LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
Data File : BF084571.D
Acq On : 20 Jan 2016 18:18
Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

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-BF123115.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	3.664	134	138	141	rVB	339837	582752	7.88%	1.027%
2	4.270	189	191	195	rBV	247752	296162	4.01%	0.522%
3	4.944	247	250	258	rVB	1513718	1708026	23.10%	3.012%
4	5.379	285	288	290	rBV	3463432	3141923	42.50%	5.540%
5	5.779	321	323	326	rVB	323933	276305	3.74%	0.487%
6	6.419	376	379	381	rBV	2518315	2190626	29.63%	3.862%
7	6.544	387	390	393	rBV	4808099	4880989	66.03%	8.606%
8	6.613	395	396	402	rVB	146053	181489	2.46%	0.320%
9	6.773	408	410	413	rBV	1393401	1372776	18.57%	2.420%
10	6.853	415	417	420	rVV	67379	91753	1.24%	0.162%
11	6.933	421	424	427	rVB	5105853	4707953	63.68%	8.301%
12	7.150	438	443	445	rBV2	43251	95178	1.29%	0.168%
13	7.344	457	460	463	rBV	3498434	3946878	53.39%	6.959%
14	7.470	465	471	474	rBV	218515	410703	5.56%	0.724%
15	7.825	497	502	504	rBV2	195500	343329	4.64%	0.605%
16	7.927	508	511	514	rVB	45915	76296	1.03%	0.135%
17	8.065	520	523	525	rBV	2298376	1931371	26.13%	3.405%
18	8.190	530	534	535	rBV	84207	123419	1.67%	0.218%
19	8.236	535	538	540	rVV	190662	395054	5.34%	0.697%
20	8.293	540	543	545	rVV	349192	555204	7.51%	0.979%
21	8.362	545	549	552	rVB3	148454	302244	4.09%	0.533%
22	8.465	552	558	560	rBV2	438869	992590	13.43%	1.750%
23	8.522	562	563	565	rVB	274657	230023	3.11%	0.406%
24	8.785	582	586	589	rBV	103605	149474	2.02%	0.264%
25	9.150	614	618	620	rBV	7474710	7392623	100.00%	13.034%
26	9.276	627	629	632	rVB	62113	81599	1.10%	0.144%
27	9.539	650	652	655	rBV	201274	247719	3.35%	0.437%
28	9.596	655	657	660	rVB	84981	99542	1.35%	0.176%
29	9.745	667	670	674	rBV2	129199	205924	2.79%	0.363%
30	9.825	674	677	679	rVV	2009516	2079409	28.13%	3.666%
31	10.236	712	713	717	rVB3	107929	215264	2.91%	0.380%
32	10.613	743	746	748	rBV	4464905	4413676	59.70%	7.782%
33	10.739	754	757	761	rBV	101119	167781	2.27%	0.296%
34	10.945	772	775	780	rVB	91100	134174	1.81%	0.237%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
Data File : BF084571.D
Acq On : 20 Jan 2016 18:18
Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.185	793	796	798	rBV2	138212	164966	2.23%	0.291%
36	11.311	804	807	809	rBV	1458919	1951839	26.40%	3.441%
37	11.482	820	822	824	rVB	117921	116010	1.57%	0.205%
38	11.882	853	857	858	rBV	66079	112073	1.52%	0.198%
39	12.008	865	868	871	rBV2	56044	102708	1.39%	0.181%
40	12.899	943	946	948	rBV	6233673	6166168	83.41%	10.872%
41	13.814	1023	1026	1032	rBV	85011	131554	1.78%	0.232%
42	13.939	1035	1037	1039	rBV	1801704	1949833	26.38%	3.438%
43	13.974	1039	1040	1042	rVB	826668	589732	7.98%	1.040%
44	14.797	1109	1112	1114	rVB	222835	246740	3.34%	0.435%
45	15.345	1158	1160	1163	rBV	764322	1164012	15.75%	2.052%

Sum of corrected areas: 56715863

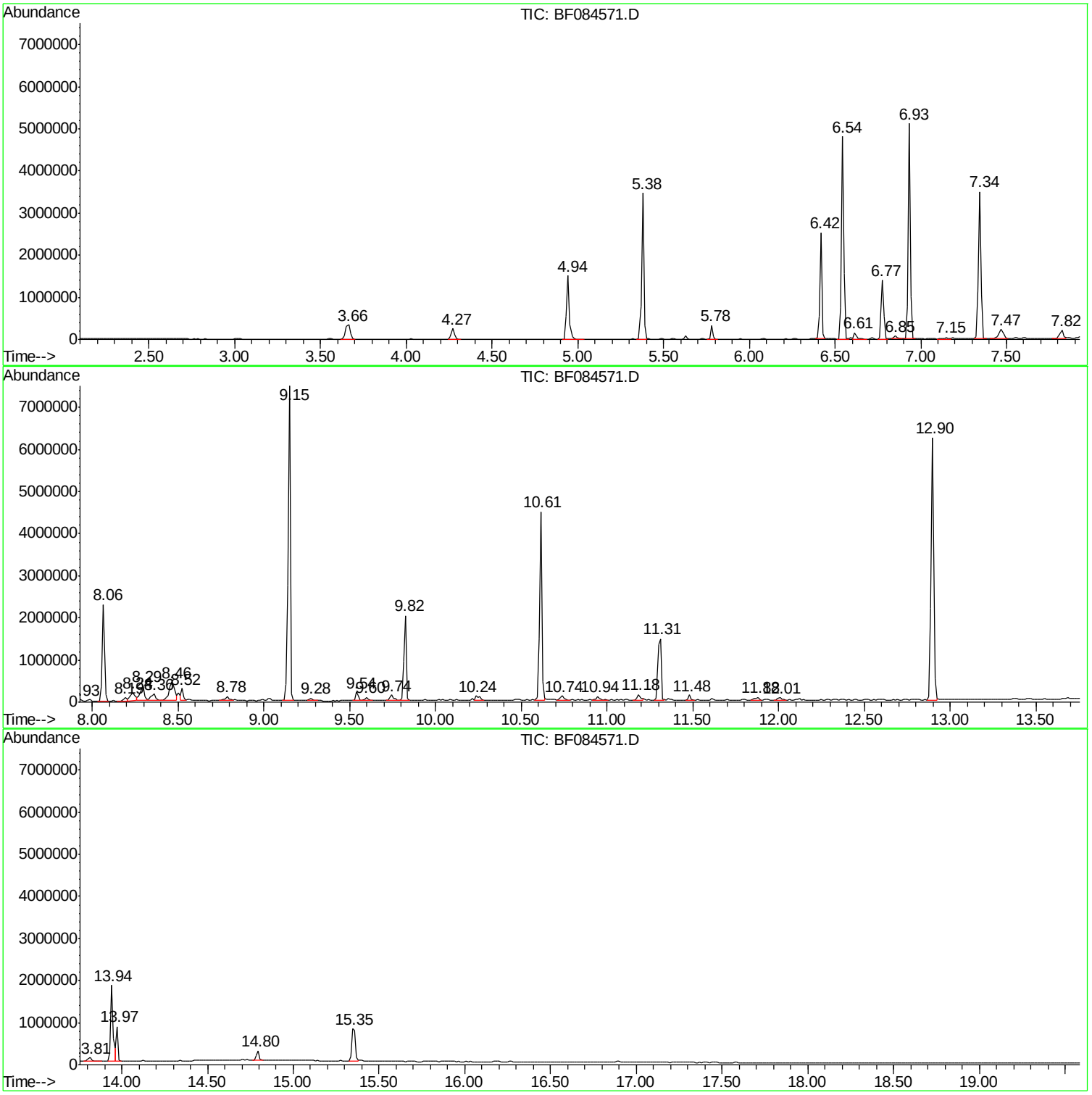
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
Data File : BF084571.D
Acq On : 20 Jan 2016 18:18
Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
Data File : BF084571.D
Acq On : 20 Jan 2016 18:18
Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

