LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084637.D
Acq On : 29 Jan 2016 15:45
Operator : SJ/IZ
Sample : H1242-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW1

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-BF012916.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	4.190	182	184	189	rBV	415574	522313	7.78%	0.952%
2	4.887	241	245	247	rBV	2229072	2795929	41.66%	5.098%
3	5.322	281	283	286	rBV	3457042	3403509	50.71%	6.206%
4	5.573	302	305	308	rBV	2110646	1886270	28.10%	3.439%
5	5.722	316	318	321	rBV	430617	408613	6.09%	0.745%
6	6.362	372	374	377	rBV	2060791	2205685	32.86%	4.022%
7	6.487	383	385	388	rBV	3677612	4718916	70.31%	8.604%
8	6.727	403	406	408	rBV	806861	1114104	16.60%	2.031%
9	6.876	417	419	422	rVB	3644340	3961411	59.02%	7.223%
10	7.287	452	455	458	rBV	2679784	3572003	53.22%	6.513%
11	7.756	493	496	501	rBV2	69626	108825	1.62%	0.198%
12	8.008	516	518	520	rBV	1751534	1518900	22.63%	2.769%
13	8.373	547	550	555	rBV	119178	143146	2.13%	0.261%
14	8.648	572	574	576	rBV	102411	87328	1.30%	0.159%
15	9.093	610	613	615	rBV	6282767	6711849	100.00%	12.238%
16	9.482	645	647	652	rVB	149770	159911	2.38%	0.292%
17	9.756	669	671	674	rBV2	1558399	1680258	25.03%	3.064%
18	10.019	688	694	697	rBV	2595106	5836742	86.96%	10.642%
19	10.179	706	708	712	rVB3	131312	252778	3.77%	0.461%
20	10.545	738	740	743	rBV2	3008298	4087452	60.90%	7.453%
21	10.671	749	751	755	rVB	97523	141288	2.11%	0.258%
22	11.242	798	801	803	rBV	1624159	1480012	22.05%	2.698%
23	11.791	847	849	851	rBV	196978	203898	3.04%	0.372%
24	12.831	937	940	942	rBV	4652123	4511303	67.21%	8.225%
25	13.757	1018	1021	1029	rBV	252372	632675	9.43%	1.154%
26	13.871	1029	1031	1033	rBV	1577628	1397415	20.82%	2.548%
27	15.254	1149	1152	1155	rBV	999569	1162985	17.33%	2.120%
28	15.791	1194	1199	1214	rVB	29627	140309	2.09%	0.256%

