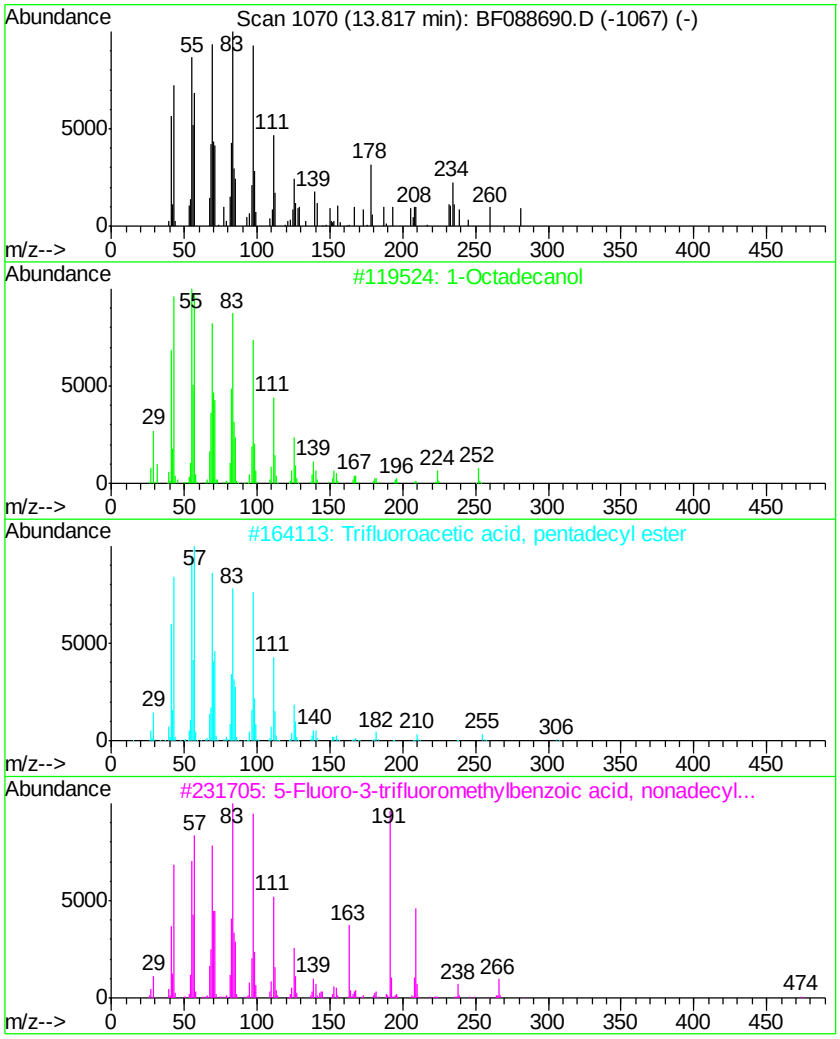
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

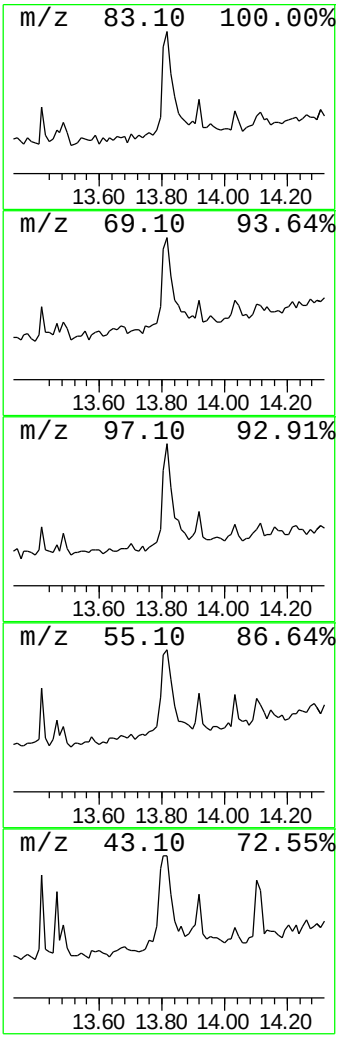
****

Peak Number 10 1-Octadecanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	2.02 ng	100333	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	93
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
3	5-Fluoro-3-trifluoromethylbenzoi...	474	C27H42F4O2	1000338-91-1	90
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	81
5	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088690.D
Acq On : 4 Jul 2016 12:36
Operator : UM/SJ
Sample : H3822-03
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D10-B3(6-12)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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown1.63	1.63	171.9	ng	5906610	1	6.79	687178	20.0
Propane, 1,1-dime...	2.02	2.3	ng	79640	1	6.79	687178	20.0
2-Pentanone, 4-hy...	4.97	6.4	ng	218444	1	6.79	687178	20.0
unknown6.56	6.56	89.8	ng	3086110	1	6.79	687178	20.0
Tridecane	10.73	2.1	ng	89301	4	11.30	829256	20.0
5-Bromo-2-thiophe...	11.91	3.0	ng	122951	4	11.30	829256	20.0
Pyrene, 2-methyl-	13.06	2.1	ng	106067	5	13.92	992896	20.0
1-Octadecanol	13.82	2.0	ng	100333	5	13.92	992896	20.0