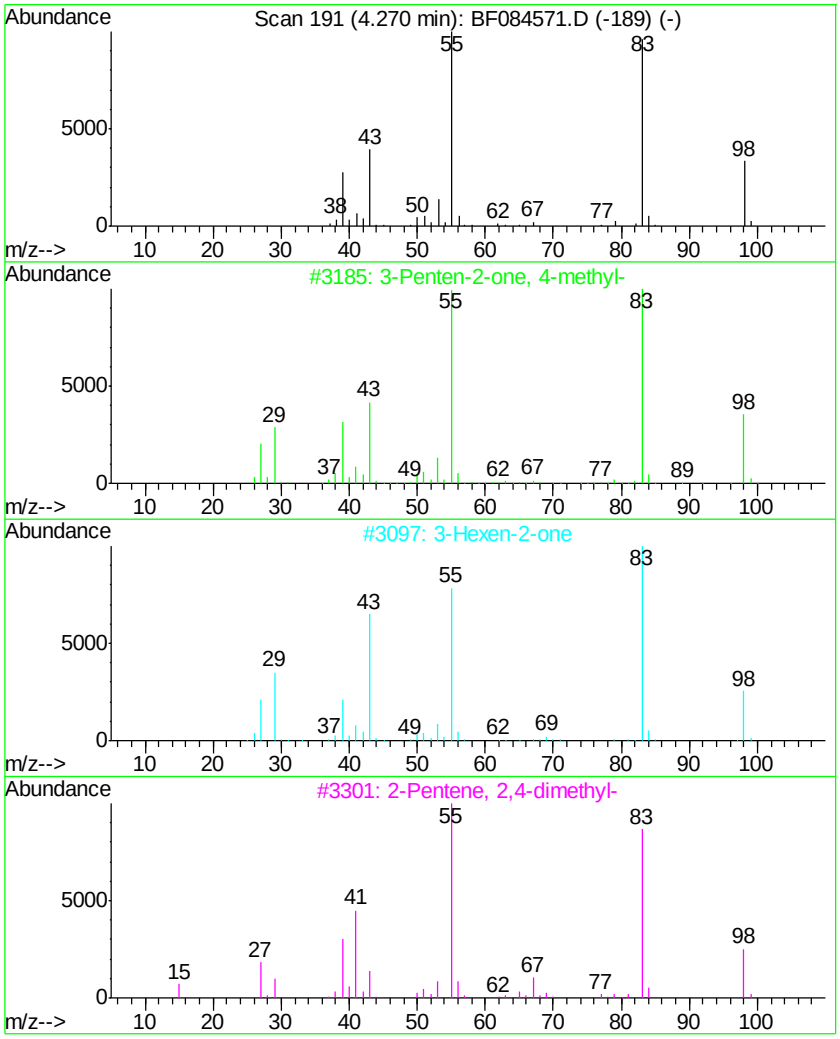
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

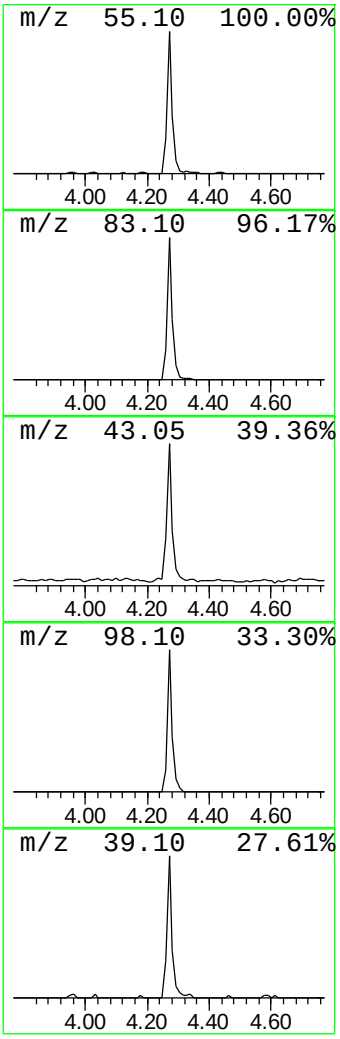
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	4.31 ng	296162	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
Data File : BF084571.D
Acq On : 20 Jan 2016 18:18
Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

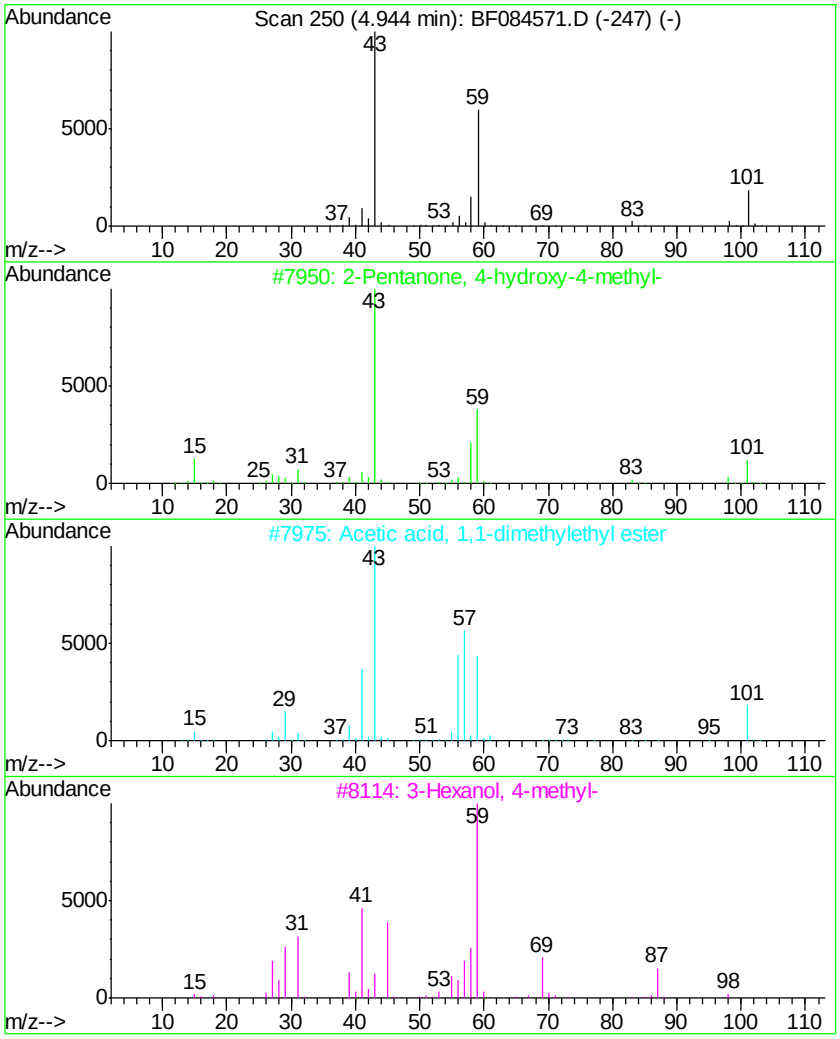
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

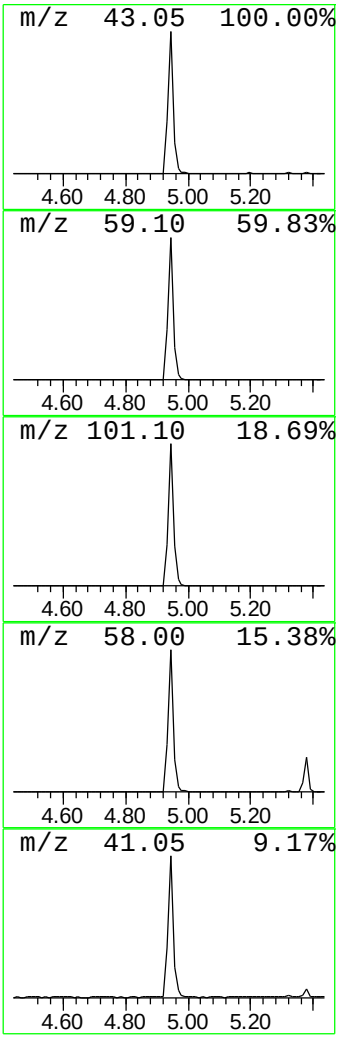
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	24.88 ng	1708030	1,4-Dichlorobenzene-d4	6.77