Sum of corrected areas: 54845827

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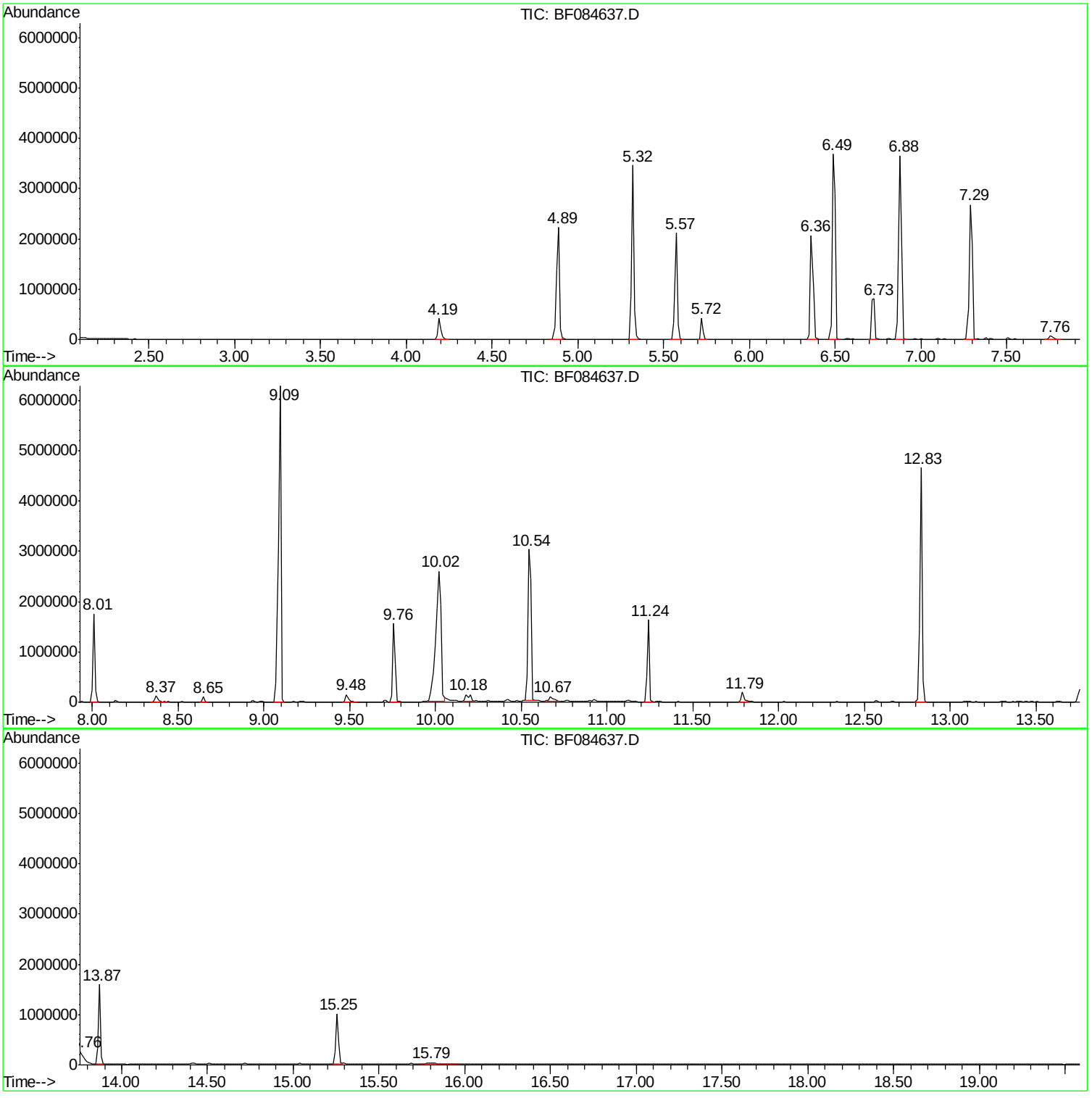
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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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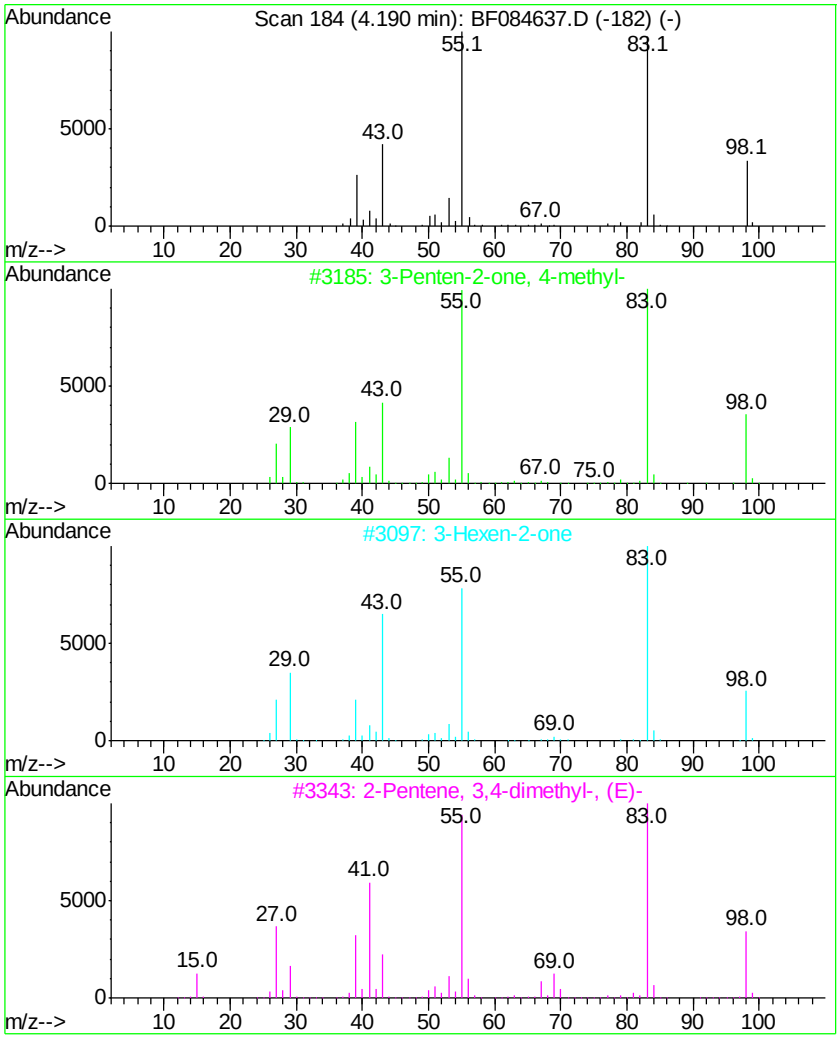
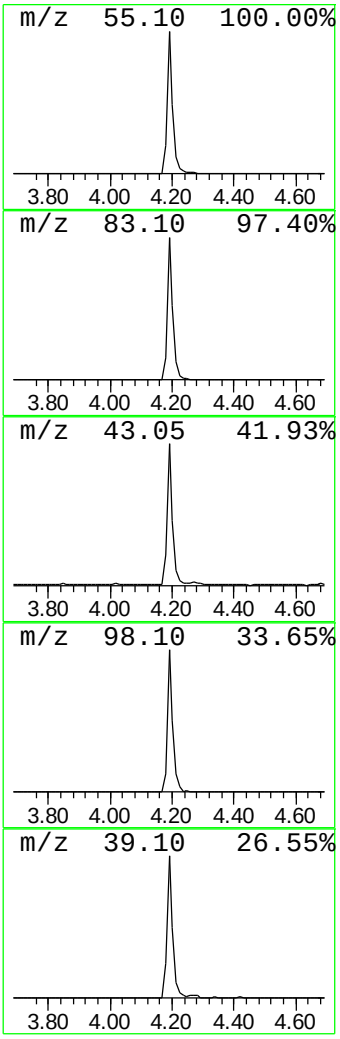
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	9.38 ng	522313	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Library Search Compound Report

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Operator : SJ/IZ
Sample : H1242-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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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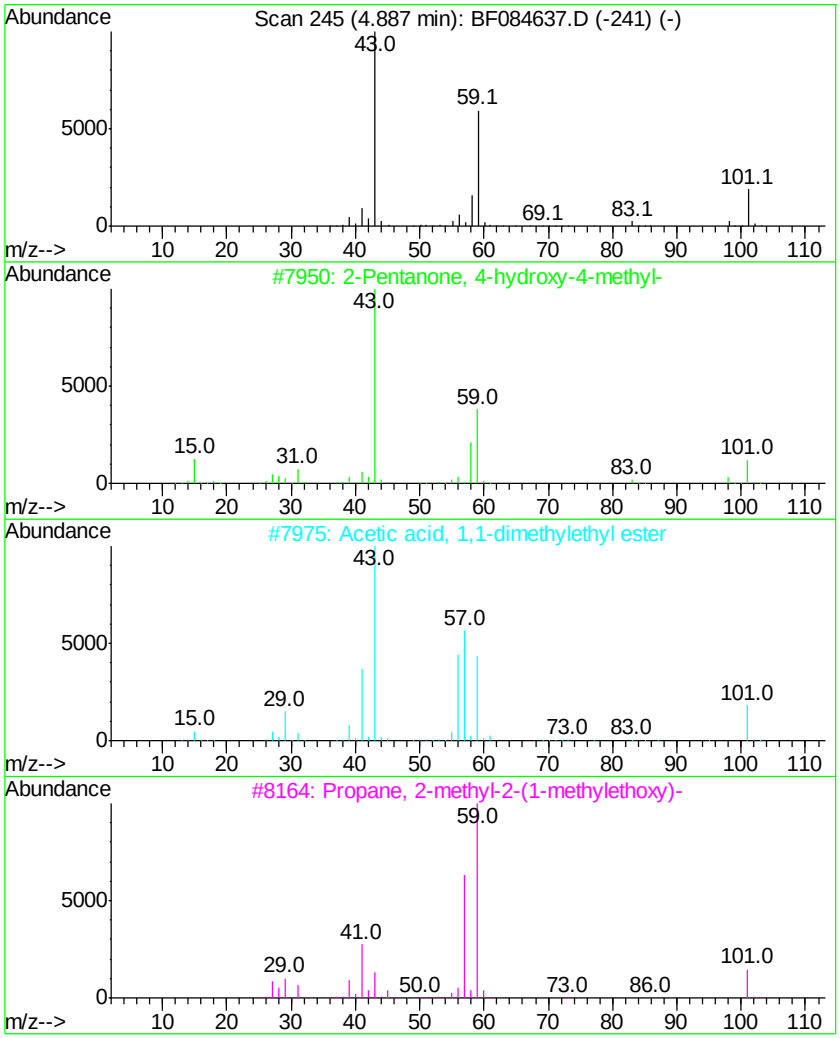
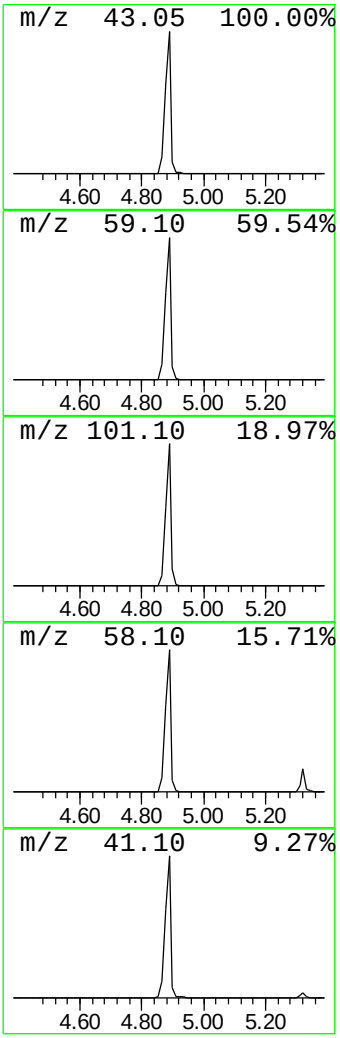
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	50.19 ng	2795930	1,4-Dichlorobenzene-d4	6.73

