LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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	1.644	3	5	8	rVB	2655071	2736603	51.97%	7.777%
2	1.735	12	13	23	rVB	389906	742289	14.10%	2.109%
3	1.873	23	25	39	rVV	2476621	5265250	100.00%	14.962%
4	2.044	39	40	57	rVB2	121596	371057	7.05%	1.054%
5	3.061	125	129	150	rVB	100240	336831	6.40%	0.957%
6	4.981	294	297	302	rVB	223157	304341	5.78%	0.865%
7	5.404	331	334	336	rBV	2530091	2600734	49.39%	7.391%
8	6.444	421	425	427	rBV	2397229	3017350	57.31%	8.574%
9	6.570	433	436	439	rBV	2176148	2612836	49.62%	7.425%
10	6.810	454	457	459	rBV	895756	856396	16.27%	2.434%
11	6.959	468	470	473	rVB	1534297	2085680	39.61%	5.927%
12	7.370	503	506	508	rBV	1821032	1737016	32.99%	4.936%
13	8.090	567	569	572	rVB	1279368	1115566	21.19%	3.170%
14	9.176	661	664	666	rVB	2154174	3158556	59.99%	8.976%
15	9.565	696	698	700	rBV	228774	234172	4.45%	0.665%
16	9.839	720	722	725	rVB2	1040681	1122835	21.33%	3.191%
17	10.628	788	791	793	rBV	1656417	1602004	30.43%	4.552%
18	10.753	801	802	806	rBV	50977	80374	1.53%	0.228%
19	11.199	840	841	847	rVB	93362	127149	2.41%	0.361%
20	11.325	849	852	854	rVV	732827	967764	18.38%	2.750%
21	11.634	877	879	882	rVB	47378	62805	1.19%	0.178%
22	12.902	988	990	993	rBV	2178485	2053416	39.00%	5.835%
23	13.805	1067	1069	1073	rBV	154721	187325	3.56%	0.532%
24	13.942	1079	1081	1084	rBV	876792	830297	15.77%	2.359%
25	14.445	1122	1125	1130	rBV	92690	154172	2.93%	0.438%
26	15.348	1201	1204	1207	rBV	504960	663880	12.61%	1.887%
27	15.805	1241	1244	1247	rBV	32472	55656	1.06%	0.158%
28	16.880	1335	1338	1346	rVB4	48972	107593	2.04%	0.306%

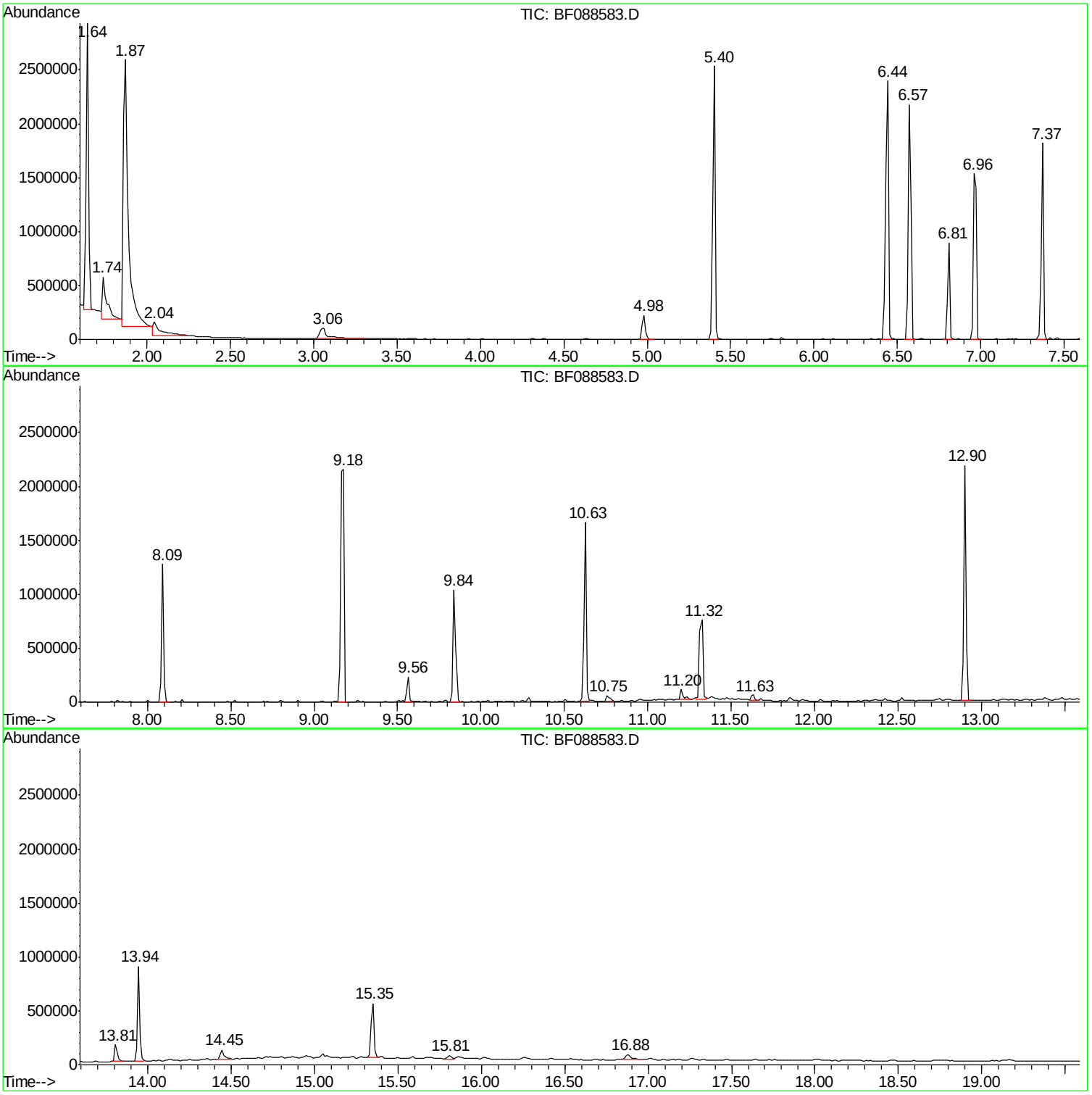
Sum of corrected areas: 35189947

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.1-5

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\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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