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
Data File : BF084571.D
Acq On : 20 Jan 2016 18:18
Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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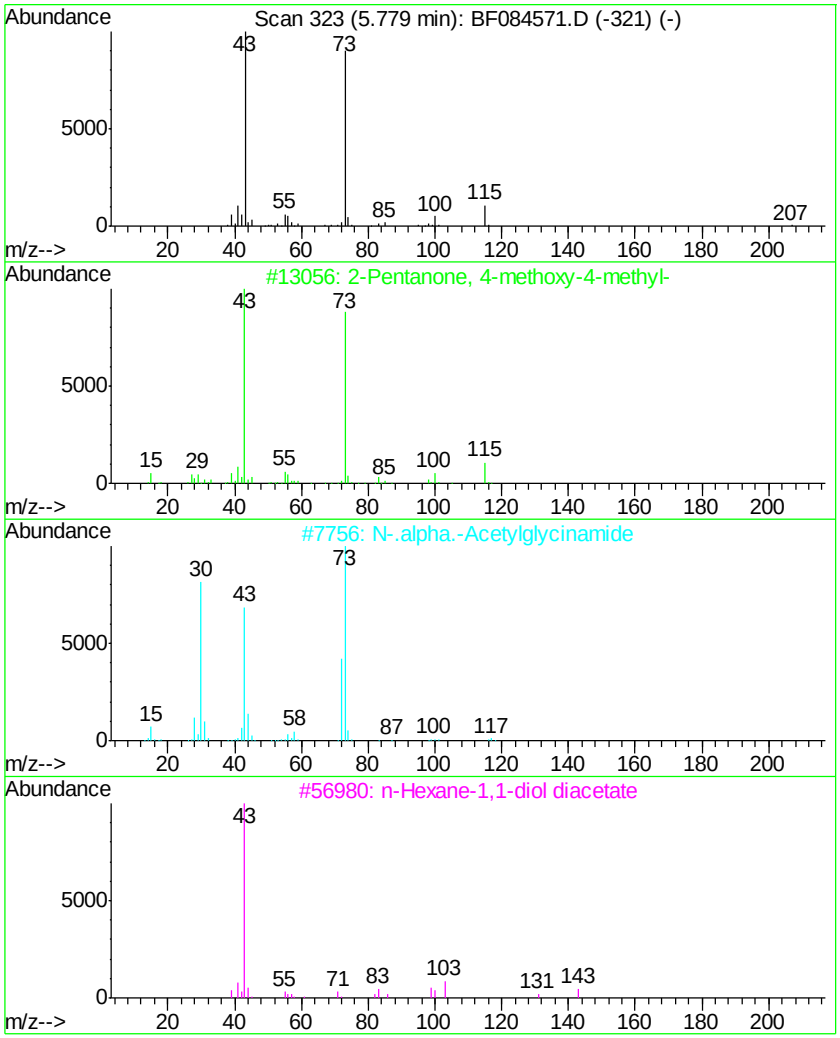
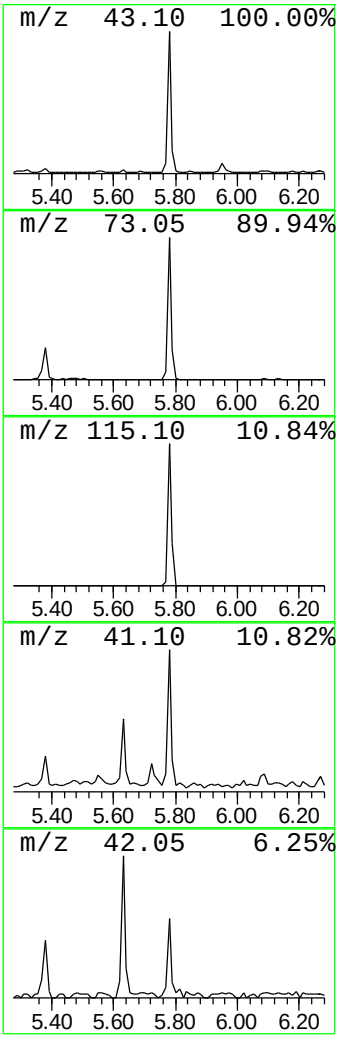
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.78	4.03 ng	276305	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3	n-Hexane-1,1-diol diacetate	202	C10H18O4	064847-81-0	12
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
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Acq On : 20 Jan 2016 18:18
Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
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TIC Library : C:\DATABASE\NIST02.L
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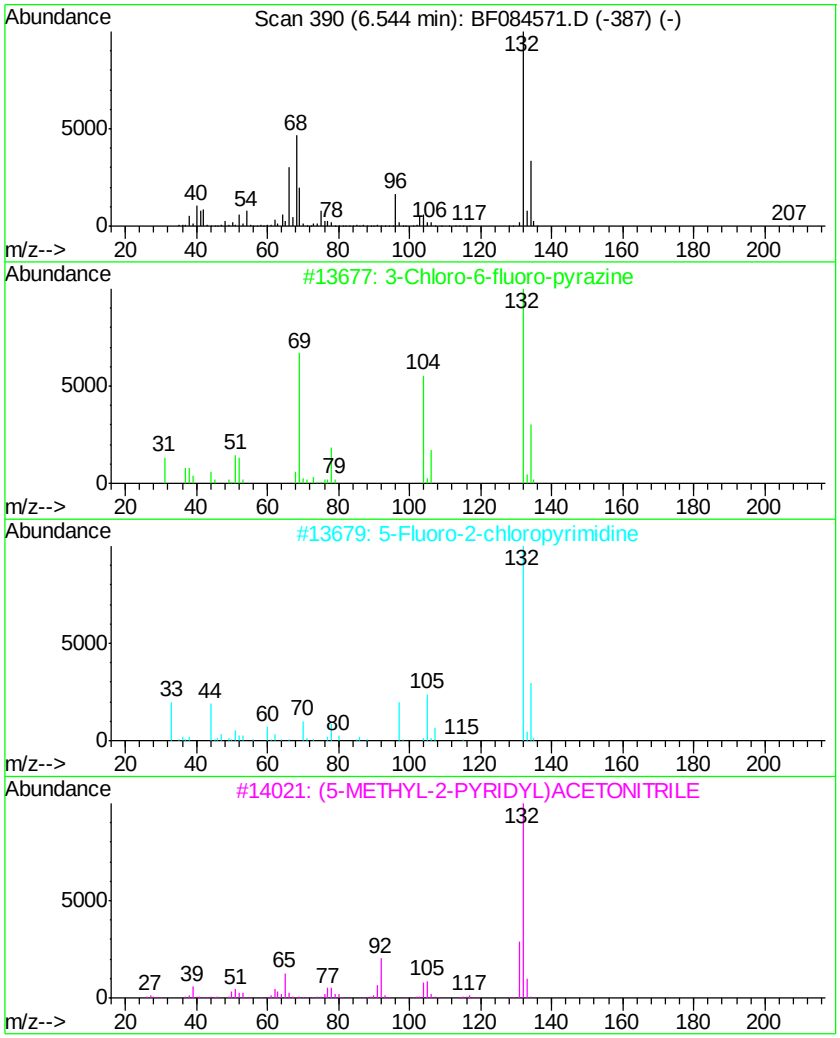
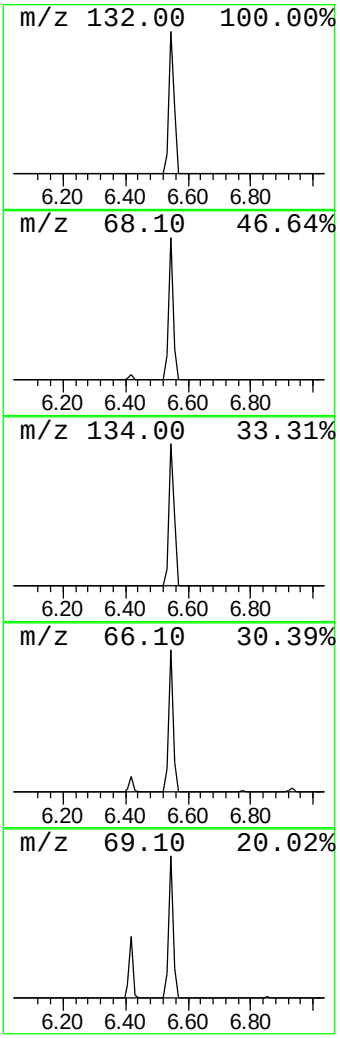
Peak Number 5 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	71.11 ng	4880990	1,4-Dichlorobenzene-d4	6.77

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	12
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9





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Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

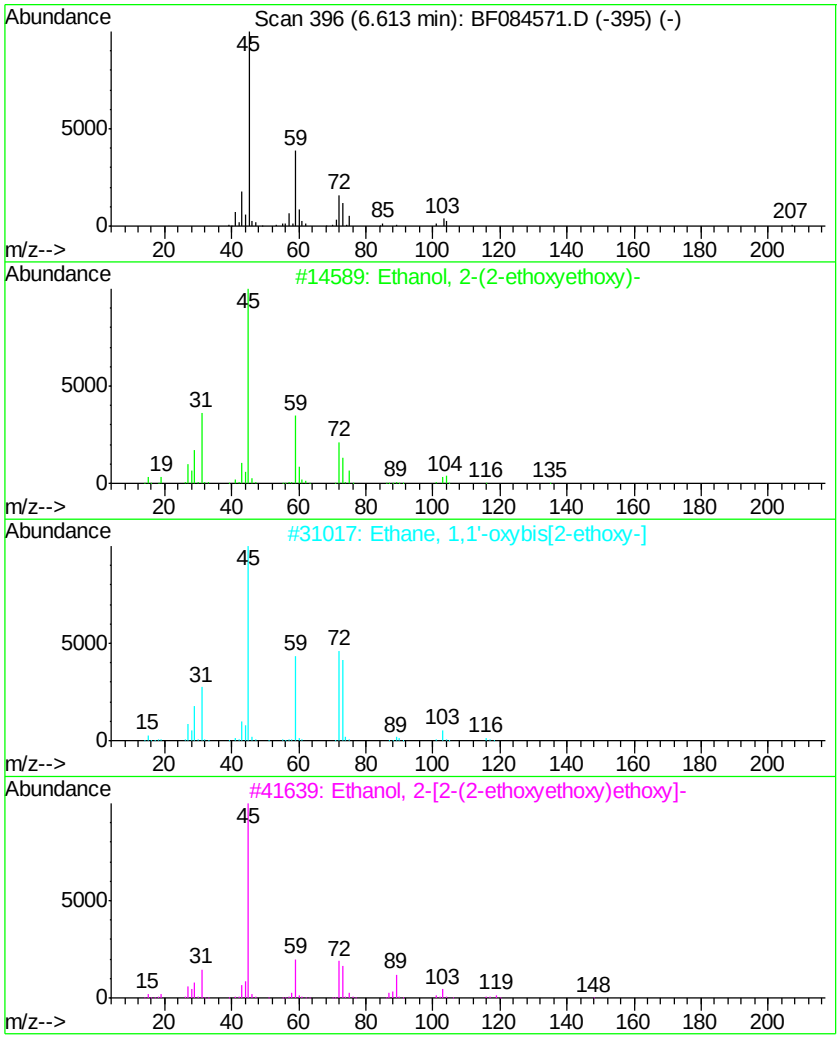
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