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





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Operator : SJ/IZ
Sample : H1242-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
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TIC Library : C:\DATABASE\NIST02.L
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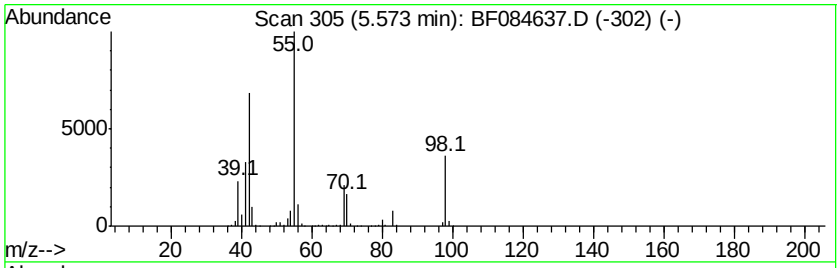
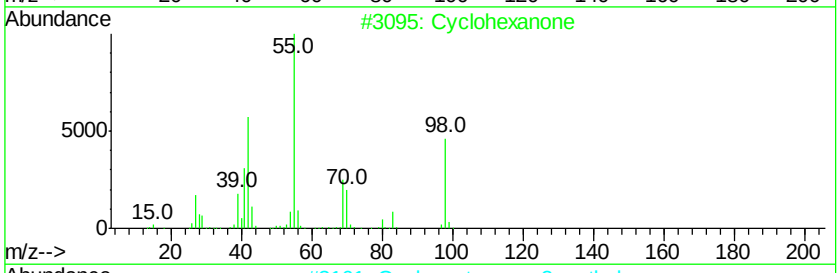
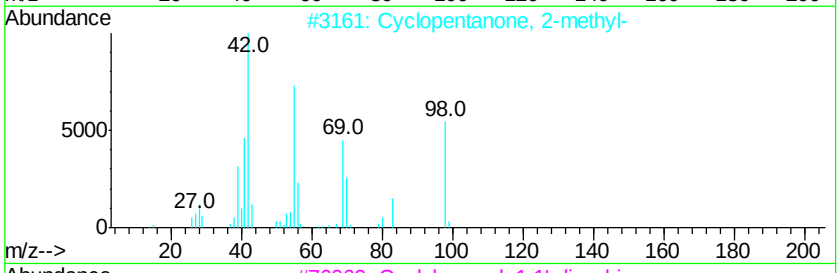
Peak Number 3 Cyclohexanone Concentration Rank 5

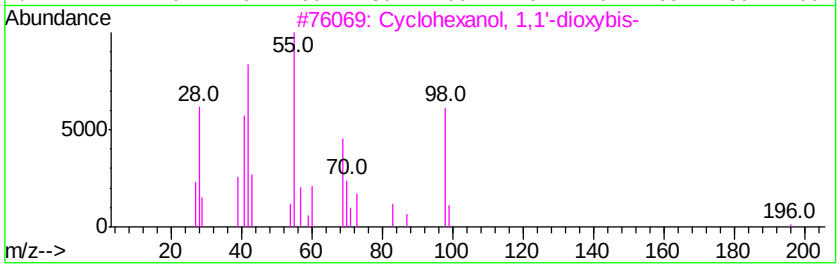
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.57	33.86 ng	1886270	1,4-Dichlorobenzene-d4	6.73

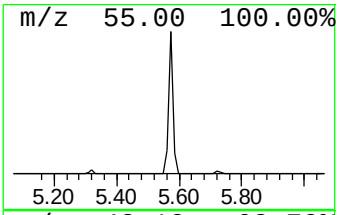
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	91
2	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	87
3	Cyclohexanol, 1,1'-dioxybis-	230	C12H22O4	002407-94-5	42
4	2(3H)-Furanone, 5-methyl-	98	C5H6O2	000591-12-8	37
5	2-Heptene, (E)-	98	C7H14	014686-13-6	37

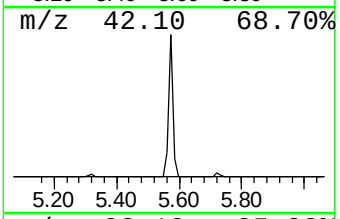


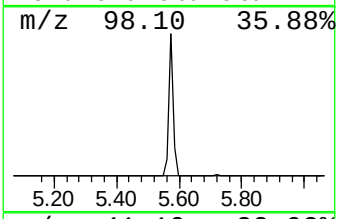


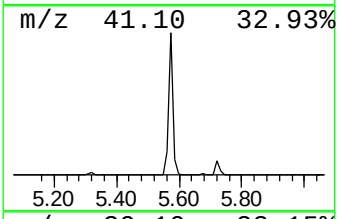


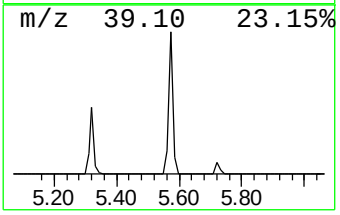












Library Search Compound Report

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Sample : H1242-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

