LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088567.D
Acq On : 1 Jul 2016 11:28
Operator : UM/SJ
Sample : H3808-25
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13-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-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	1.667	4	7	10	rVB	4583329	5943850	100.00%	14.672%
2	1.735	12	13	23	rVB	490640	787199	13.24%	1.943%
3	1.861	23	24	40	rVV	2431635	5859888	98.59%	14.465%
4	2.055	40	41	87	rVB	139137	822275	13.83%	2.030%
5	4.981	294	297	300	rBV	122176	160930	2.71%	0.397%
6	5.404	331	334	336	rBV	2067465	2324776	39.11%	5.739%
7	6.433	421	424	427	rBV	2057975	2093733	35.23%	5.168%
8	6.570	433	436	439	rBV	2294653	2155526	36.26%	5.321%
9	6.810	454	457	459	rBV	730003	801294	13.48%	1.978%
10	6.959	468	470	473	rVB	1708084	1684448	28.34%	4.158%
11	7.370	503	506	508	rBV	1367927	1571032	26.43%	3.878%
12	8.090	566	569	571	rBV	1243958	1114729	18.75%	2.752%
13	9.165	660	663	666	rBV	2305967	2524640	42.47%	6.232%
14	9.565	695	698	700	rBV	615467	638077	10.74%	1.575%
15	9.839	719	722	725	rVB	1203060	1204939	20.27%	2.974%
16	10.628	788	791	793	rBV	1320069	1518358	25.55%	3.748%
17	11.325	849	852	854	rVB	880570	1262896	21.25%	3.117%
18	11.554	870	872	877	rBV	157448	270375	4.55%	0.667%
19	12.376	942	944	952	rBV	663611	784692	13.20%	1.937%
20	12.902	987	990	993	rBV	2438142	2563852	43.13%	6.329%
21	13.382	1027	1032	1034	rBV2	473676	594823	10.01%	1.468%
22	13.817	1067	1070	1077	rBV	184134	303068	5.10%	0.748%
23	13.942	1077	1081	1084	rBV	1450681	1676627	28.21%	4.139%
24	14.525	1129	1132	1136	rBV2	37121	101724	1.71%	0.251%
25	14.720	1146	1149	1151	rVB	40599	69229	1.16%	0.171%
26	14.800	1154	1156	1159	rVV2	264477	286950	4.83%	0.708%
27	14.902	1163	1165	1167	rVB	120927	115427	1.94%	0.285%
28	15.177	1186	1189	1191	rVB	121448	156869	2.64%	0.387%