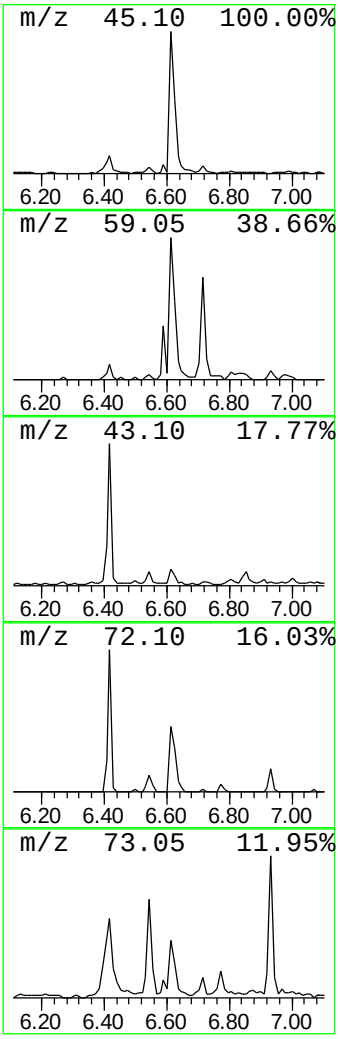
****

Peak Number 6 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	2.64 ng	181489	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	72
2	Ethane, 1,1'-oxybis[2-ethoxy-]	162	C8H18O3	000112-36-7	64
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	59
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	50
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
Data File : BF084571.D
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Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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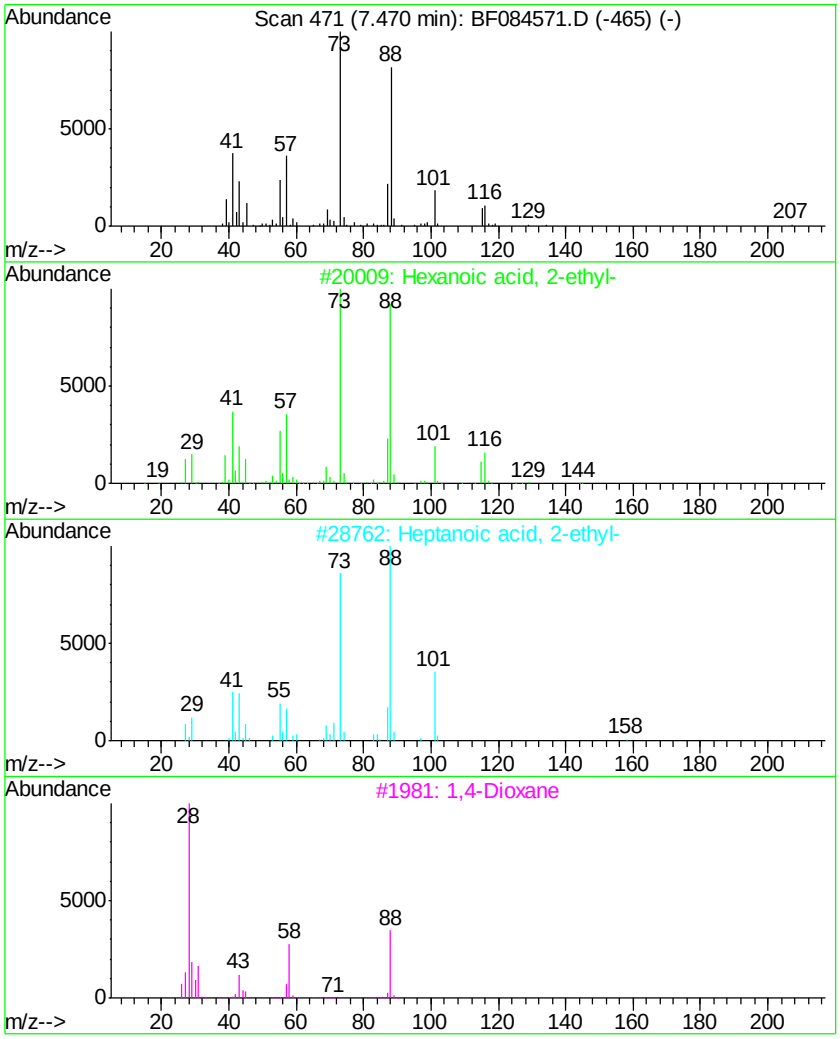
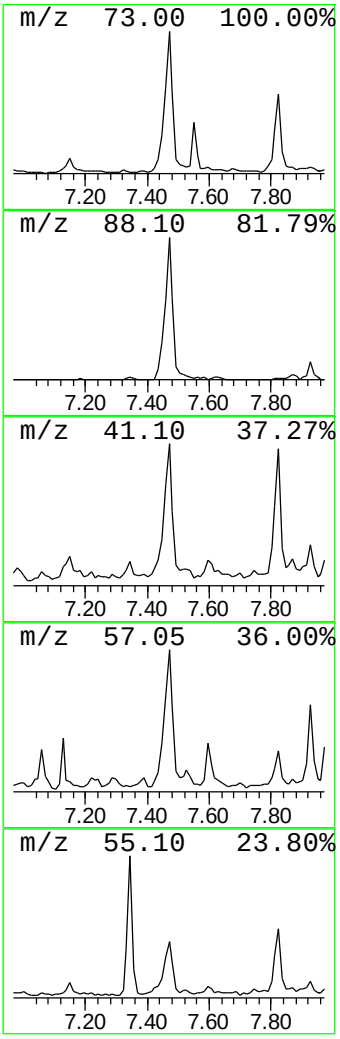
Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	4.25 ng	410703	Naphthalene-d8	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3	1,4-Dioxane	88	C4H8O2	000123-91-1	47
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
5	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	36