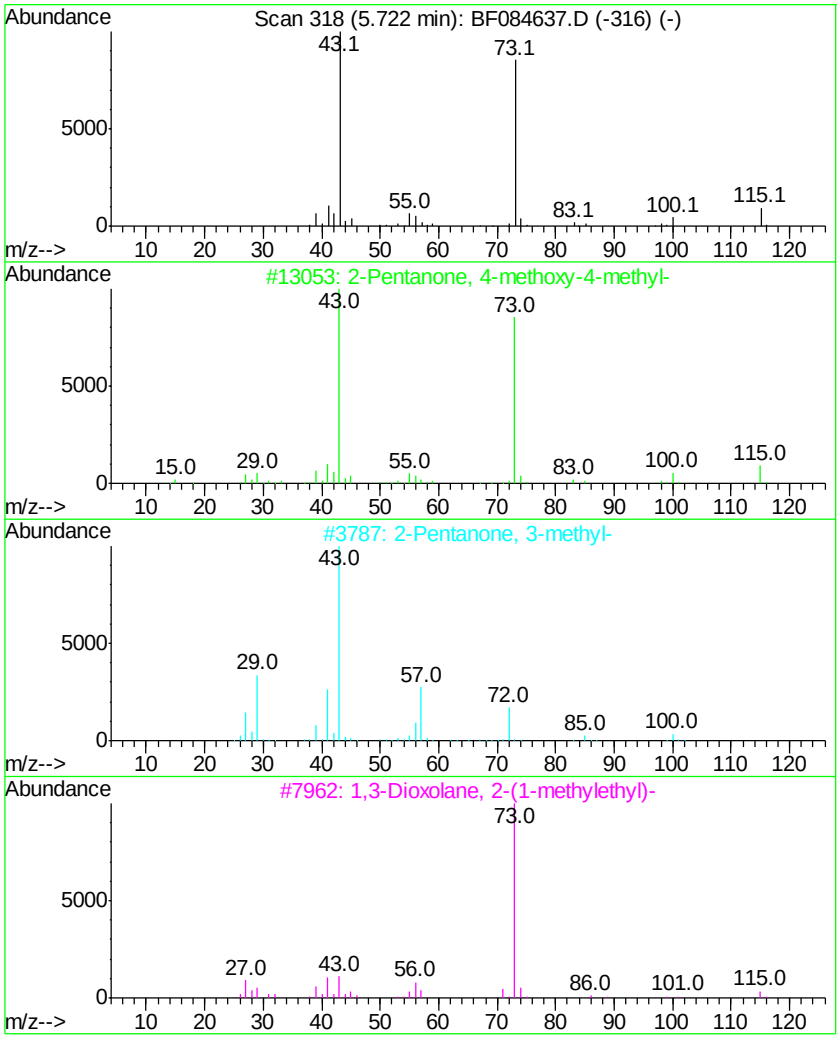
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

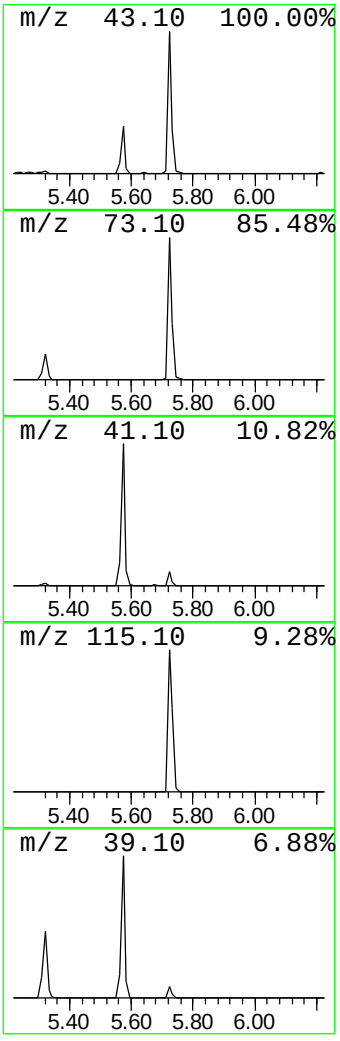
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	7.34 ng	408613	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
4	N-Formylmorpholine	115	C5H9NO2	004394-85-8	9
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