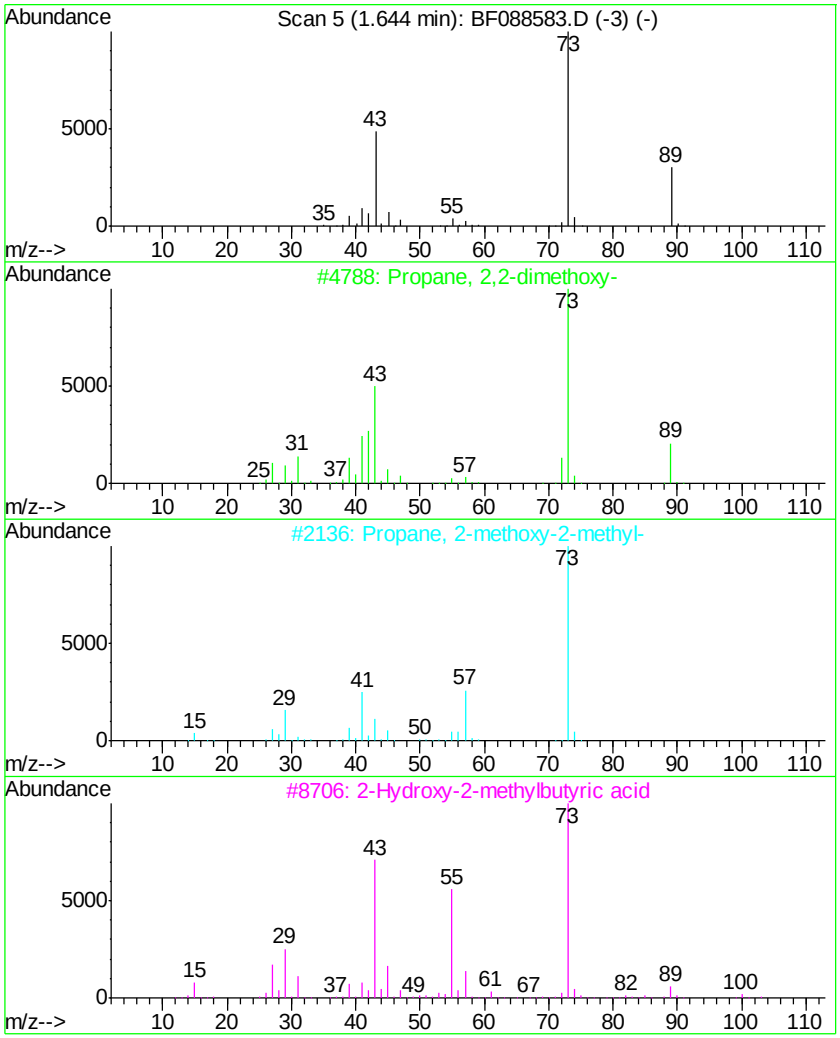
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

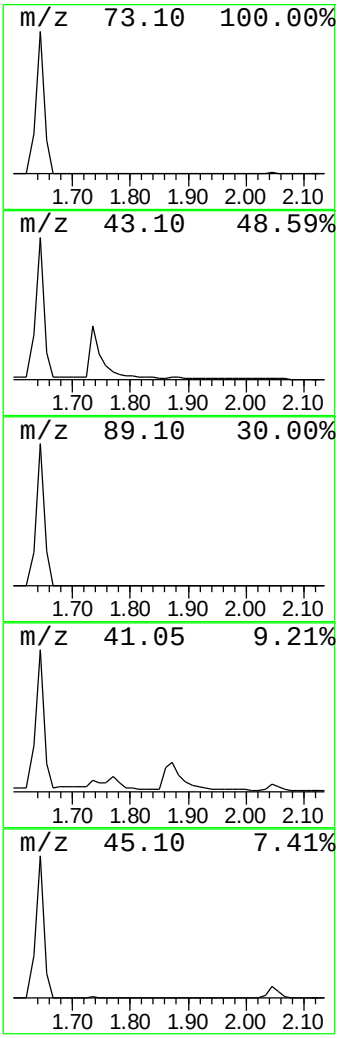
****

Peak Number 1 unknown1.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.64	63.91 ng	2736600	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	40
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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