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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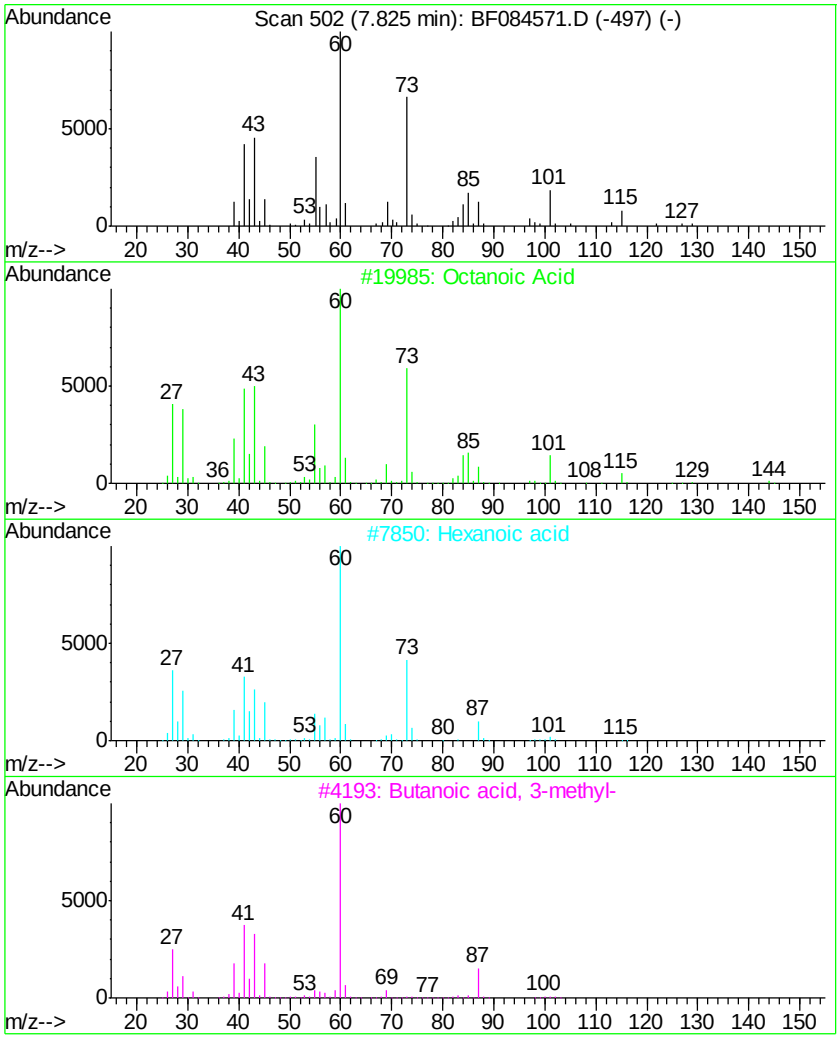
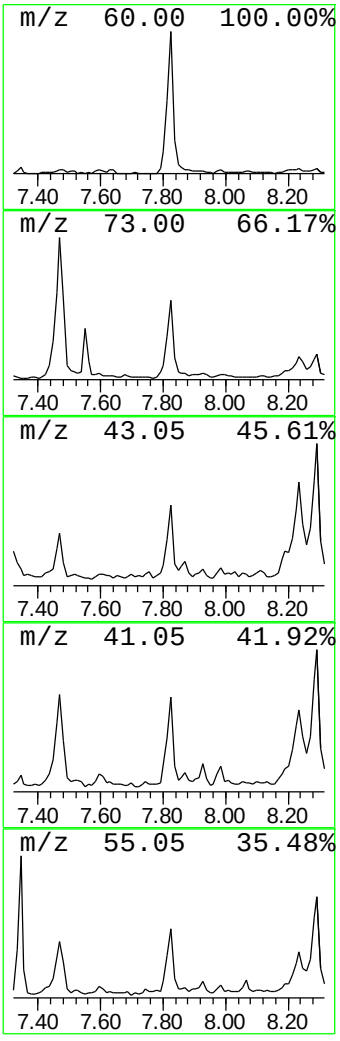
Peak Number 9 Octanoic Acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	3.56 ng	343329	Naphthalene-d8	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic Acid	144	C8H16O2	000124-07-2	78
2	Hexanoic acid	116	C6H12O2	000142-62-1	59
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	53
4	Heptanoic acid	130	C7H14O2	000111-14-8	50
5	Pentanoic acid	102	C5H10O2	000109-52-4	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
Data File : BF084571.D
Acq On : 20 Jan 2016 18:18
Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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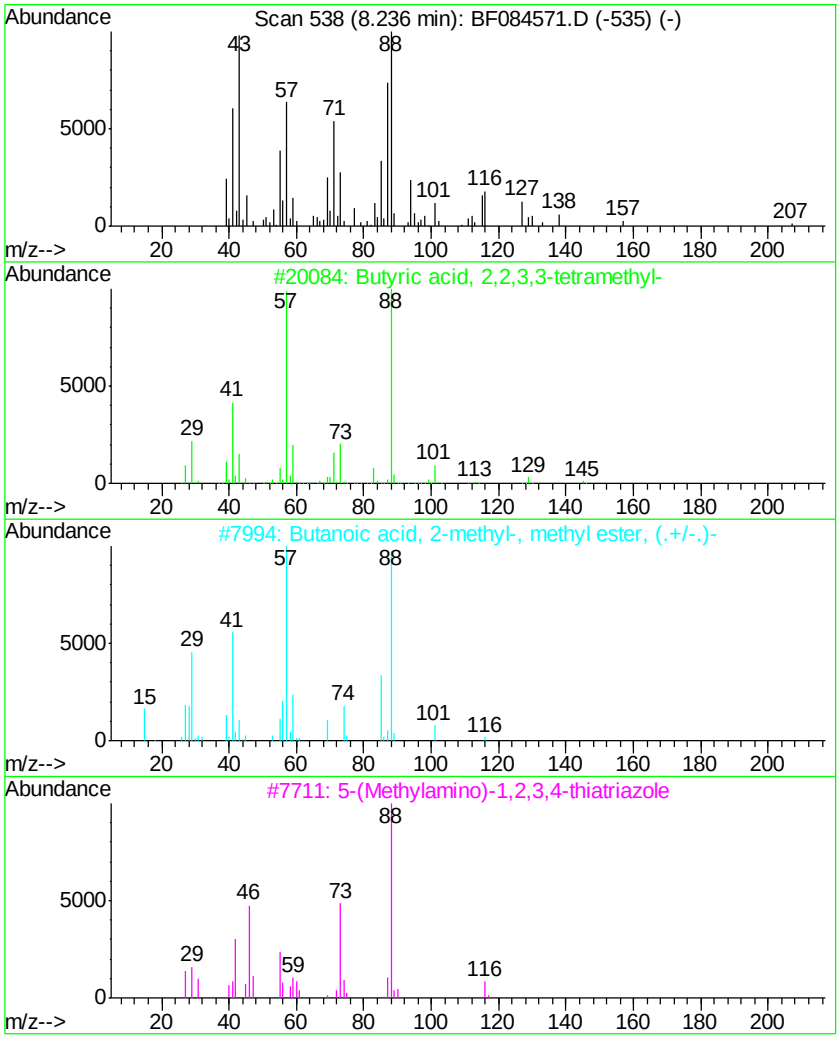
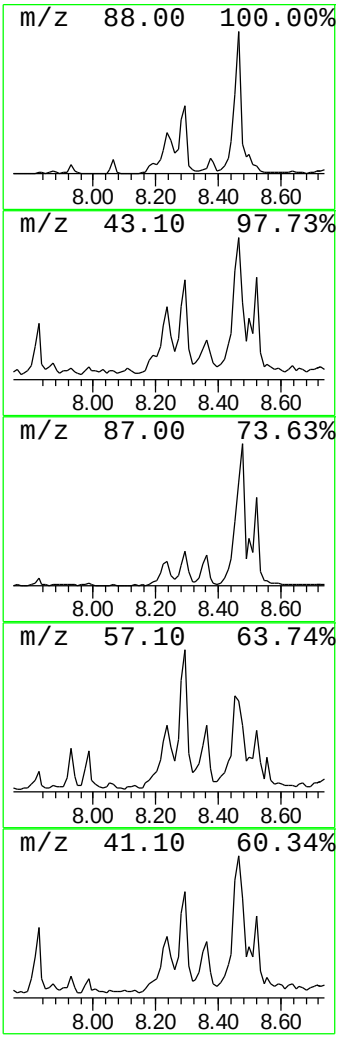
Peak Number 10 unknown8.24 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.24	4.09 ng	395054	Naphthalene-d8	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	35
2	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	053955-81-0	27
3	5-(Methylamino)-1,2,3,4-thiatria...	116	C2H4N4S	052098-72-3	27
4	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	25
5	3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
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Sample : H1177-01
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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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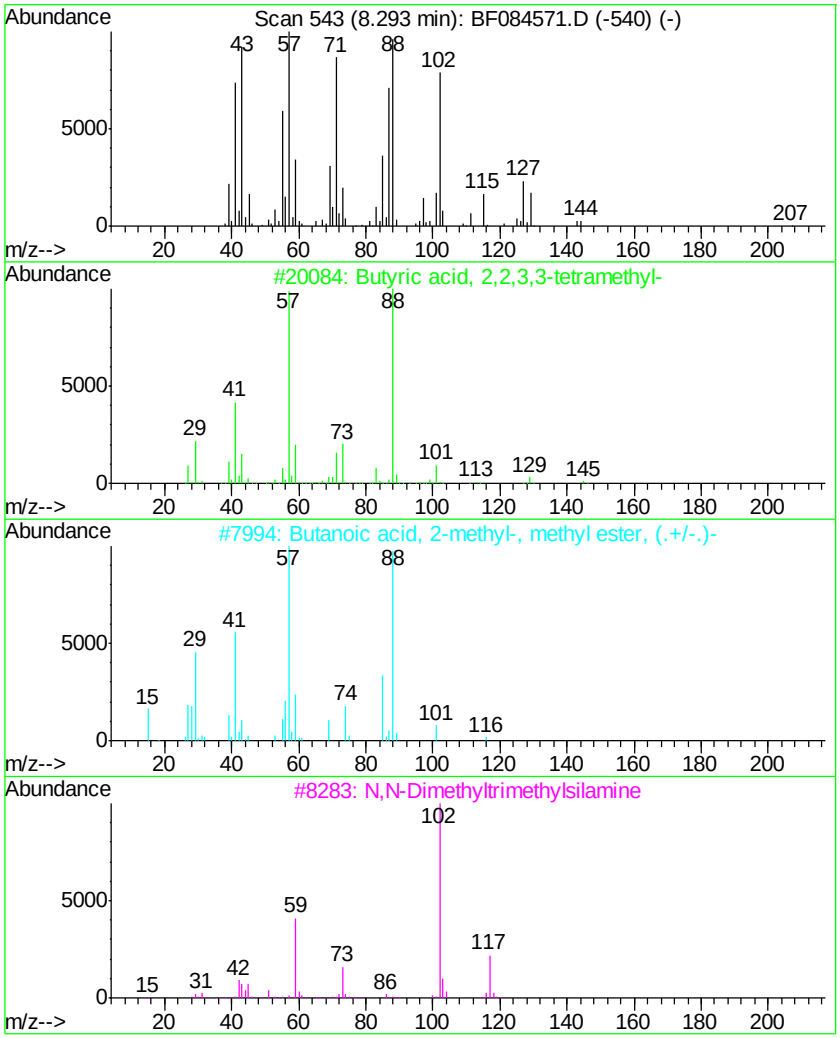
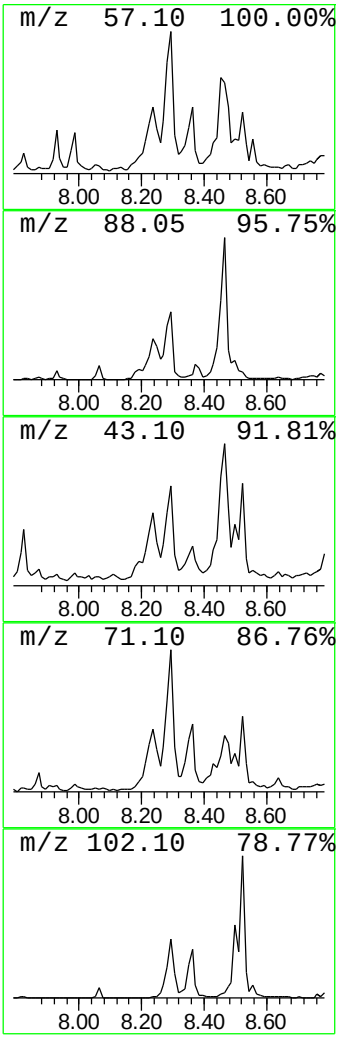
Peak Number 11 unknown8.29 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.29	5.75 ng	555204	Naphthalene-d8	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	22
2	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	053955-81-0	14
3	N,N-Dimethyltrimethylsilamine	117	C5H15NSi	002083-91-2	14
4	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	14
5	Butane, 2,2'-[methylenebis(oxy)]...	188	C11H24O2	054699-28-4	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
Data File : BF084571.D
Acq On : 20 Jan 2016 18:18
Operator : SJ/UM
Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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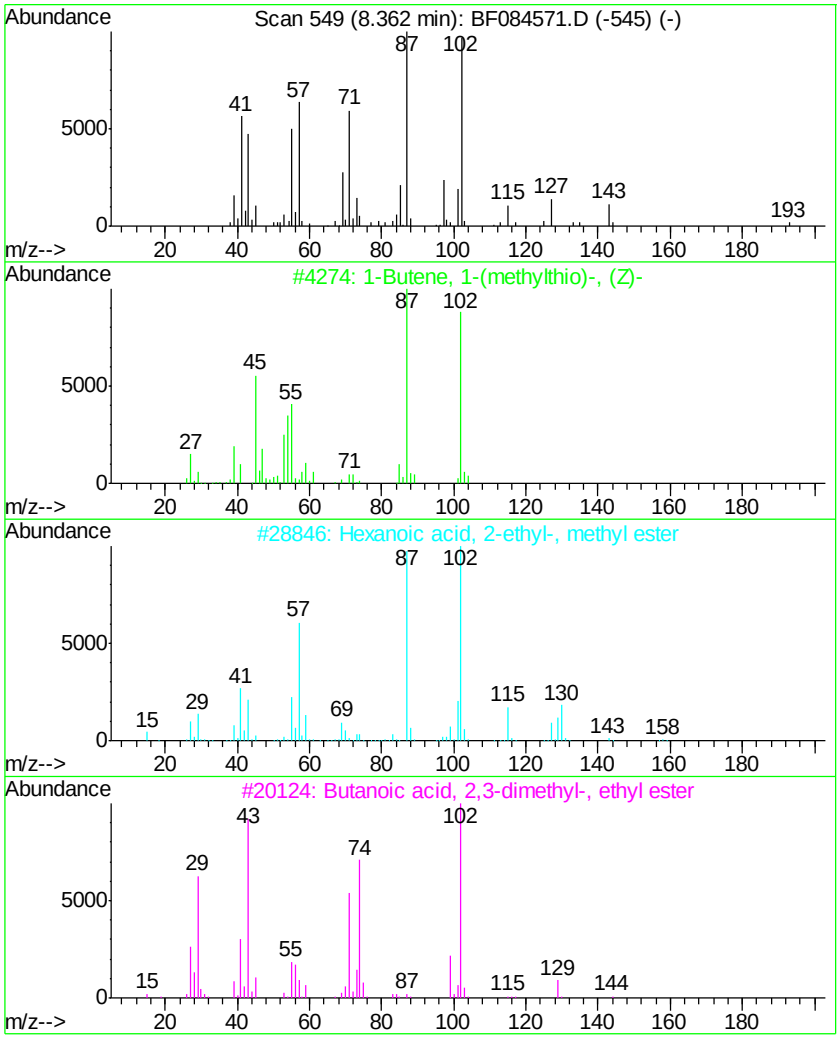
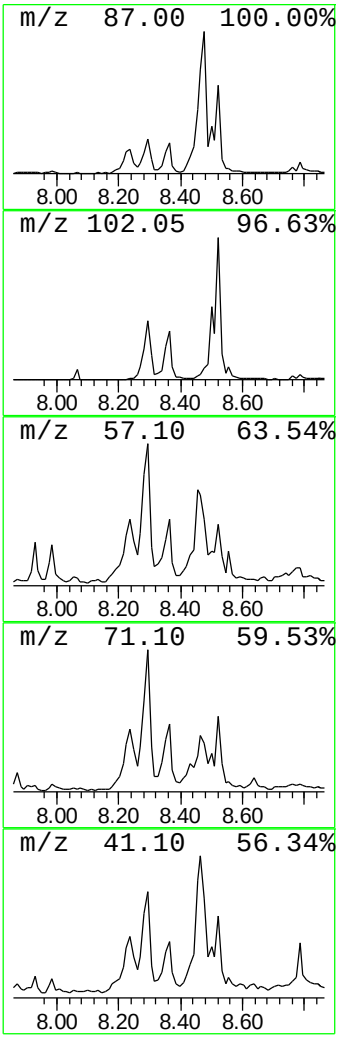
Peak Number 12 unknown8.36 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.36	3.13 ng	302244	Naphthalene-d8	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	43
2	Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	33
3	Butanoic acid, 2,3-dimethyl-, et...	144	C8H16O2	054004-42-1	25
4	Pentanoic acid, 2-methyl-, ethyl...	144	C8H16O2	039255-32-8	25
5	Butanoic acid, 2,2-dimethyl-3-ox...	144	C7H12O3	038923-57-8	25