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TIC Library : C:\DATABASE\NIST02.L
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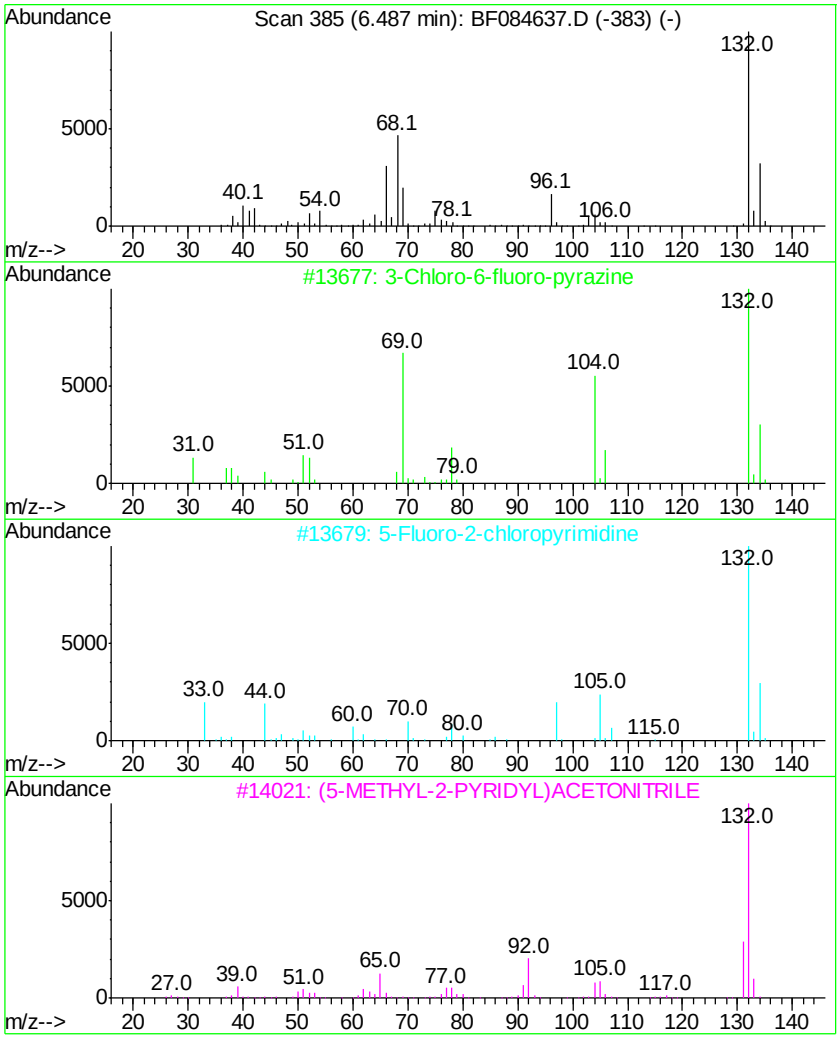
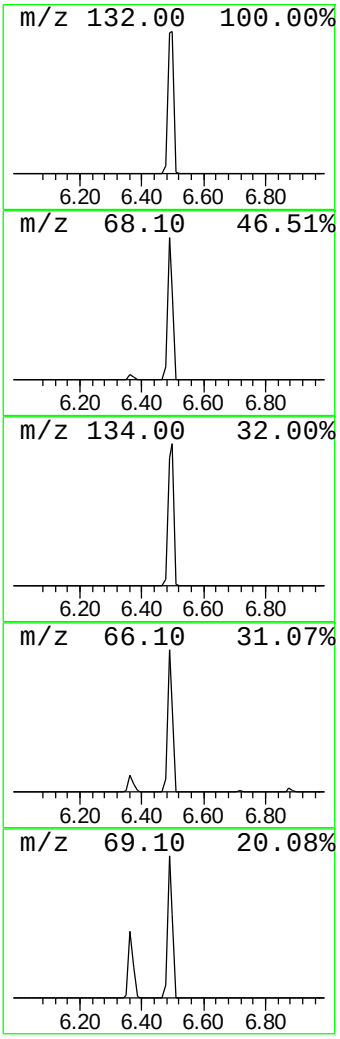
Peak Number 5 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	84.71 ng	4718920	1,4-Dichlorobenzene-d4	6.73

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Instrument : BNA_F
ClientSampleId : TW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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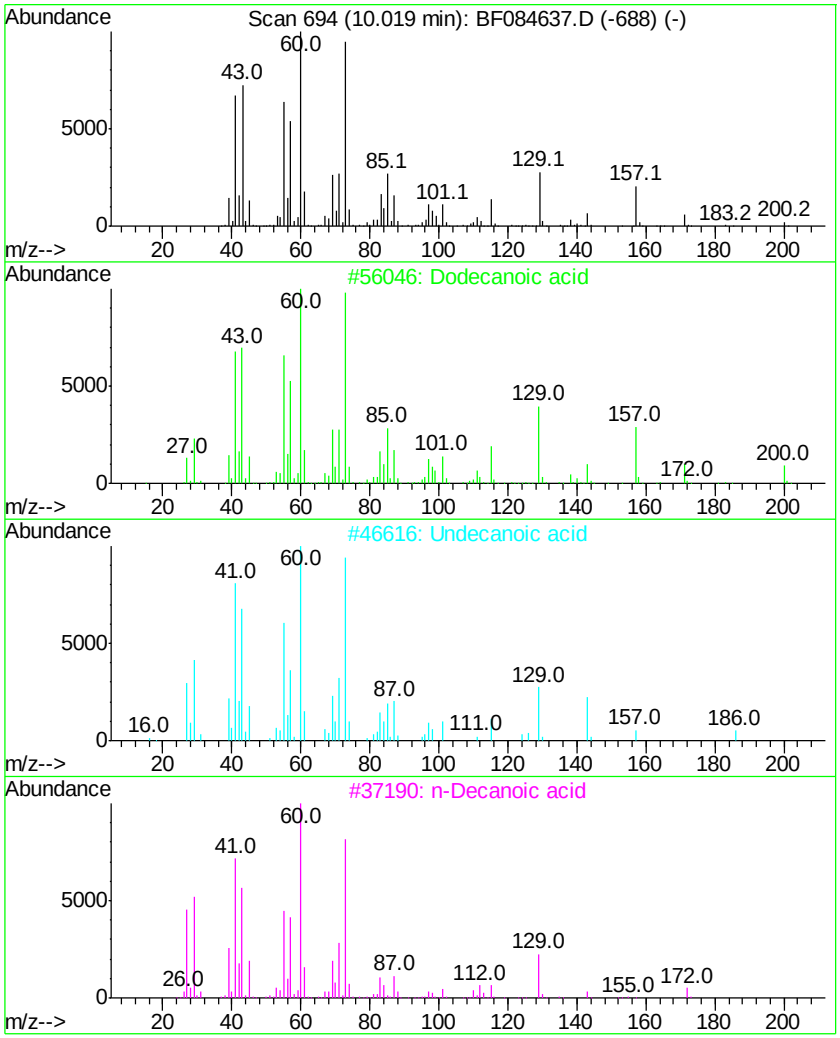
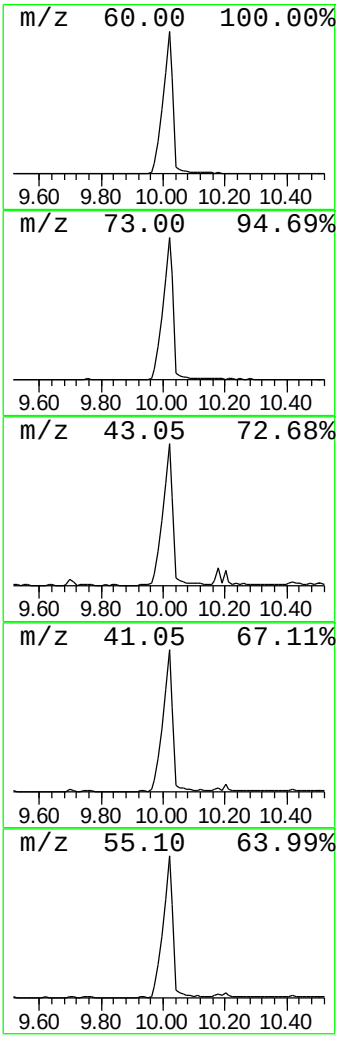
Peak Number 7 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	69.47 ng	5836740	Acenaphthene-d10	9.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	91
2	Undecanoic acid	186	C11H22O2	000112-37-8	80
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Nonanoic acid	158	C9H18O2	000112-05-0	53
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43