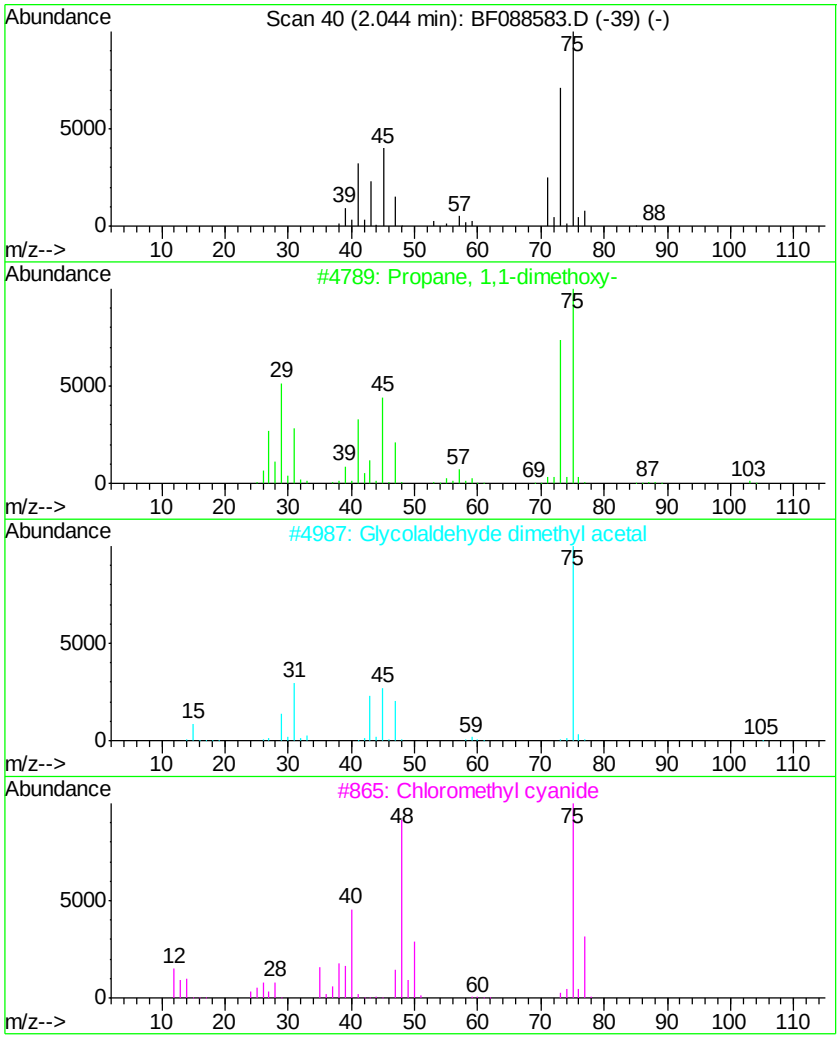
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

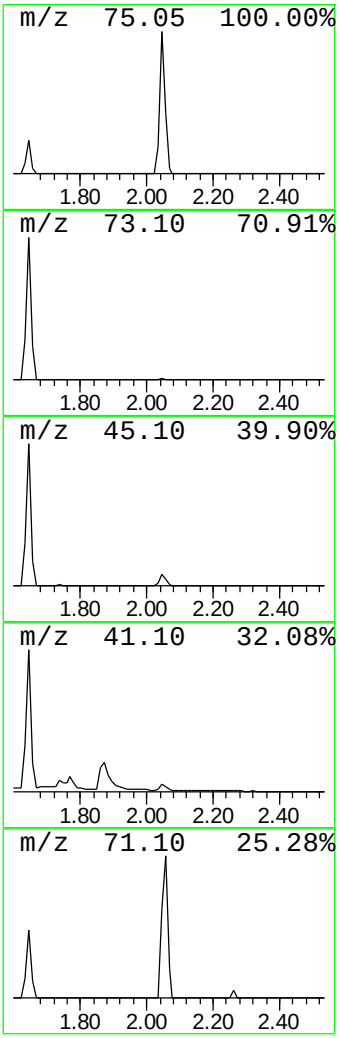
****

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.04	8.67 ng	371057	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	36
3	Chloromethyl cyanide	75	C2H2ClN	000107-14-2	7
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7
5	Formamide, N-methylthio	75	C2H5NS	018952-41-5	5





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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

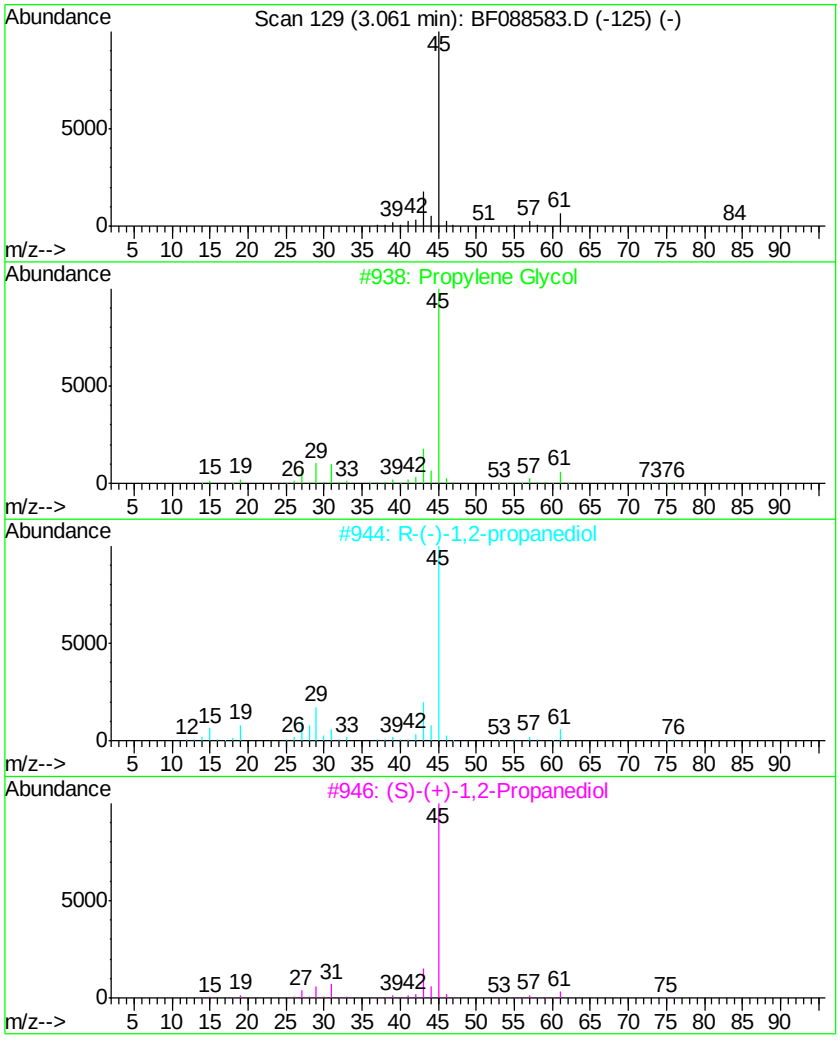
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