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Acq On : 20 Jan 2016 18:18
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Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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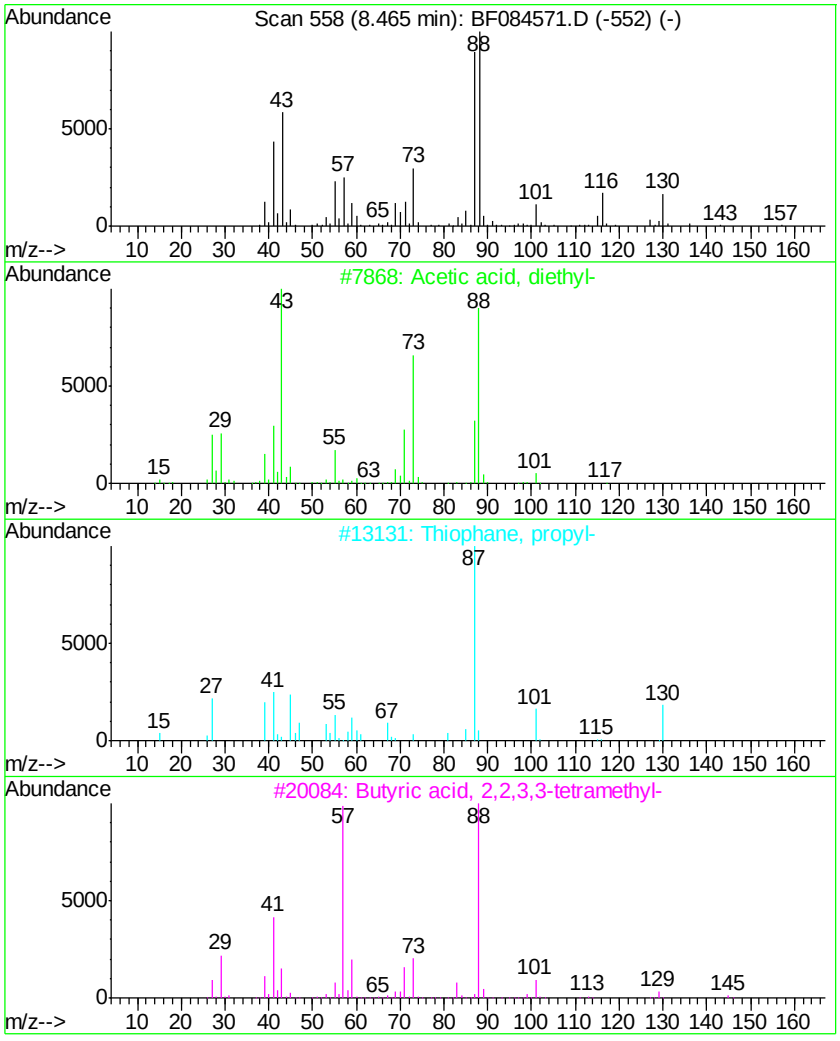
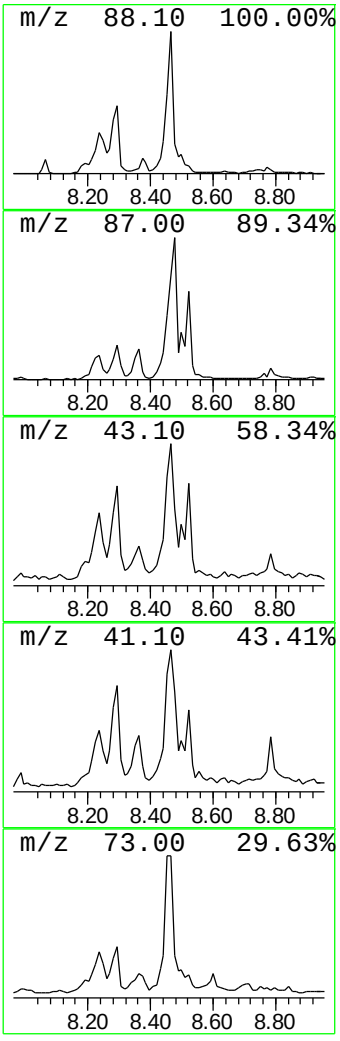
Peak Number 13 unknown8.46 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	10.28 ng	992590	Naphthalene-d8	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	47
2	Thiophane, propyl-	130	C7H14S	001551-34-4	38
3	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	32
4	Heptanoic acid, 2,6-dimethyl-, m...	172	C10H20O2	033315-72-9	32
5	5-(Methylamino)-1,2,3,4-thiatria...	116	C2H4N4S	052098-72-3	32