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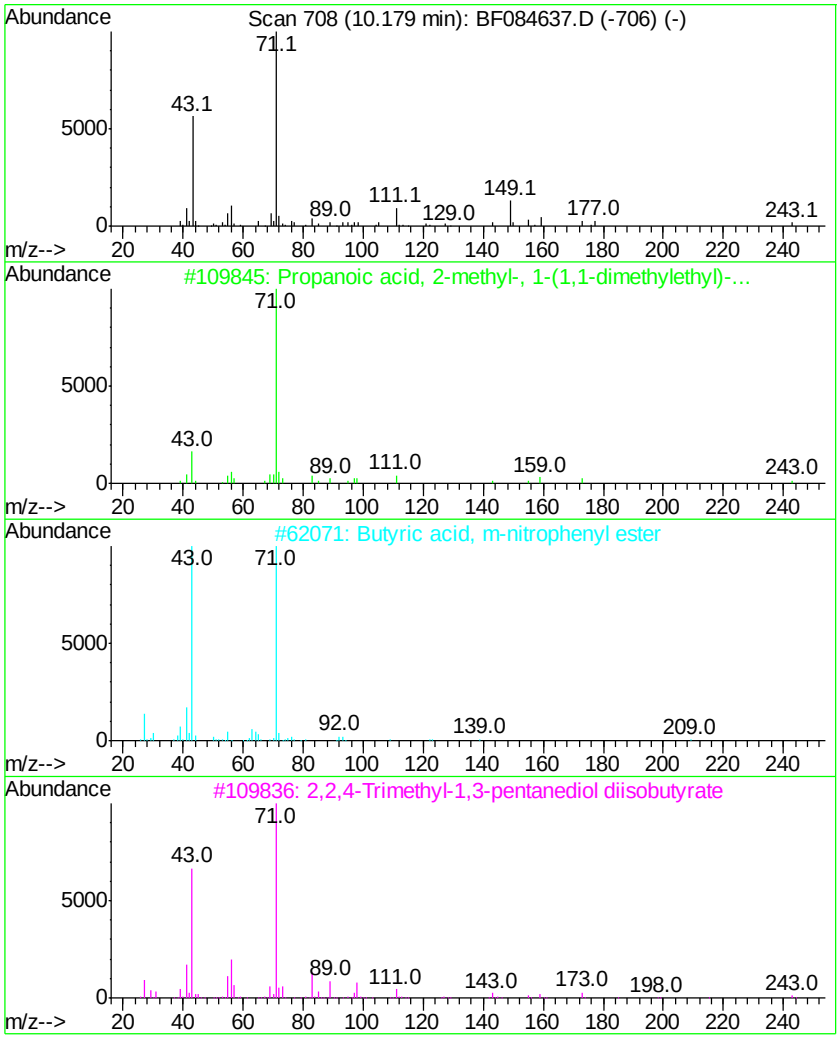
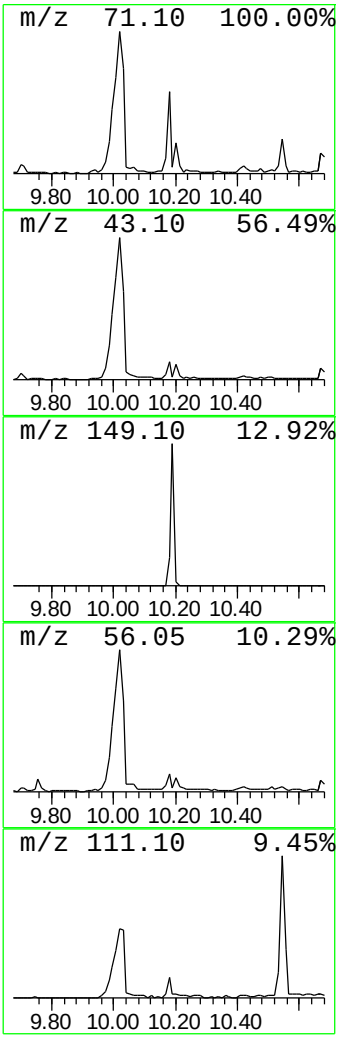
Peak Number 8 Propanoic acid, 2-methyl-, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	3.01 ng	252778	Acenaphthene-d10	9.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	50
2	Butyric acid, m-nitrophenyl ester	209	C10H11NO4	014617-97-1	50
3	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	45
4	Butane, 1-bromo-2-methyl-	150	C5H11Br	010422-35-2	42
5	Butane, 1-bromo-2-methyl-, (S)-	150	C5H11Br	000534-00-9	42