29	15.348	1201	1204	1207	rBV	890919	1118768	18.82%	2.762%

Sum of corrected areas: 40510994

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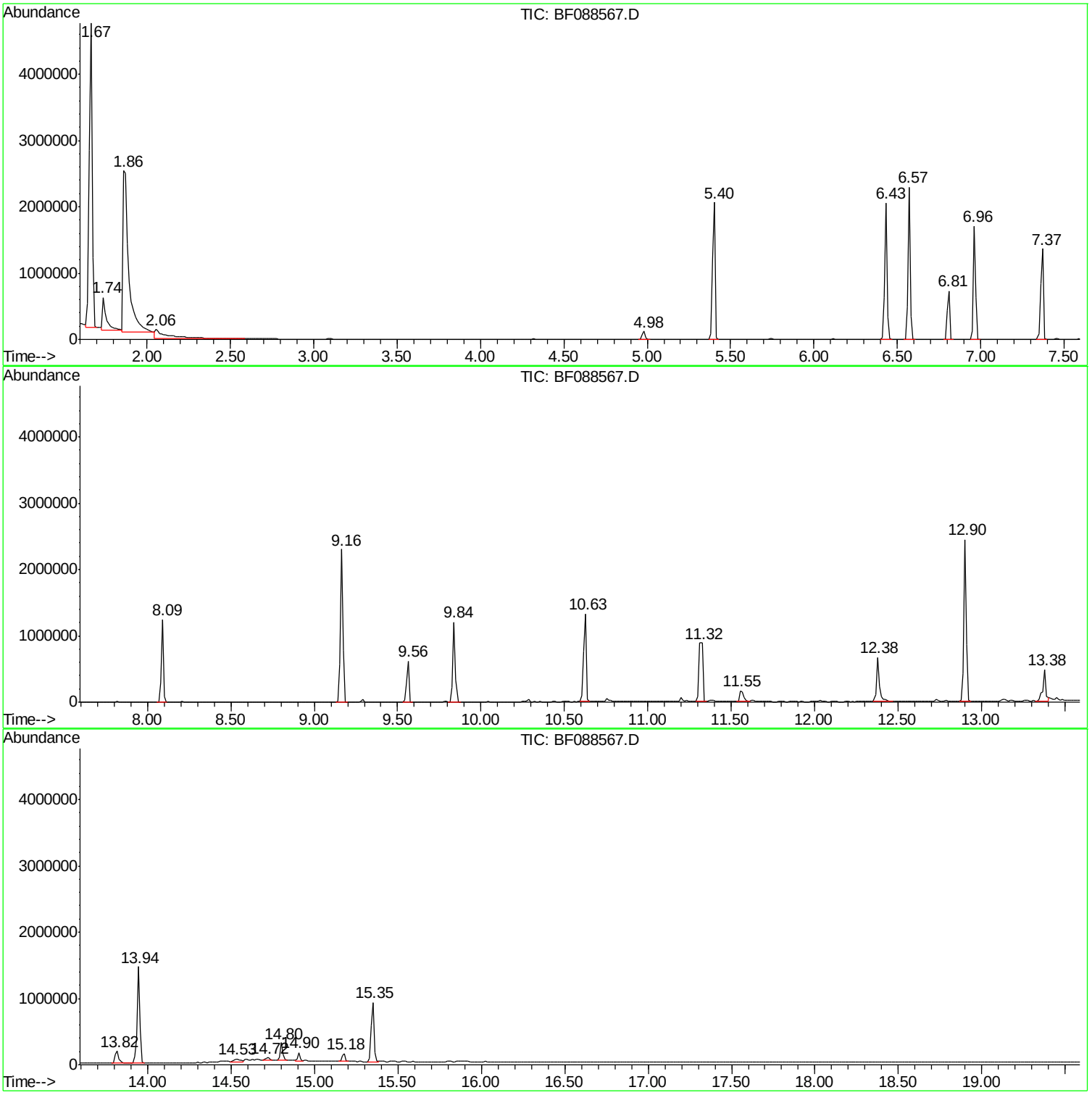
BNA_F
ClientSampleId :
SB-13-COMP

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



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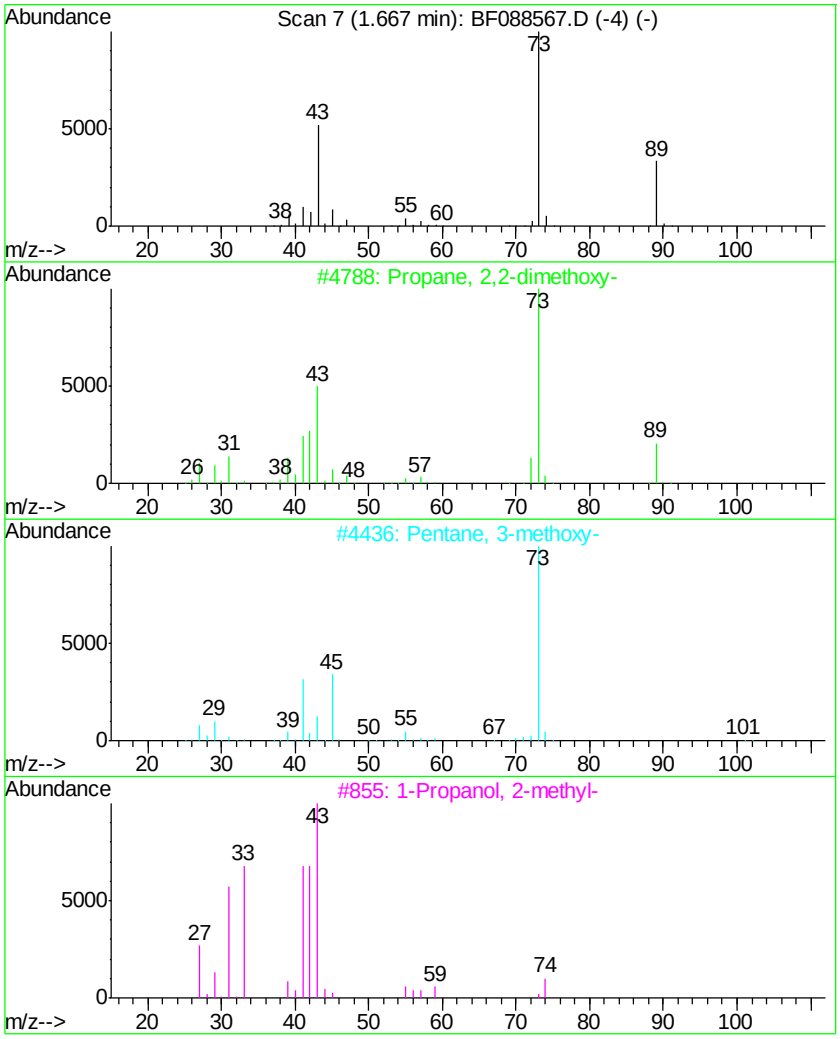
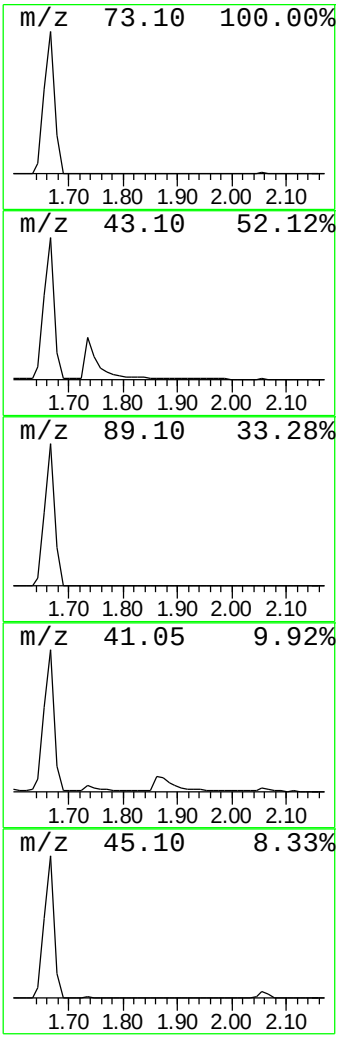
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	148.36 ng	5943850	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	56
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SB-13-COMP

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

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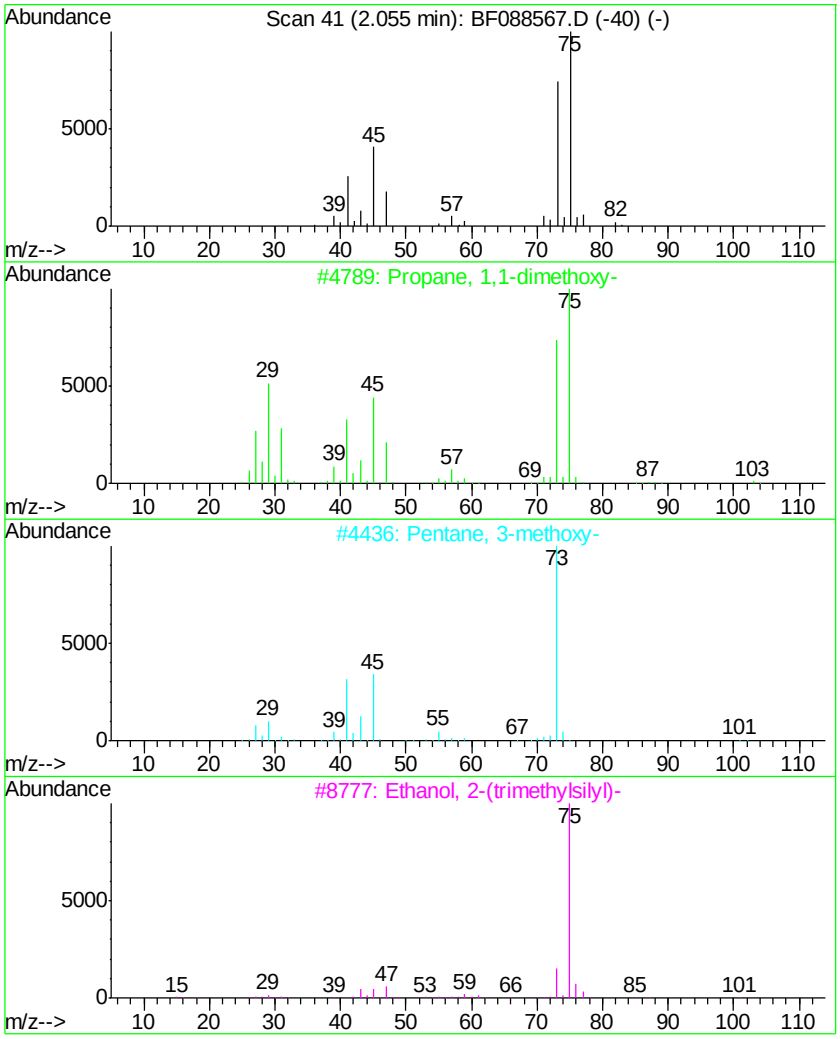
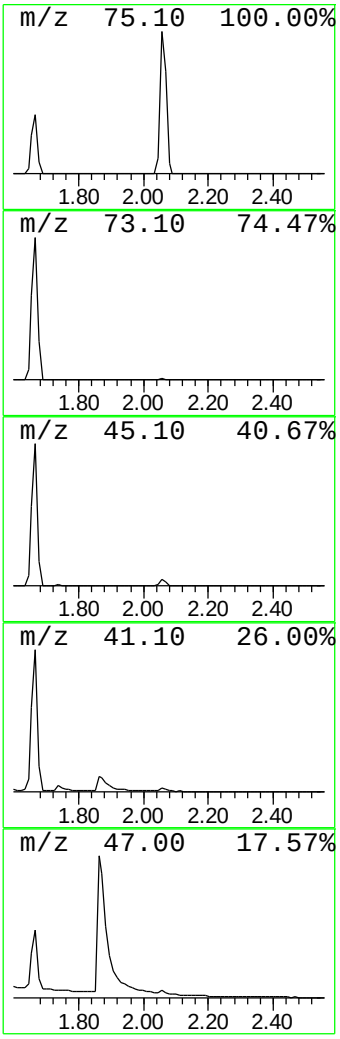
Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	20.52 ng	822275	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	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3	Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	9
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9





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Instrument : BNA_F
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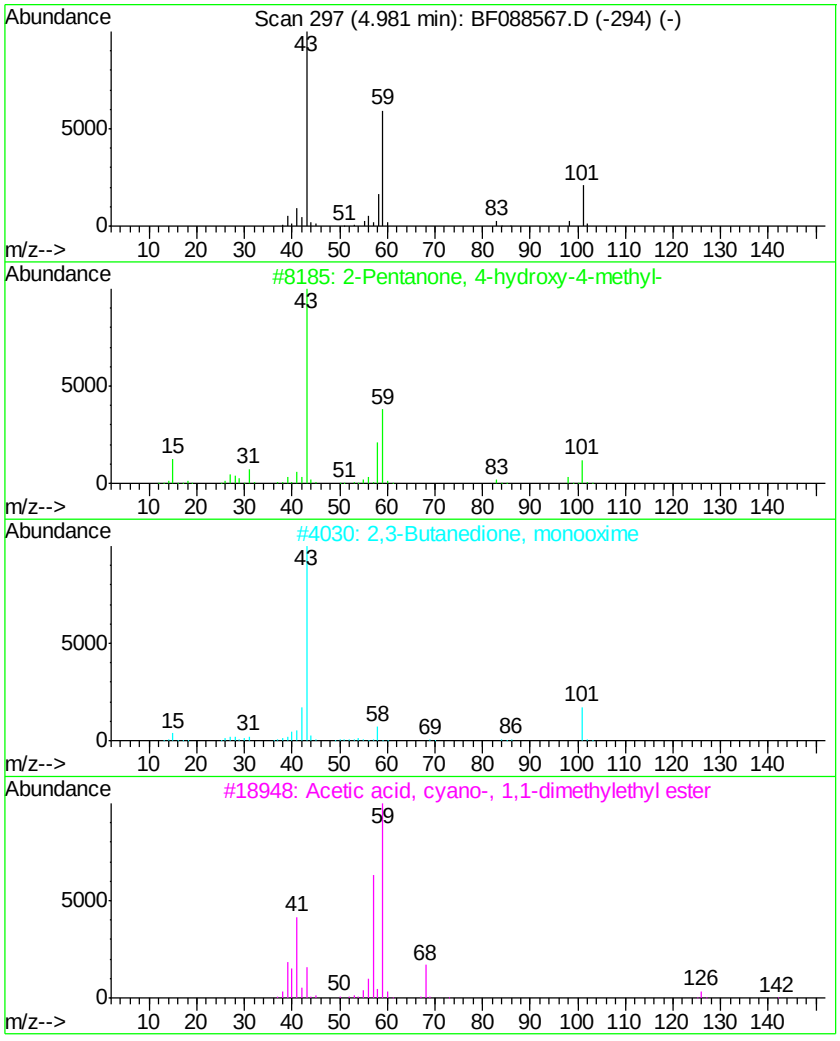
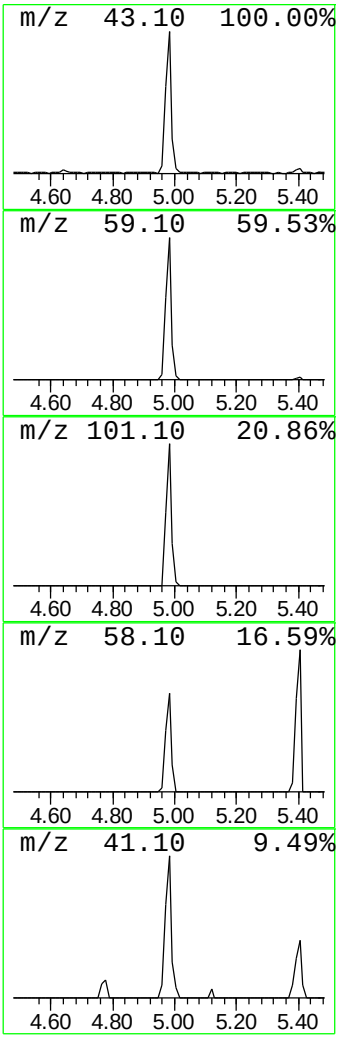
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	4.02 ng	160930	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	53
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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TIC Library : C:\Database\NIST11.L
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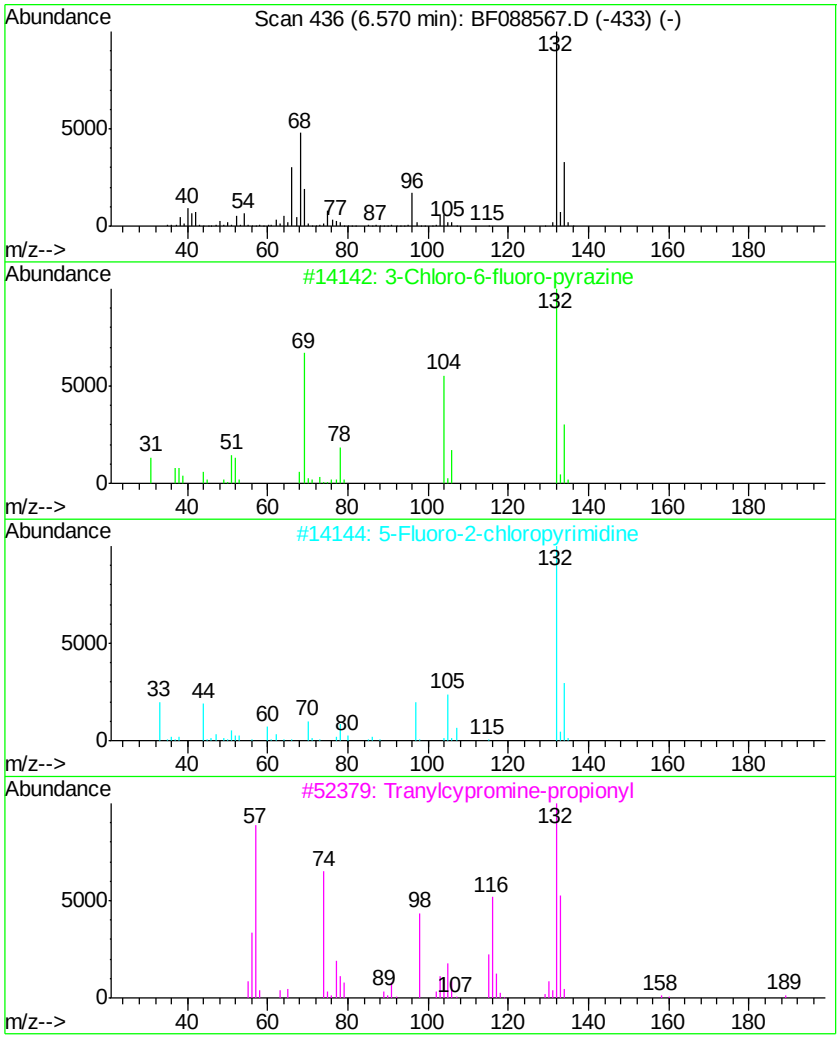
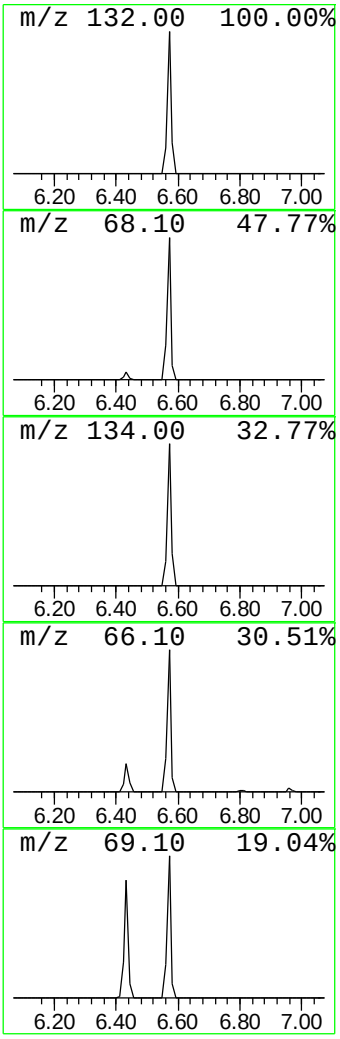
Peak Number 6 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	53.80 ng	2155530	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