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Sample : H1177-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

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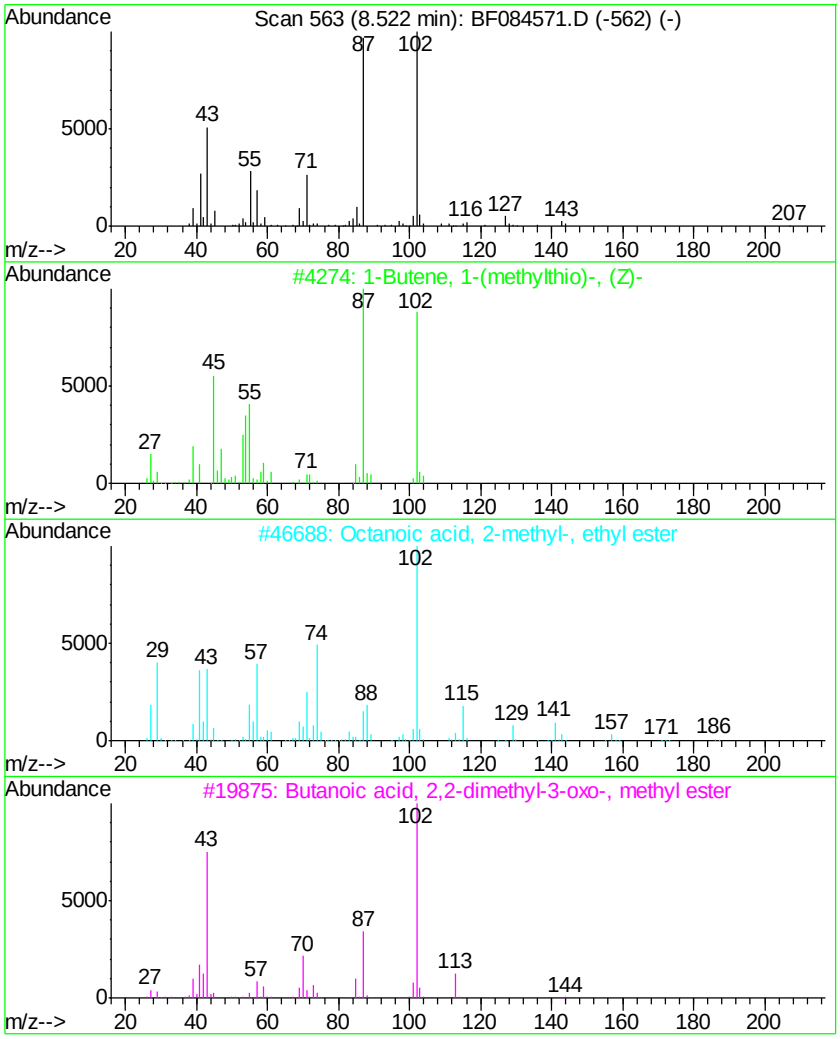
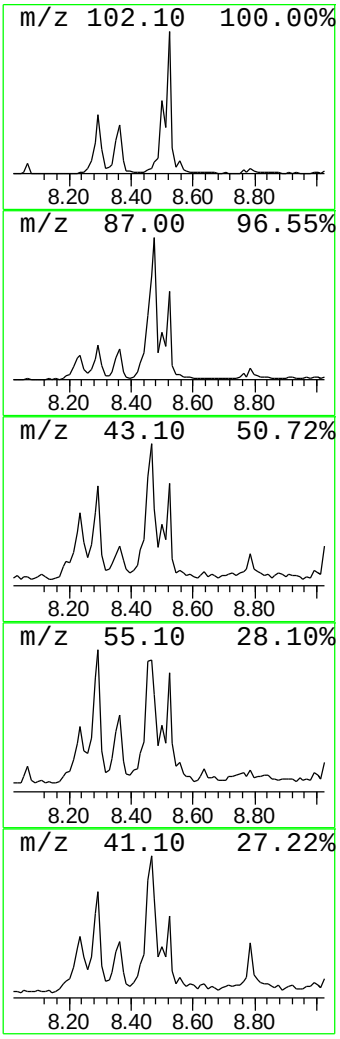
Peak Number 14 unknown8.52 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	2.38 ng	230023	Naphthalene-d8	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	38
2	Octanoic acid, 2-methyl-, ethyl ...	186	C11H22O2	030982-02-6	25
3	Butanoic acid, 2,2-dimethyl-3-ox...	144	C7H12O3	038923-57-8	25
4	4-Methyl-2-pentyl acetate	144	C8H16O2	000108-84-9	17
5	Butanoic acid, 2,3-dimethyl-, et...	144	C8H16O2	054004-42-1	16





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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LAR9887

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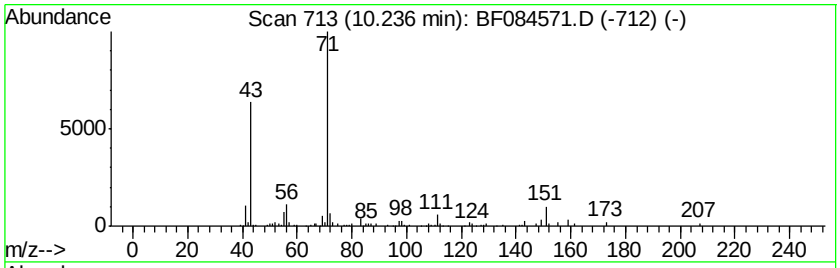
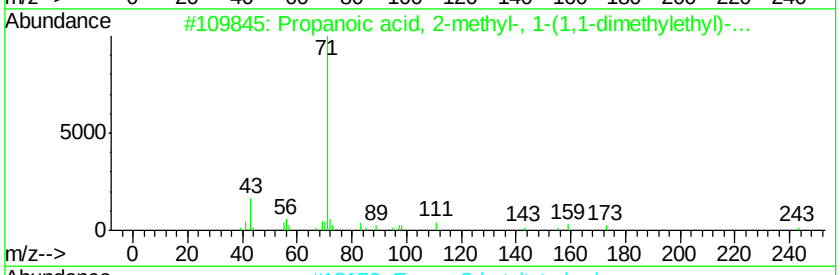
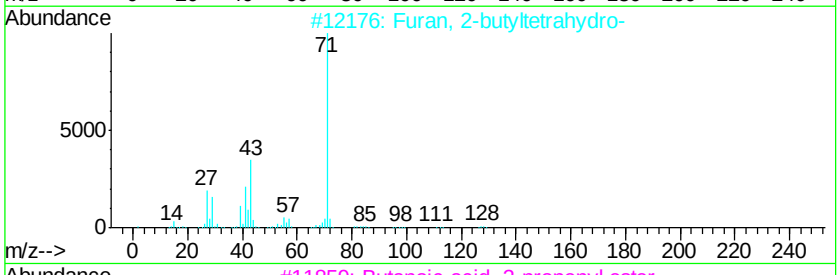
Peak Number 15 Propanoic acid, 2-methyl-, ... Concentration Rank 16