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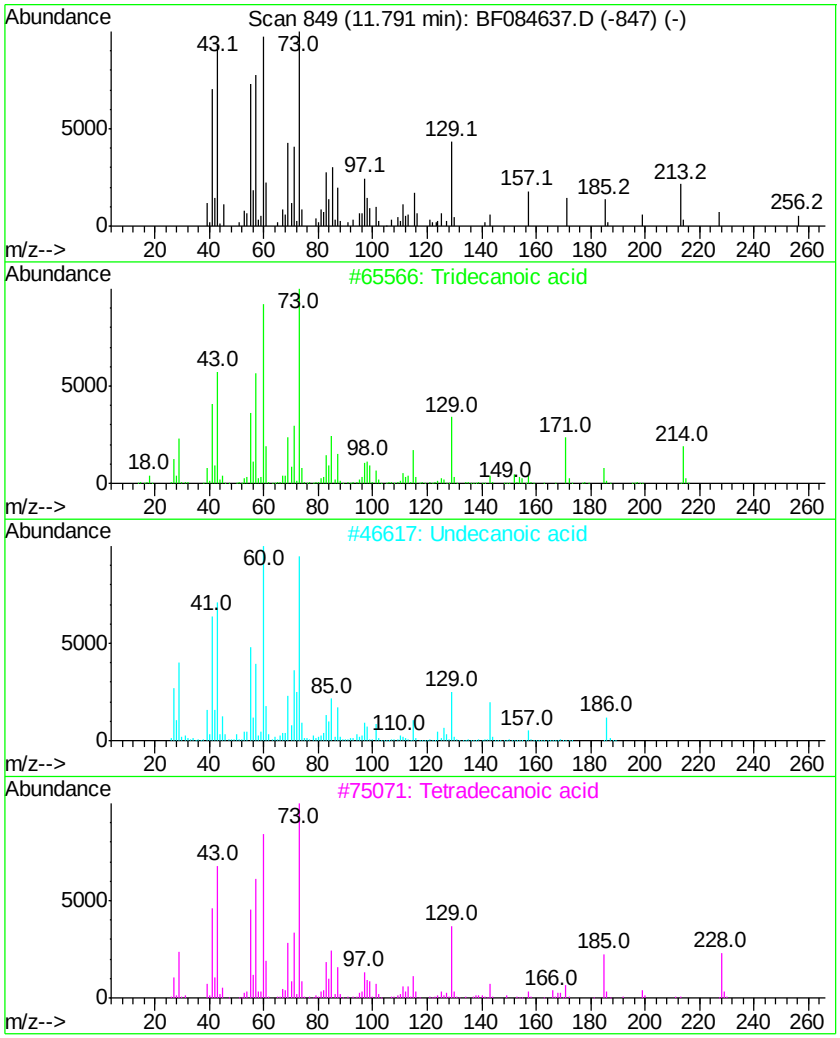
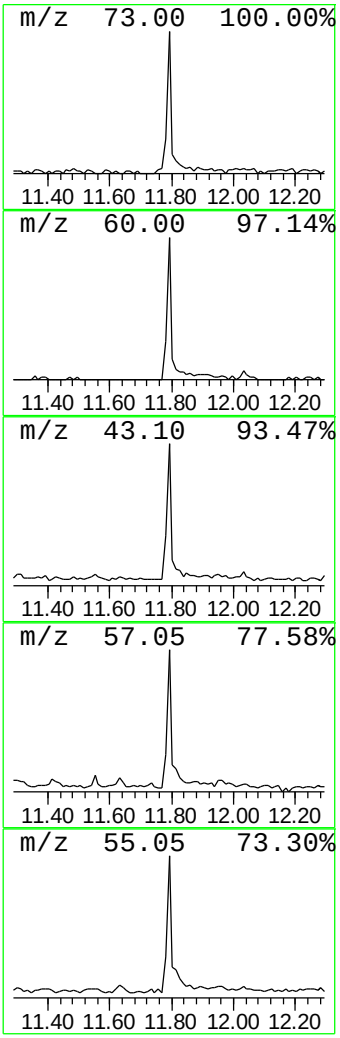
Peak Number 9 Tridecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	2.76 ng	203898	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	87
2	Undecanoic acid	186	C11H22O2	000112-37-8	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	47
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	45





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084637.D
Acq On : 29 Jan 2016 15:45
Operator : SJ/IZ
Sample : H1242-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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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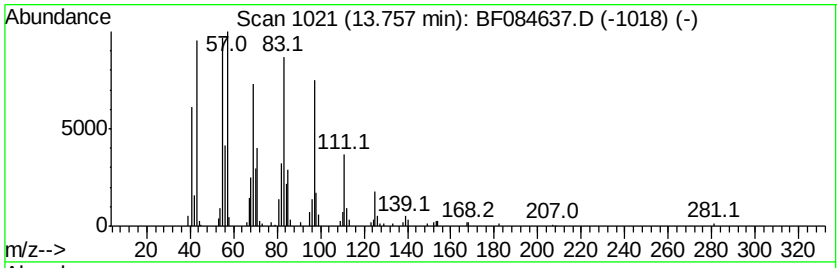
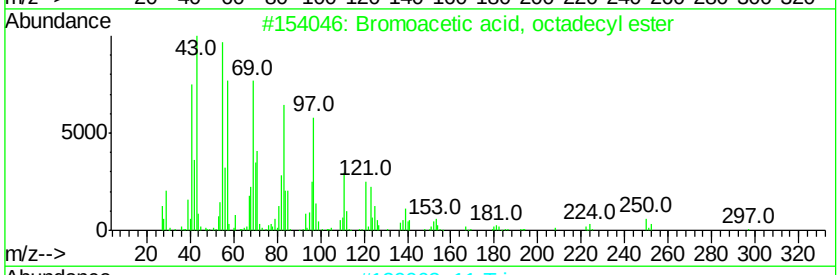
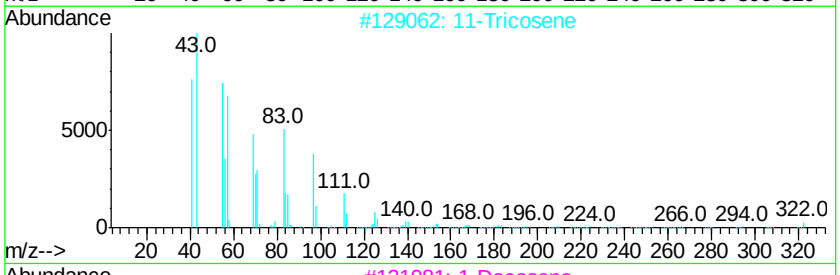
Peak Number 10 Bromoacetic acid, octadecyl... Concentration Rank 7

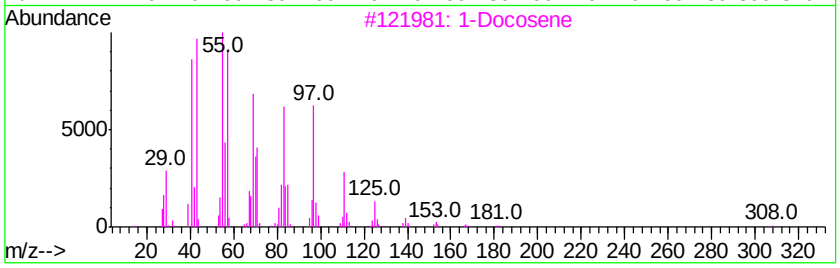
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	9.05 ng	632675	Chrysene-d12	13.87

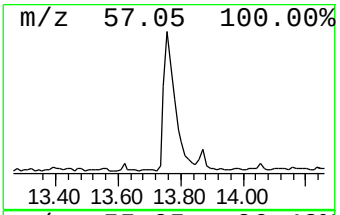
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	11-Tricosene	322	C23H46	052078-56-5	86
3	1-Docosene	308	C22H44	001599-67-3	81
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	80
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	74

