LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085596.D
Acq On : 20 Mar 2016 4:20
Operator : UM/SJ
Sample : H1790-05
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-8A-(0-10)

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-BF031816.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	2.447	7	14	18	rVB2	15683	55154	1.56%	0.186%
2	2.698	34	36	43	rVB	115654	169204	4.77%	0.570%
3	4.618	201	204	207	rBV	27124	39135	1.10%	0.132%
4	5.053	240	242	247	rBV2	201287	363770	10.26%	1.226%
5	5.464	275	278	281	rBV	2699178	2855114	80.56%	9.625%
6	6.493	365	368	370	rBV	2481974	3025909	85.38%	10.201%
7	6.619	377	379	382	rBV	2507996	3261019	92.01%	10.994%
8	6.847	397	399	404	rBV	561874	817376	23.06%	2.756%
9	7.007	411	413	416	rVB	2408441	2520963	71.13%	8.499%
10	7.419	446	449	451	rBV	2076863	2108516	59.49%	7.108%
11	8.139	509	512	516	rBV2	1124473	1445362	40.78%	4.873%
12	8.847	572	574	577	rBV	104359	88246	2.49%	0.298%
13	8.950	580	583	585	rVB	59636	52685	1.49%	0.178%
14	9.213	603	606	609	rBV	3489859	3544060	100.00%	11.948%
15	9.888	663	665	667	rBV	1079918	1025331	28.93%	3.457%
16	9.922	667	668	670	rVB	139762	103398	2.92%	0.349%
17	10.093	681	683	686	rVB	60083	49138	1.39%	0.166%
18	10.436	711	713	715	rVB	65905	52544	1.48%	0.177%
19	10.676	731	734	737	rBV2	1728784	2020111	57.00%	6.810%
20	11.373	793	795	797	rBV	1092922	974864	27.51%	3.287%
21	12.094	854	858	867	rBV	26377	51887	1.46%	0.175%
22	12.779	916	918	920	rBV	186921	155859	4.40%	0.525%
23	12.962	931	934	936	rBV	3293804	3203124	90.38%	10.799%
24	13.488	978	980	982	rBV	86069	87607	2.47%	0.295%
25	14.002	1023	1025	1028	rBV	670308	677238	19.11%	2.283%