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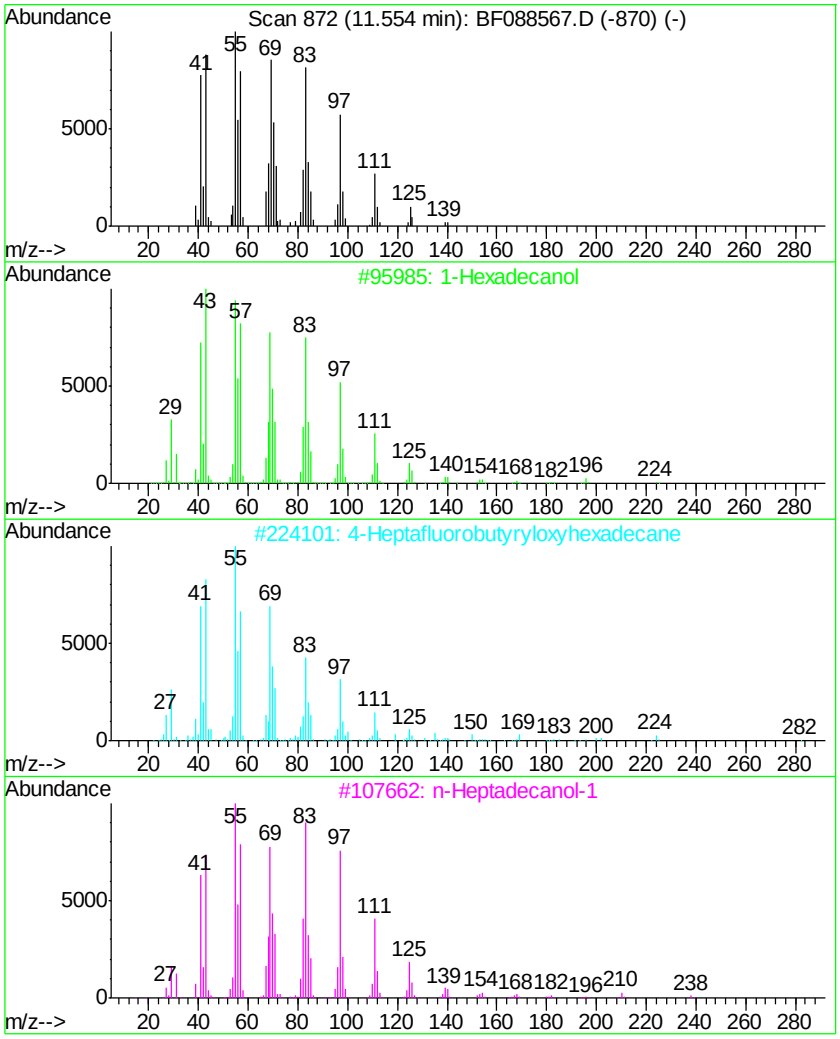
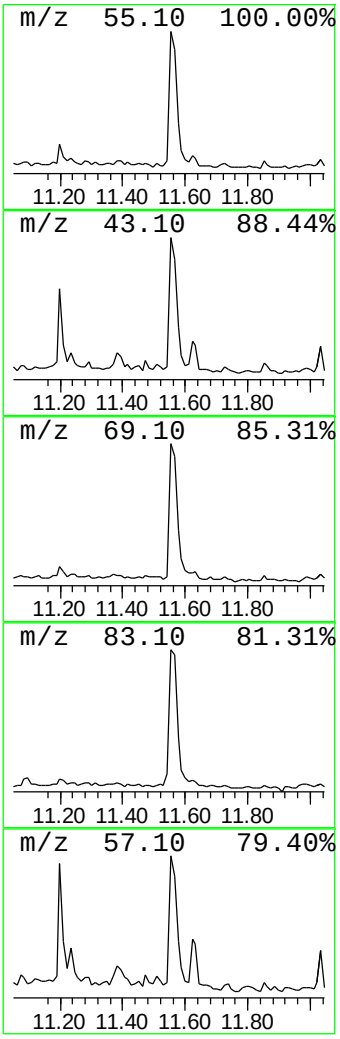
****

Peak Number 8 1-Hexadecanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	4.28 ng	270375	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	95
2	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	91





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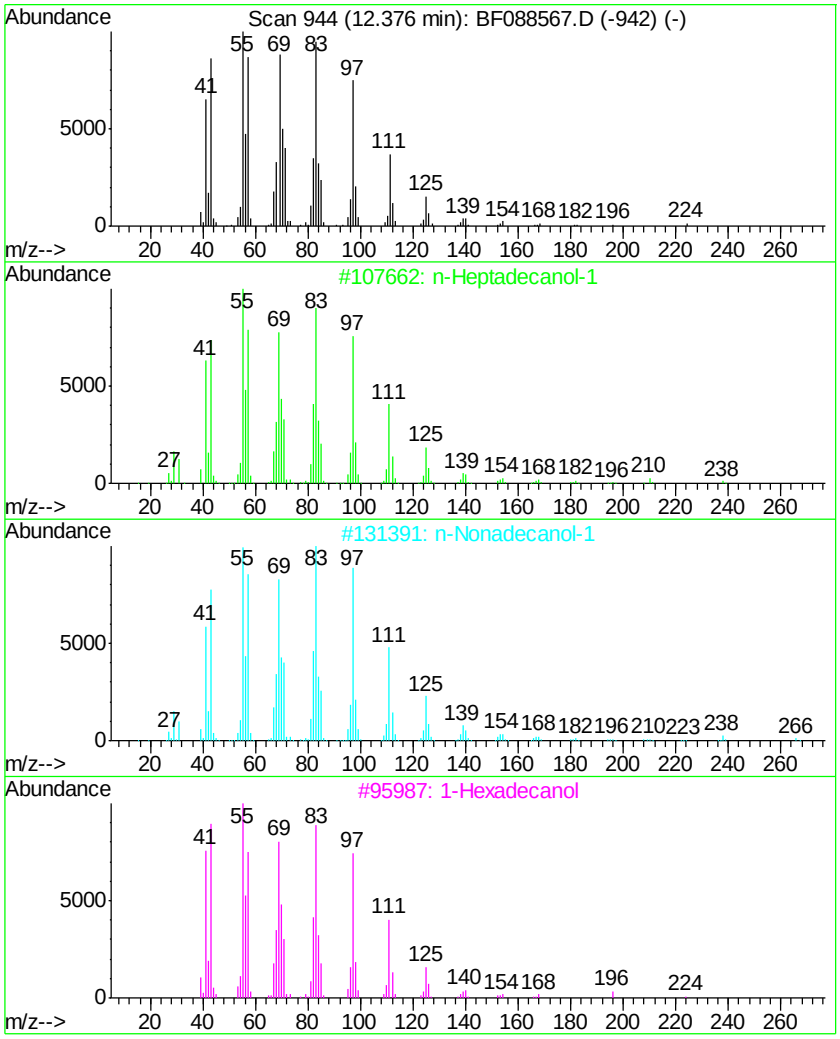
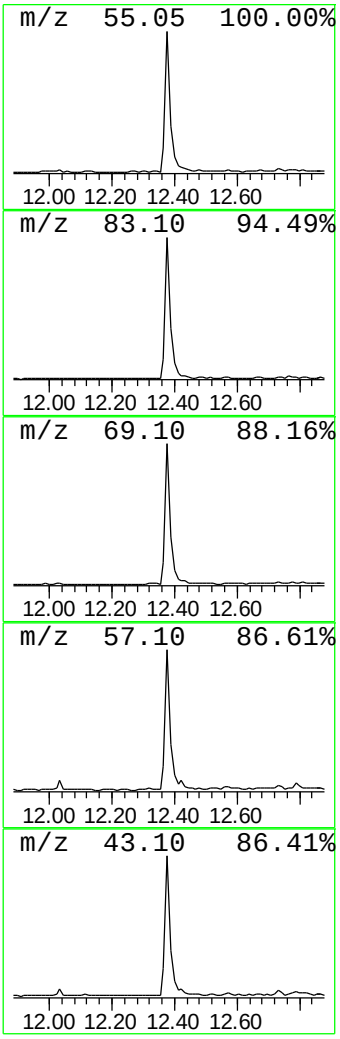
Peak Number 9 n-Heptadecanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	12.43 ng	784692	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	1-Hexadecanol	242	C16H34O	036653-82-4	93
4	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	93
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91





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TIC Library : C:\Database\NIST11.L