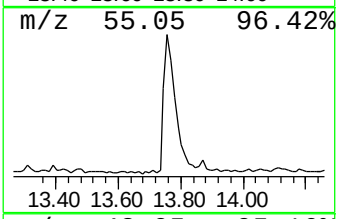


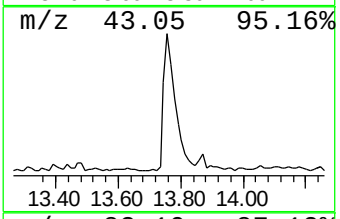


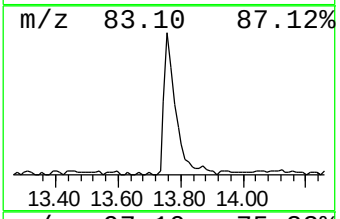


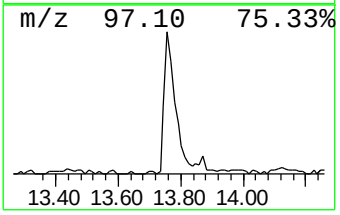












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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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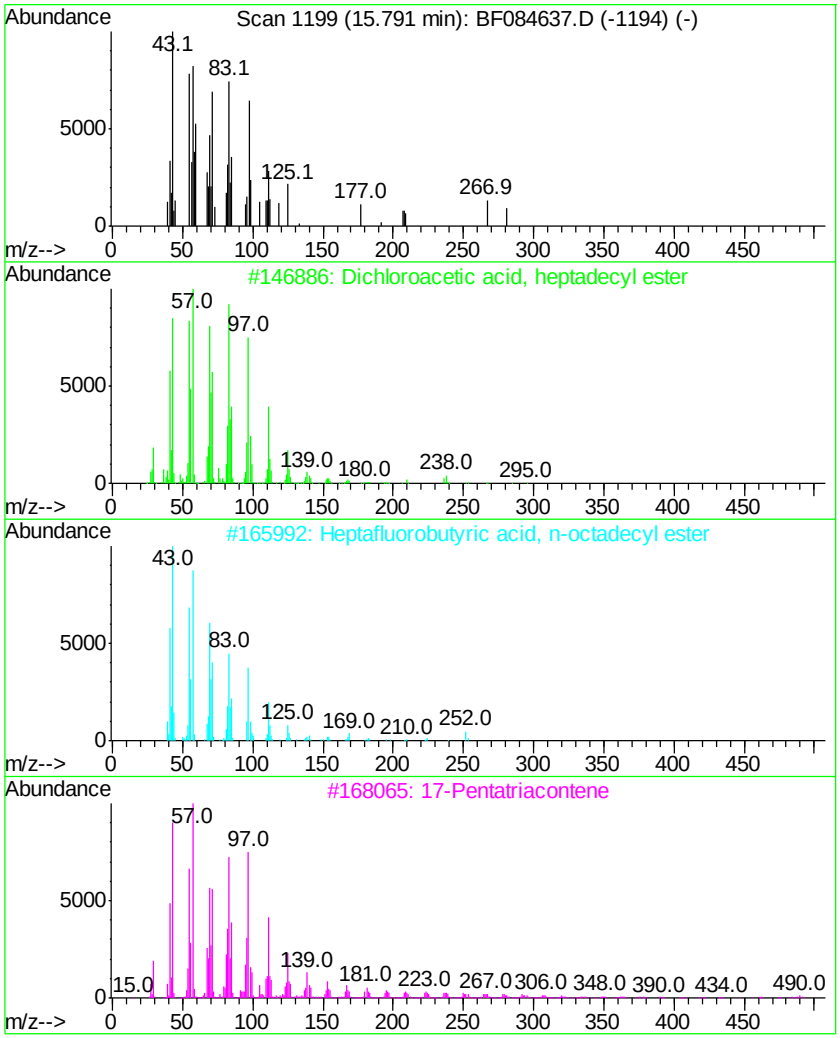
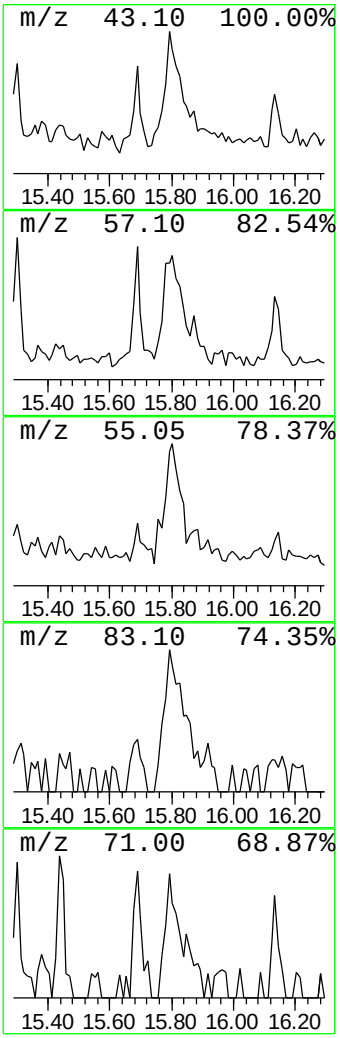
Peak Number 11 Dichloroacetic acid, heptad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.41 ng	140309	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	64
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	64
3	17-Pentatriacontene	491	C35H70	006971-40-0	59
4	2-Heptafluorobutyroxypentadecane	424	C19H31F7O2	1000245-50-0	59
5	4-Heptafluorobutyroxytridecane	396	C17H27F7O2	1000245-49-6	59





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.19	9.4	ng	522313	1	6.73	1114100	20.0
2-Pentanone, 4-hy...	4.89	50.2	ng	2795930	1	6.73	1114100	20.0
Cyclohexanone	5.57	33.9	ng	1886270	1	6.73	1114100	20.0
2-Pentanone, 4-me...	5.72	7.3	ng	408613	1	6.73	1114100	20.0
unknown6.49	6.49	84.7	ng	4718920	1	6.73	1114100	20.0
Dodecanoic acid	10.02	69.5	ng	5836740	3	9.76	1680260	20.0
Propanoic acid, 2...	10.18	3.0	ng	252778	3	9.76	1680260	20.0
Tridecanoic acid	11.79	2.8	ng	203898	4	11.24	1480010	20.0
Bromoacetic acid,...	13.76	9.1	ng	632675	5	13.87	1397420	20.0
Dichloroacetic ac...	15.79	2.4	ng	140309	6	15.25	1162990	20.0