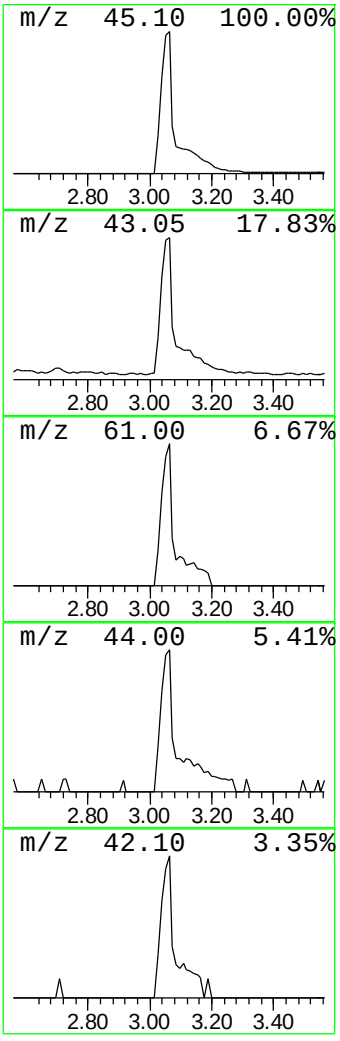
****

Peak Number 5 unknown3.06 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	7.87 ng	336831	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	43
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Formamide	45	CH3NO	000075-12-7	7





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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

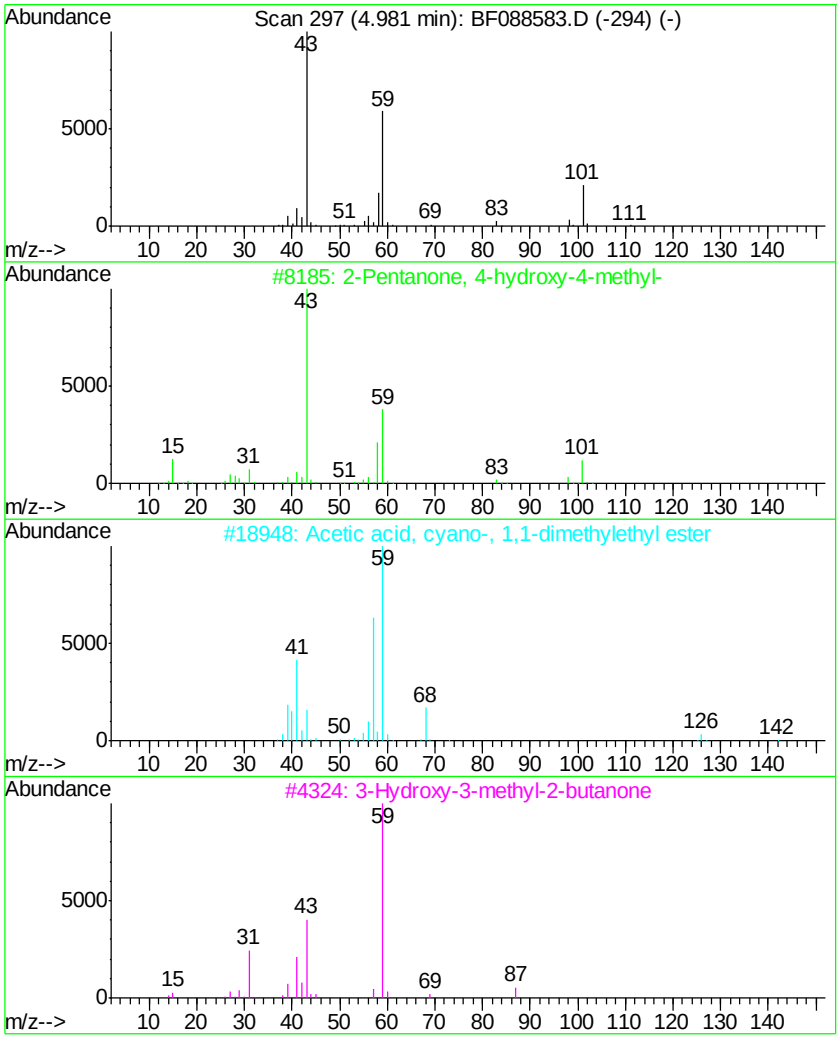
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

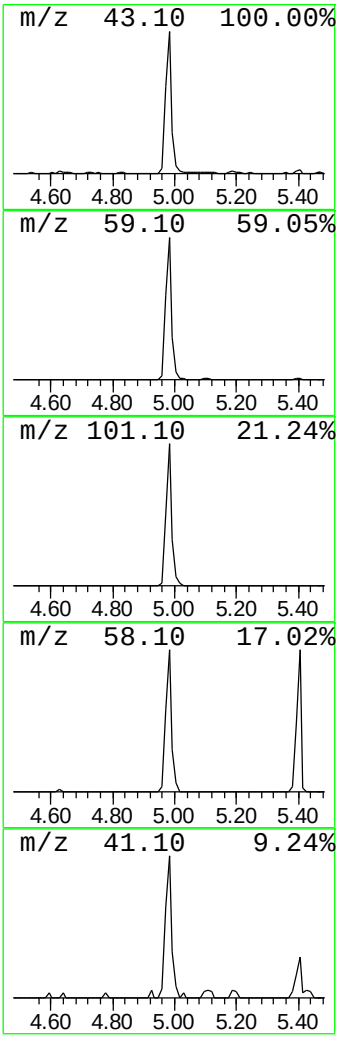
****

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	7.11 ng	304341	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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