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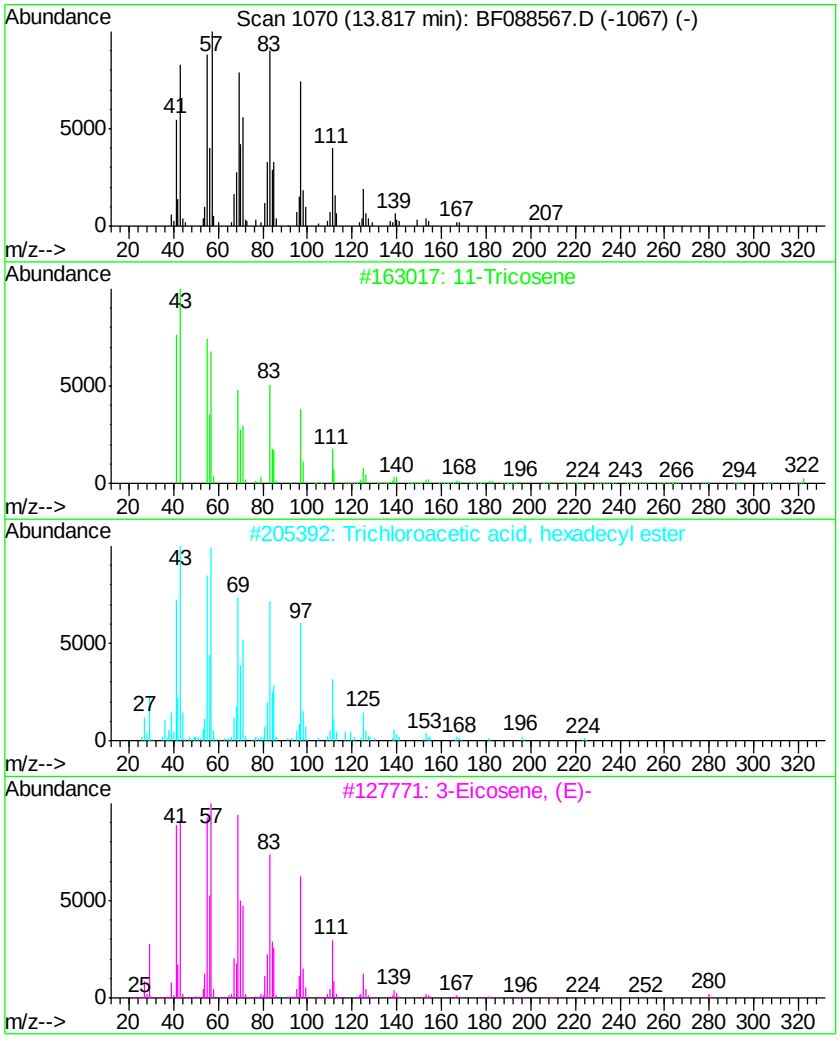
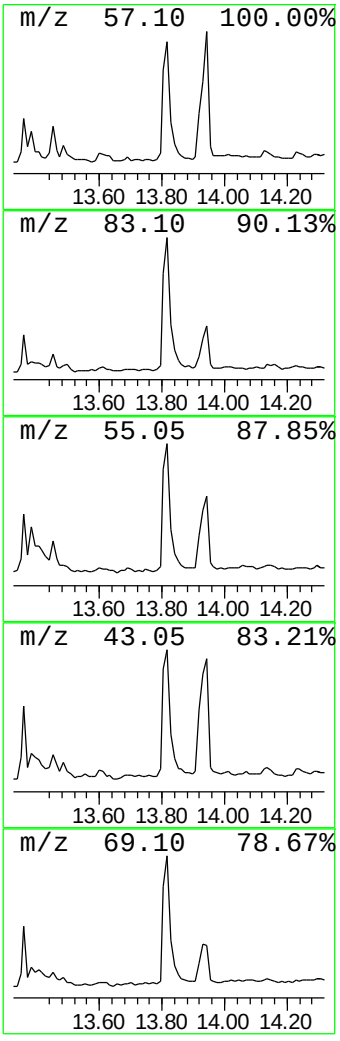
Peak Number 10 11-Tricosene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.62 ng	303068	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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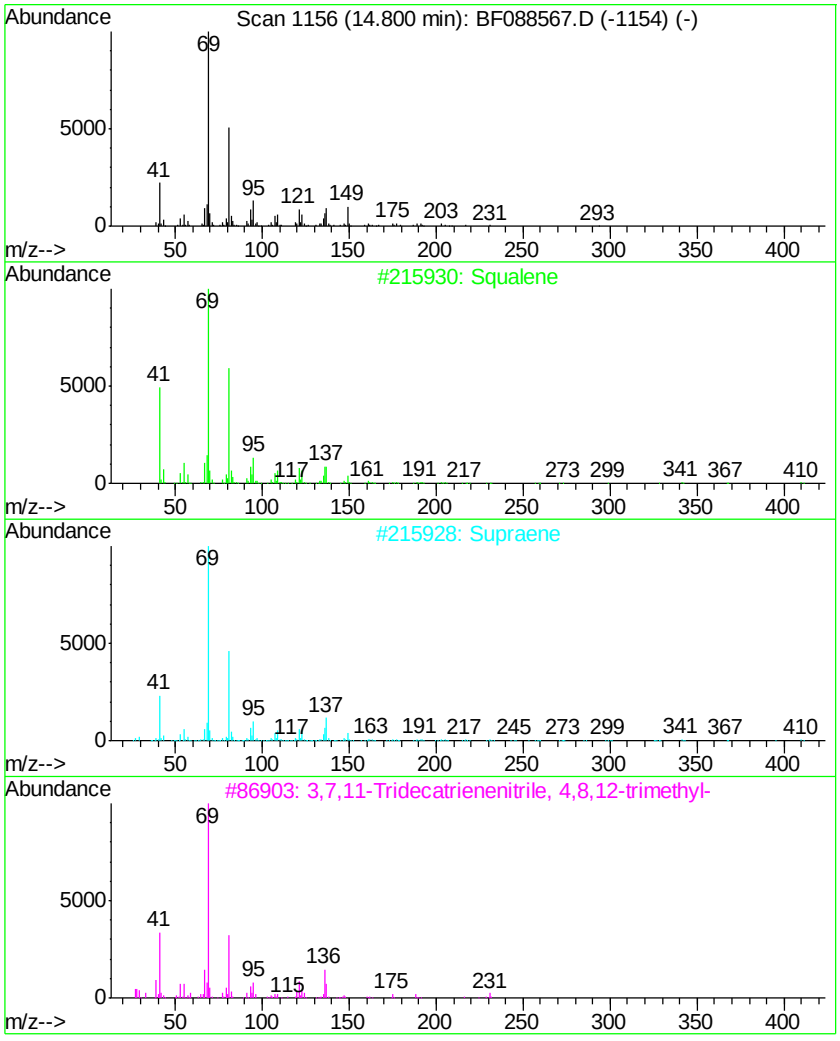
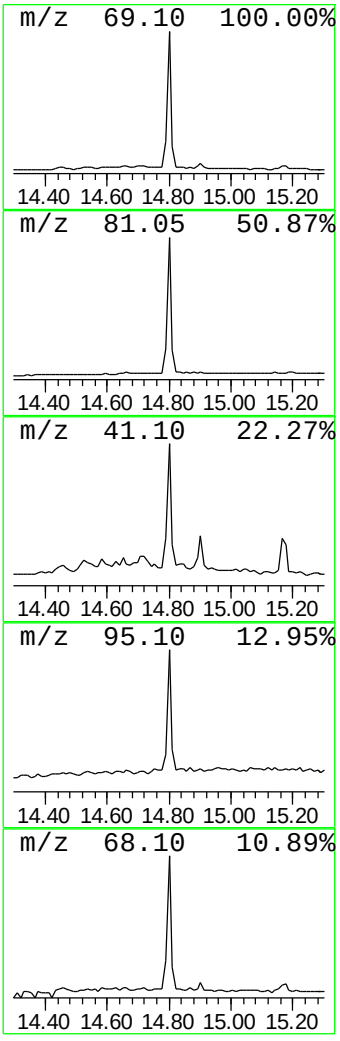
Peak Number 11 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	5.13 ng	286950	Perylene-d12	15.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
4	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50





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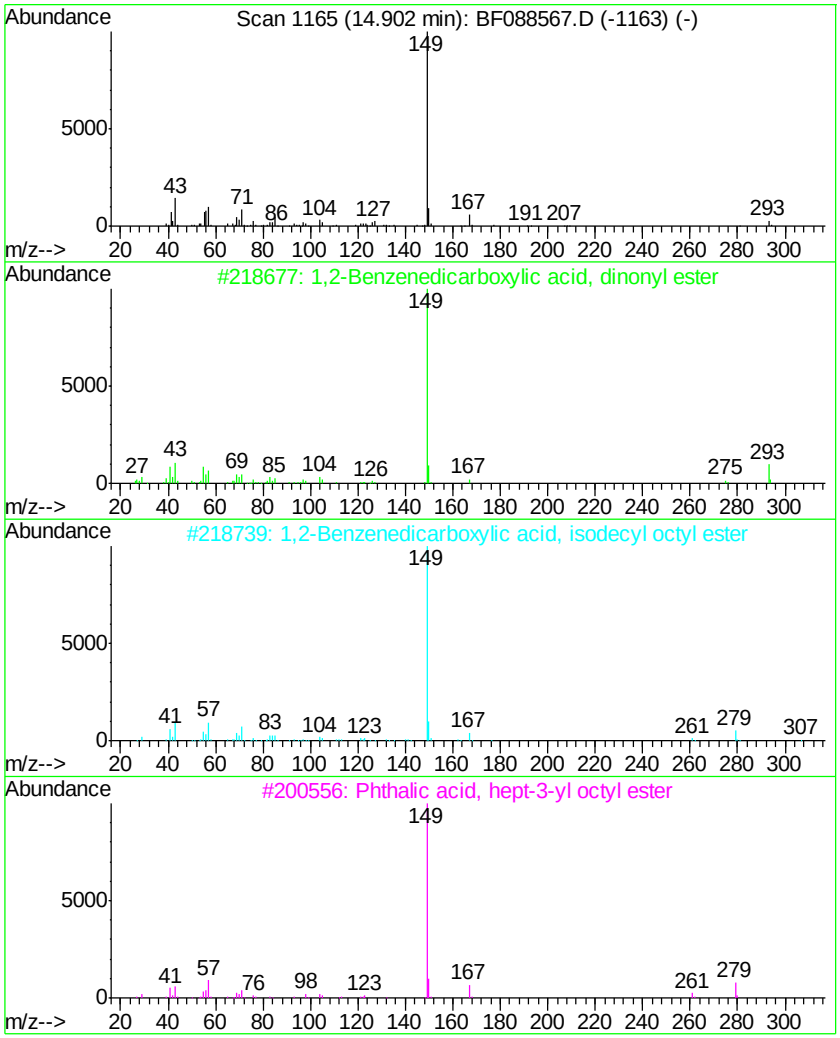
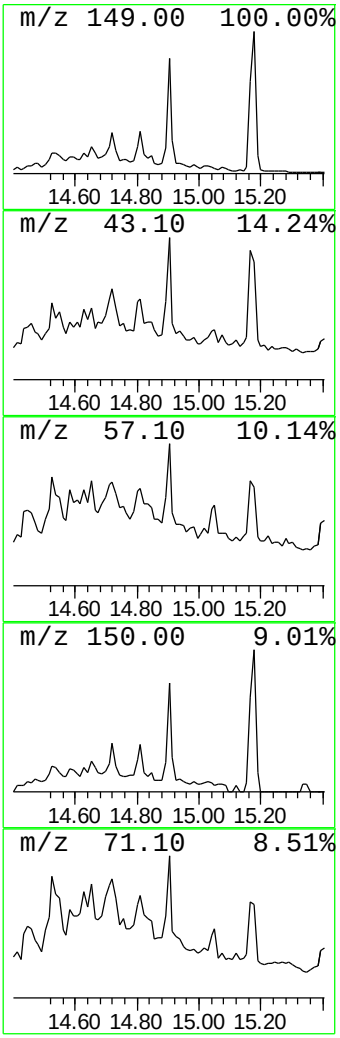
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1,2-Benzenedicarboxylic aci... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.06 ng	115427	Perylene-d12	15.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	86