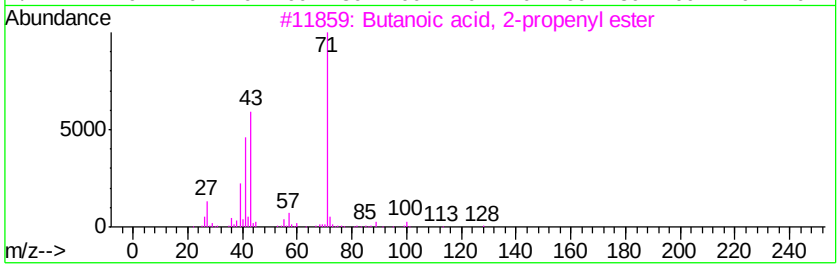
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	2.07 ng	215264	Acenaphthene-d10	9.82

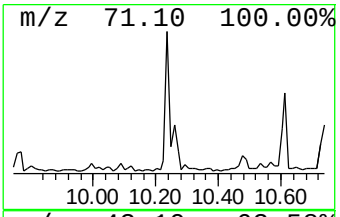
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	72
2	Furan, 2-butyltetrahydro-	128	C8H16O	001004-29-1	53
3	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	50
4	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	50
5	Propanoic acid, 2-methyl-, 2-eth...	286	C16H30O4	074367-30-9	50

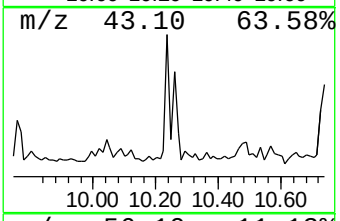


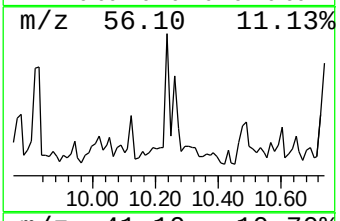


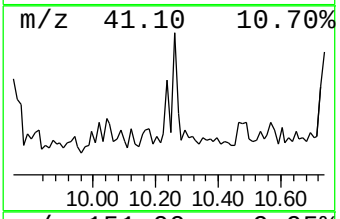


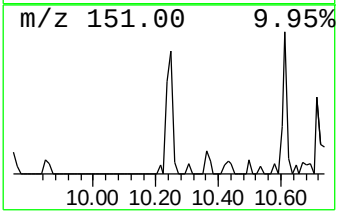












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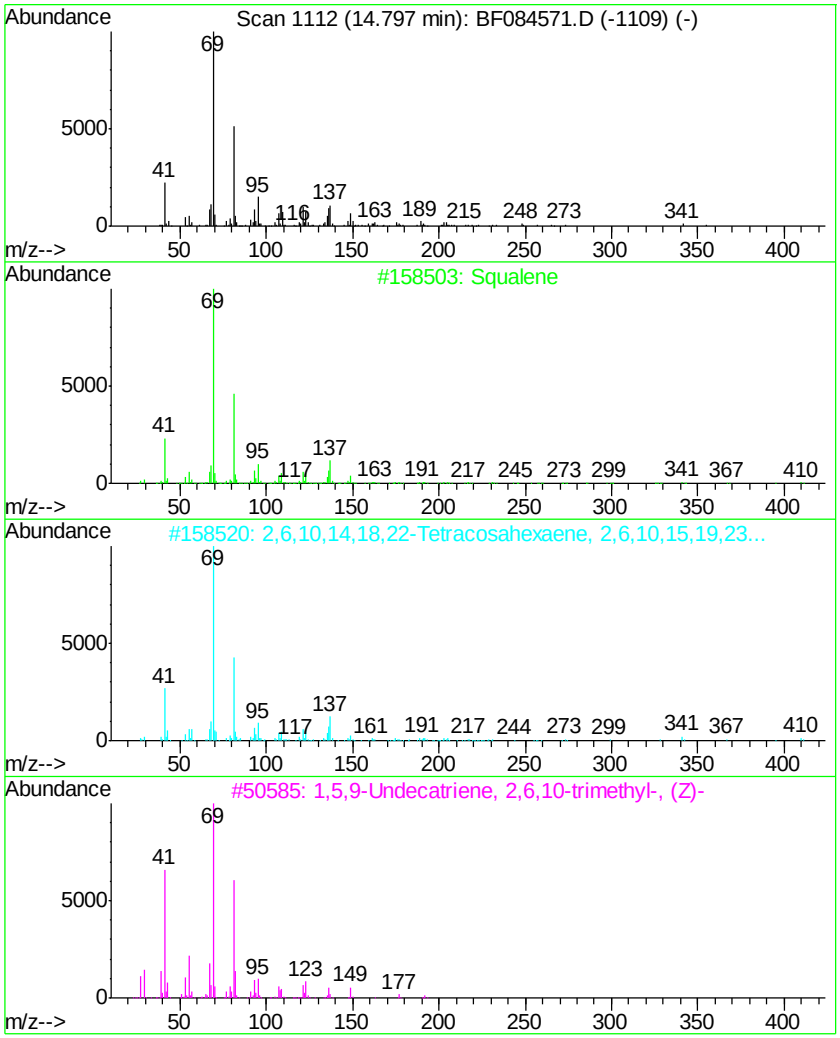
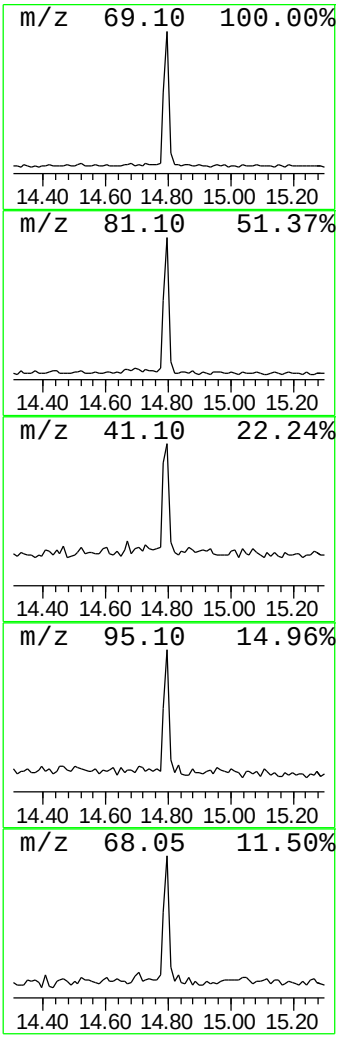
Peak Number 16 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.24 ng	246740	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.27	4.3	ng	296162	1	6.77	1372780	20.0
2-Pentanone, 4-hy...	4.94	24.9	ng	1708030	1	6.77	1372780	20.0
2-Pentanone, 4-me...	5.78	4.0	ng	276305	1	6.77	1372780	20.0
unknown6.54	6.54	71.1	ng	4880990	1	6.77	1372780	20.0
Ethanol, 2-(2-eth...	6.61	2.6	ng	181489	1	6.77	1372780	20.0
Hexanoic acid, 2-...	7.47	4.3	ng	410703	2	8.06	1931370	20.0
Octanoic Acid	7.82	3.6	ng	343329	2	8.06	1931370	20.0
unknown8.24	8.24	4.1	ng	395054	2	8.06	1931370	20.0
unknown8.29	8.29	5.8	ng	555204	2	8.06	1931370	20.0
unknown8.36	8.36	3.1	ng	302244	2	8.06	1931370	20.0
unknown8.46	8.46	10.3	ng	992590	2	8.06	1931370	20.0
unknown8.52	8.52	2.4	ng	230023	2	8.06	1931370	20.0
Propanoic acid, 2...	10.24	2.1	ng	215264	3	9.82	2079410	20.0
Squalene	14.80	4.2	ng	246740	6	15.36	1164010	20.0