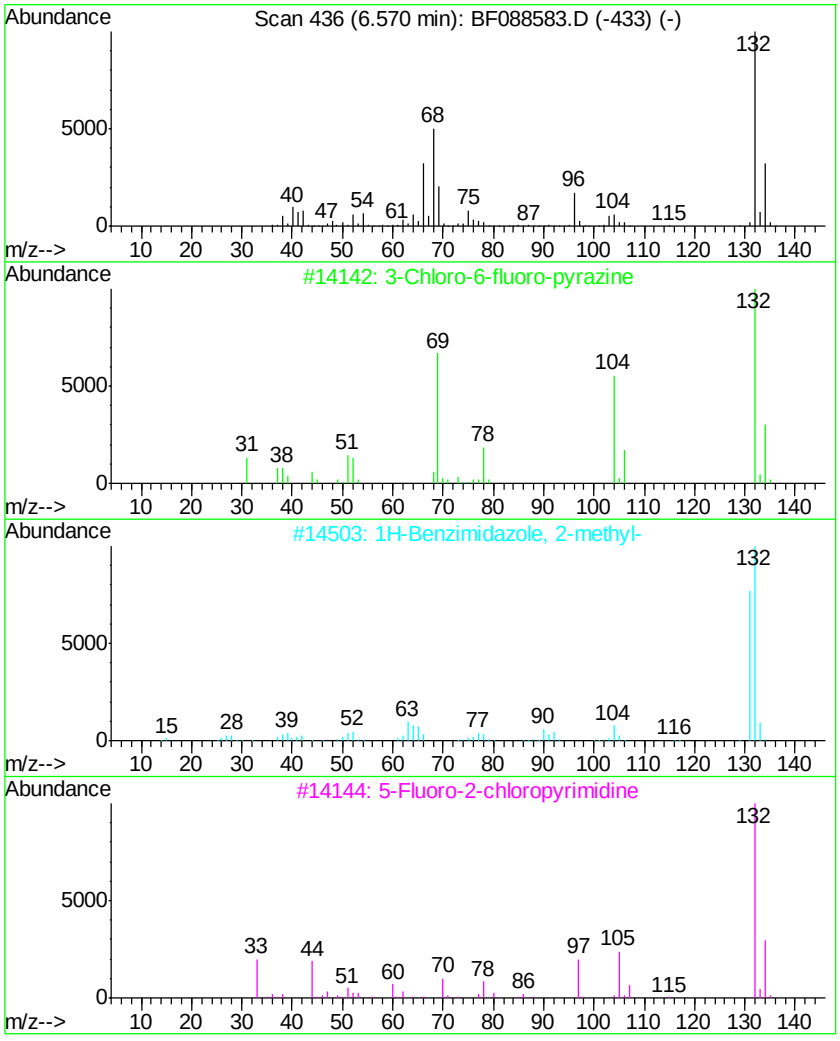
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

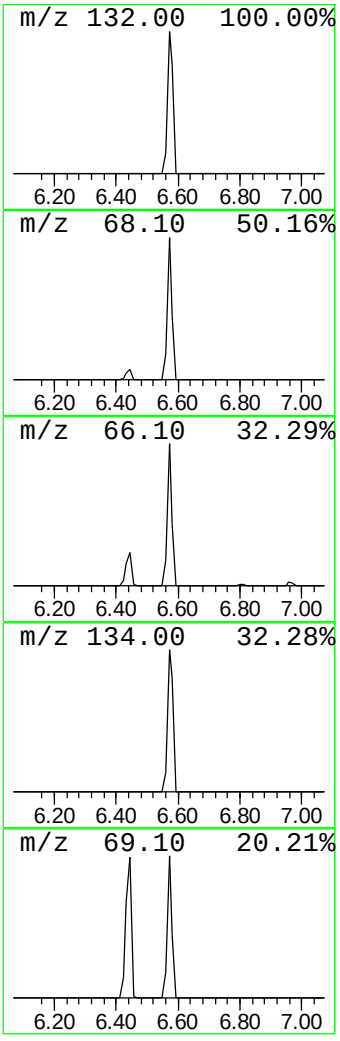
****

Peak Number 7 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	61.02 ng	2612840	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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