2	1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	86
3	Phthalic acid, hept-3-yl octyl e...	376	C23H36O4	1000356-99-2	80
4	Phthalic acid, 4-chloro-2-methyl...	486	C29H39ClO4	1000356-38-0	80
5	Phthalic acid, 2-fluorophenyl he...	484	C30H41FO4	1000356-50-1	80





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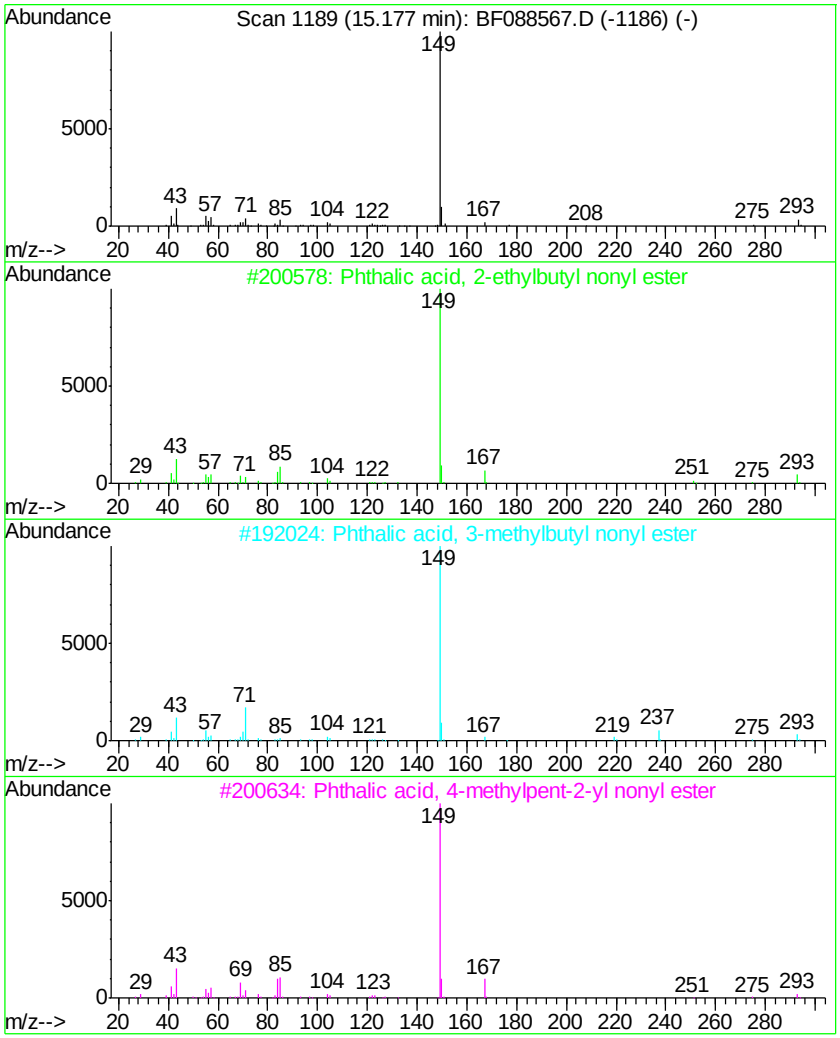
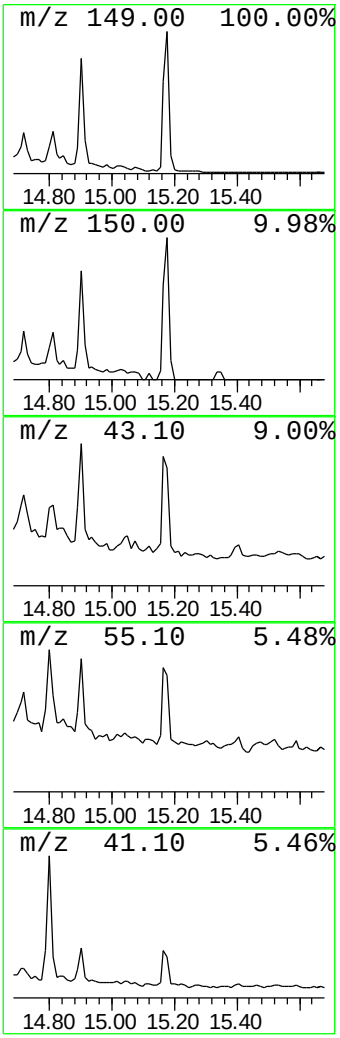
Peak Number 13 Phthalic acid, 2-ethylbutyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	2.80 ng	156869	Perylene-d12	15.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 2-ethylbutyl nony...	376	C23H36O4	1000356-89-4	86
2	Phthalic acid, 3-methylbutyl non...	362	C22H34O4	1000356-81-0	83
3	Phthalic acid, 4-methylpent-2-yl...	376	C23H36O4	1000356-87-9	78
4	Phthalic acid, hex-2-yn-4-yl non...	372	C23H32O4	1000315-19-5	78
5	Phthalic acid, 6-ethyl-3-octyl p...	376	C23H36O4	1000315-17-5	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088567.D
Acq On : 1 Jul 2016 11:28
Operator : UM/SJ
Sample : H3808-25
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13-COMP

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
Propane, 2,2-dime...	1.67	148.4	ng	5943850	1	6.81	801294	20.0
Propane, 1,1-dime...	2.06	20.5	ng	822275	1	6.81	801294	20.0
2-Pentanone, 4-hy...	4.98	4.0	ng	160930	1	6.81	801294	20.0
unknown6.57	6.57	53.8	ng	2155530	1	6.81	801294	20.0
1-Hexadecanol	11.55	4.3	ng	270375	4	11.32	1262900	20.0
n-Heptadecanol-1	12.38	12.4	ng	784692	4	11.32	1262900	20.0
11-Tricosene	13.82	3.6	ng	303068	5	13.94	1676630	20.0
Squalene	14.80	5.1	ng	286950	6	15.35	1118770	20.0
1,2-Benzenedicarb...	14.90	2.1	ng	115427	6	15.35	1118770	20.0
Phthalic acid, 2-...	15.18	2.8	ng	156869	6	15.35	1118770	20.0