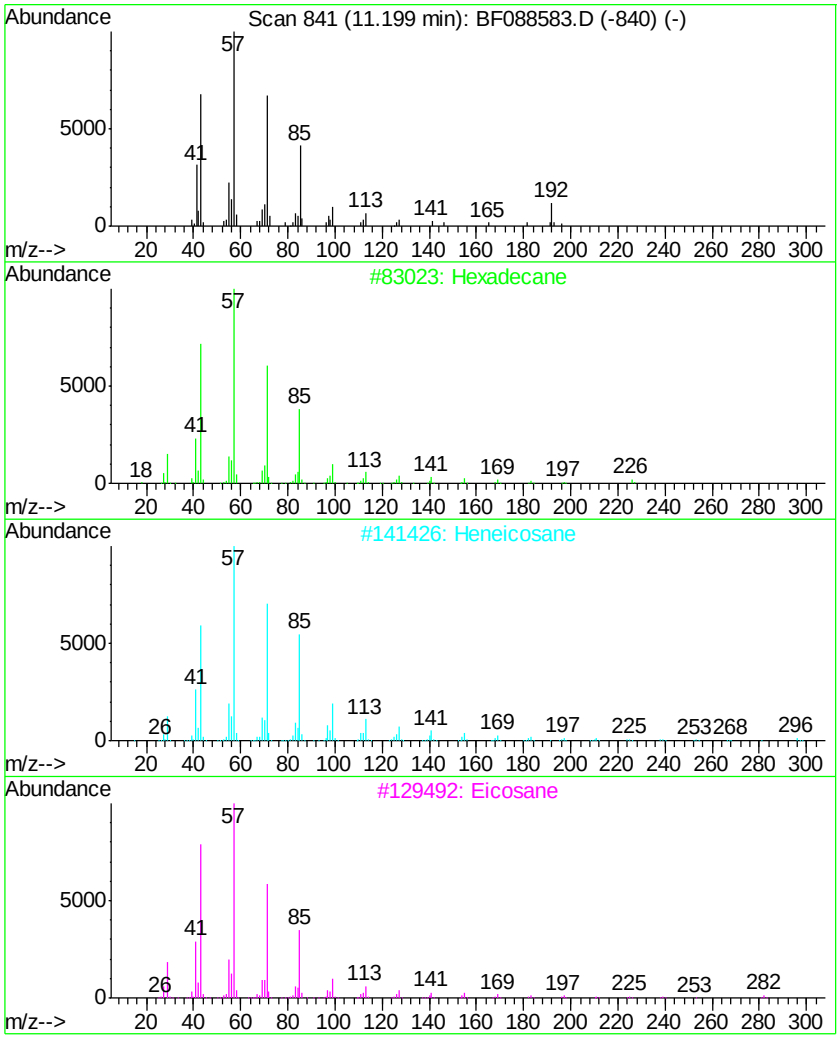
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

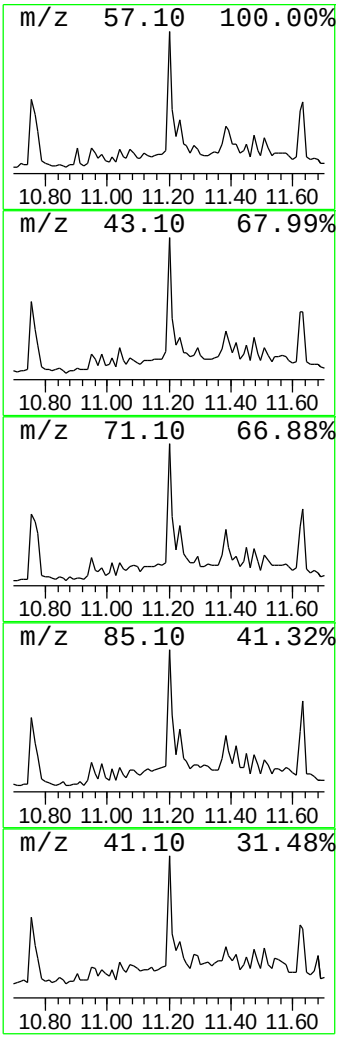
****

Peak Number 9 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	2.63 ng	127149	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Heneicosane	296	C21H44	000629-94-7	86
3	Eicosane	282	C20H42	000112-95-8	80
4	Heptacosane	380	C27H56	000593-49-7	80
5	Pentadecane	212	C15H32	000629-62-9	80





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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

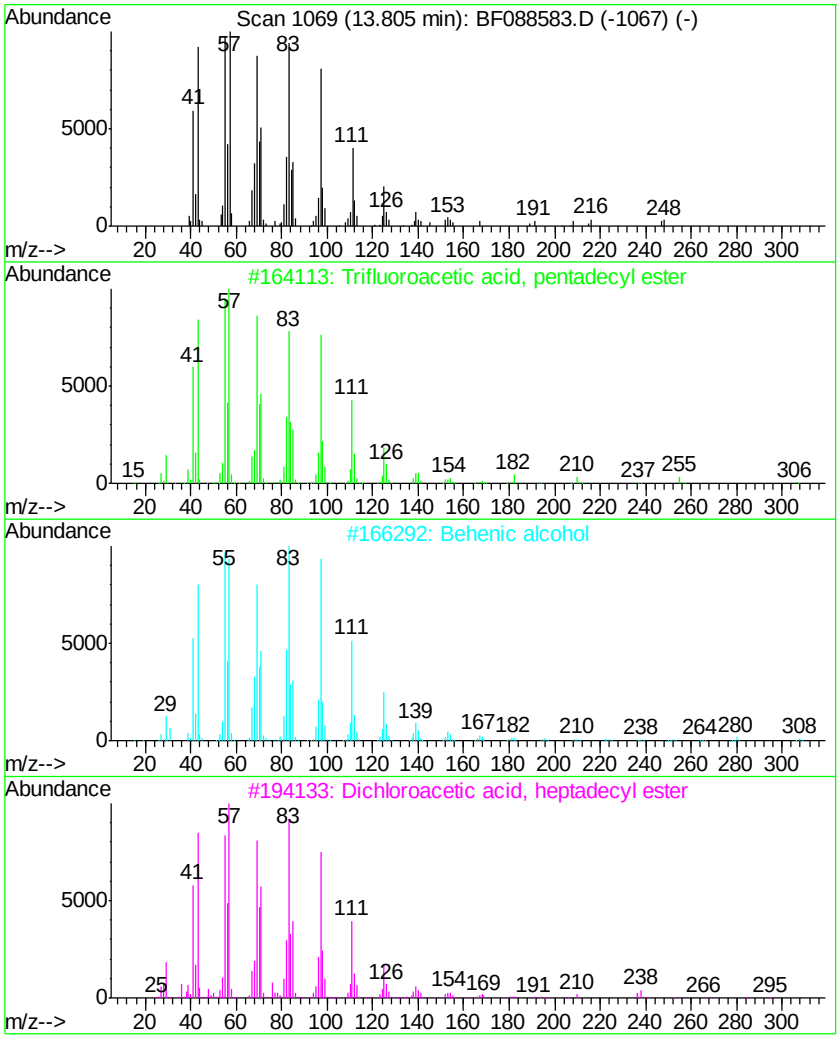
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

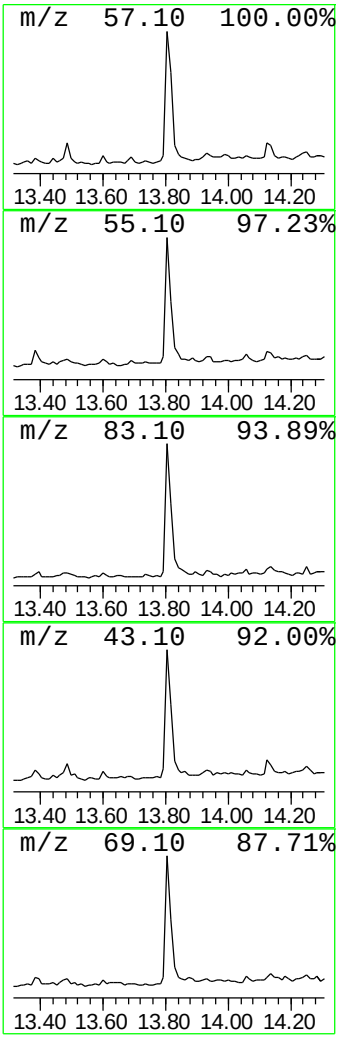
****

Peak Number 10 Trifluoroacetic acid, penta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	4.51 ng	187325	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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

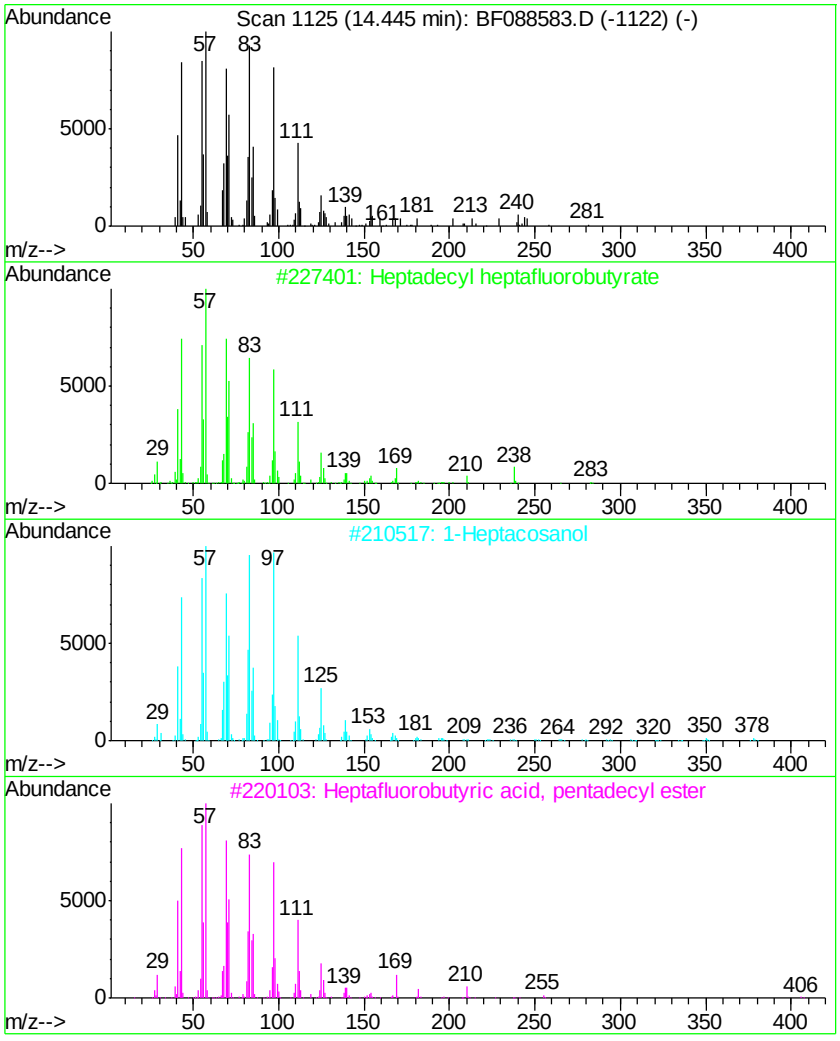
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

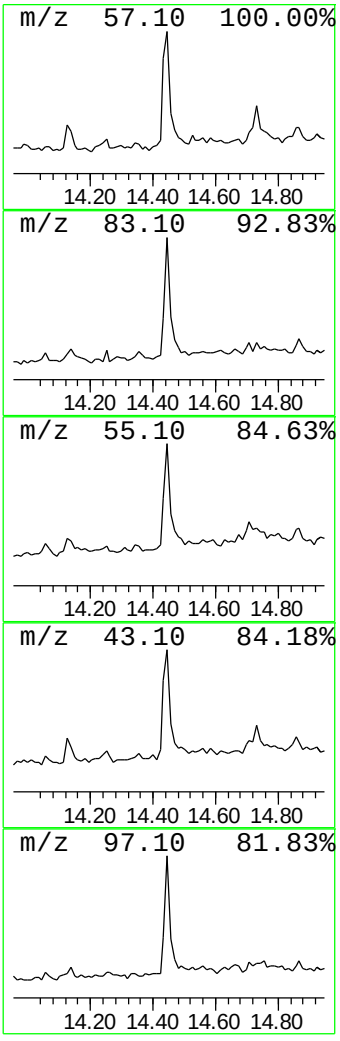
****

Peak Number 11 Heptadecyl heptafluorobutyrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	3.71 ng	154172	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	93
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	Octacosanol	410	C28H58O	000557-61-9	89
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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

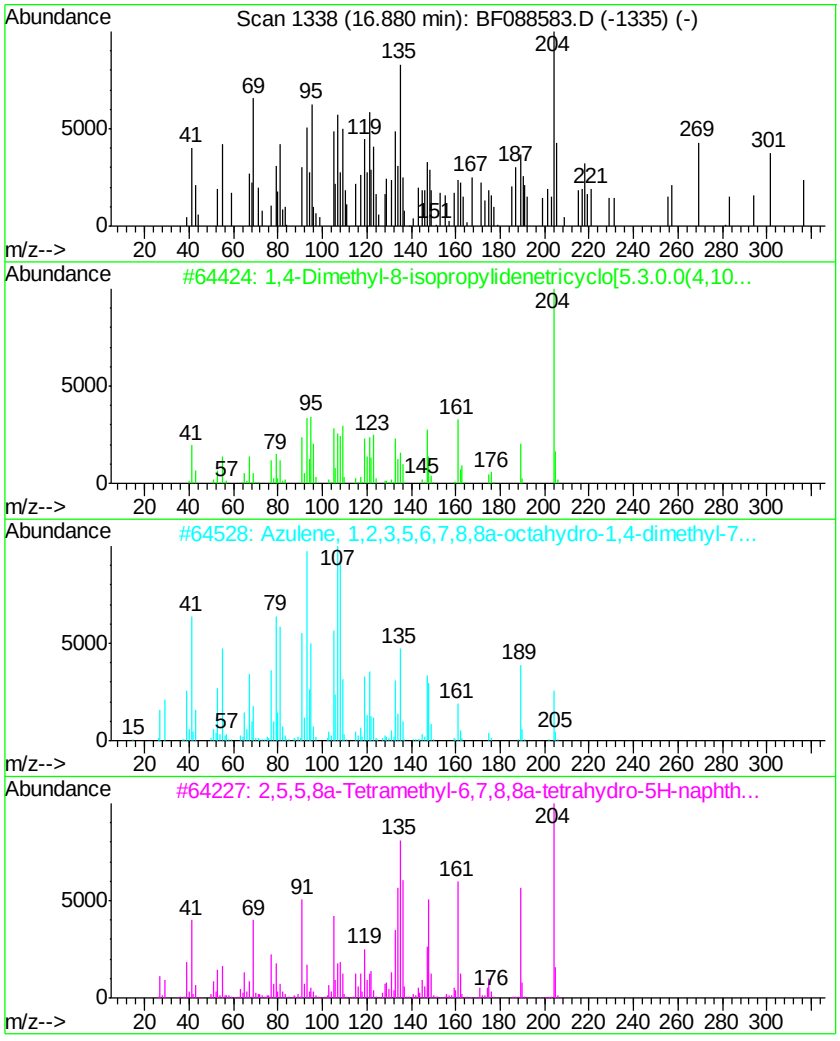
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

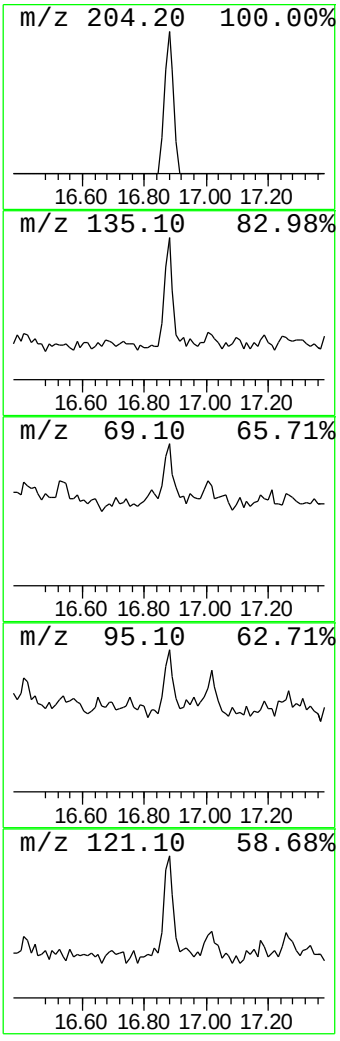
****

Peak Number 12 1,4-Dimethyl-8-isopropylide... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.88	3.24 ng	107593	Perylene-d12	15.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	78
2	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	53
3	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	43
4	Aciphyllene	204	C15H24	087745-31-1	42
5	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088583.D
Acq On : 1 Jul 2016 19:15
Operator : UM/SJ
Sample : H3836-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-5

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
unknown1.64	1.64	63.9	ng	2736600	1	6.81	856396	20.0
Propane, 1,1-dime...	2.04	8.7	ng	371057	1	6.81	856396	20.0
unknown3.06	3.06	7.9	ng	336831	1	6.81	856396	20.0
2-Pentanone, 4-hy...	4.98	7.1	ng	304341	1	6.81	856396	20.0
unknown6.57	6.57	61.0	ng	2612840	1	6.81	856396	20.0
Hexadecane	11.20	2.6	ng	127149	4	11.32	967764	20.0
Trifluoroacetic a...	13.81	4.5	ng	187325	5	13.94	830297	20.0
Heptadecyl heptaf...	14.45	3.7	ng	154172	5	13.94	830297	20.0
1,4-Dimethyl-8-is...	16.88	3.2	ng	107593	6	15.35	663880	20.0