26	15.431	1147	1150	1153	rBV	564776	702013	19.81%	2.367%
27	16.060	1196	1205	1215	rBV2	37221	212877	6.01%	0.718%

Sum of corrected areas: 29662504

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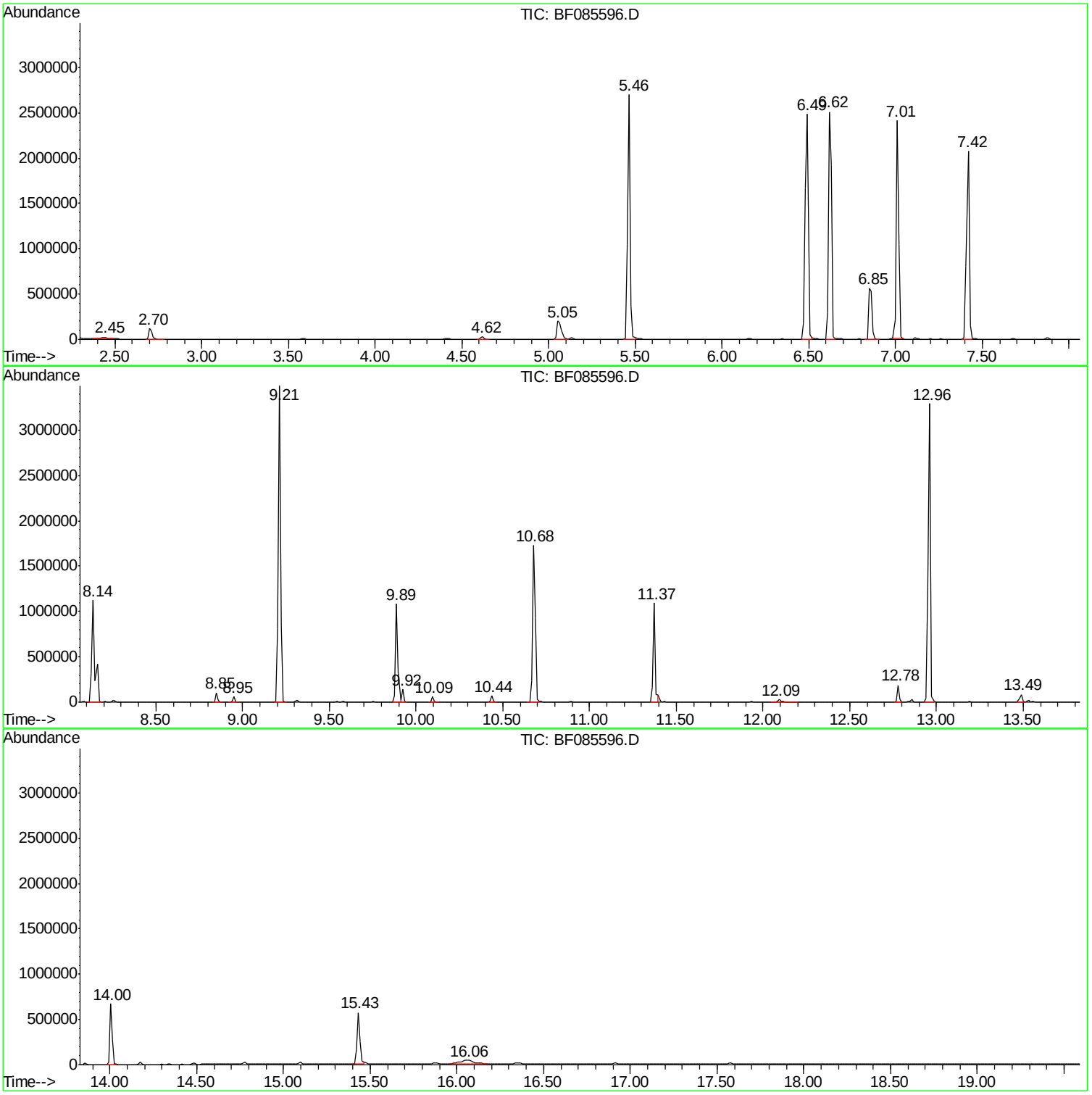
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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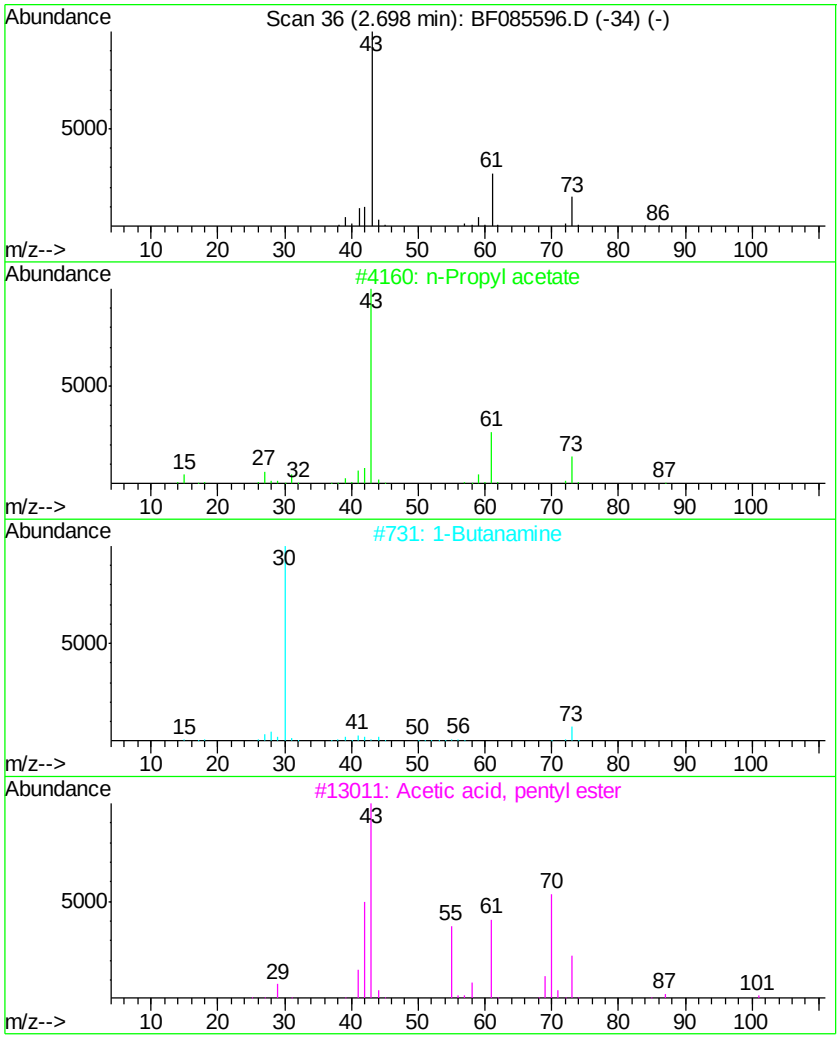
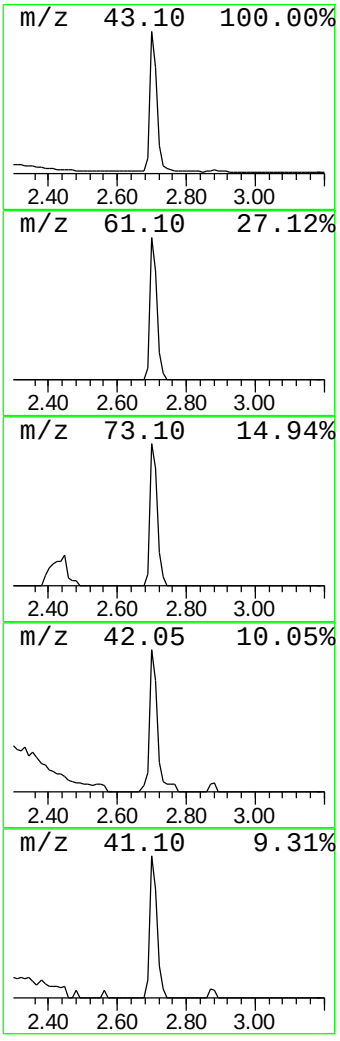
Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.70	4.14 ng	169204	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	9
3	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9
4	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
5	Isobutylamine	73	C4H11N	000078-81-9	5





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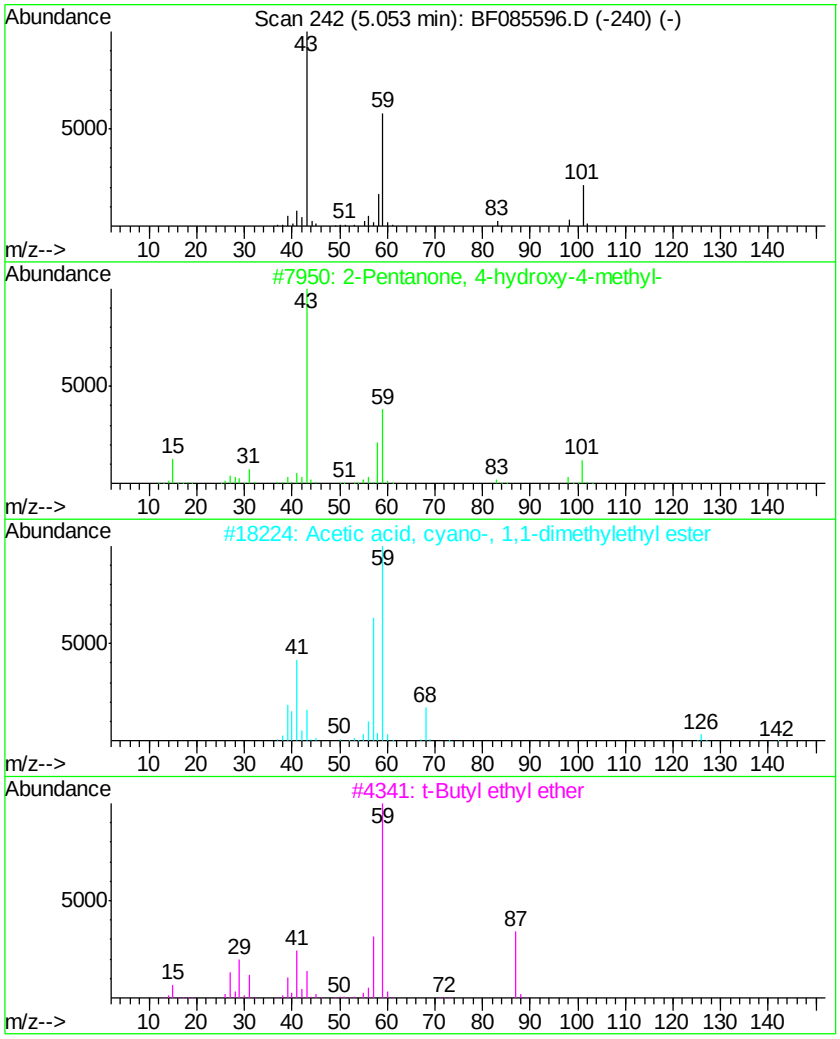
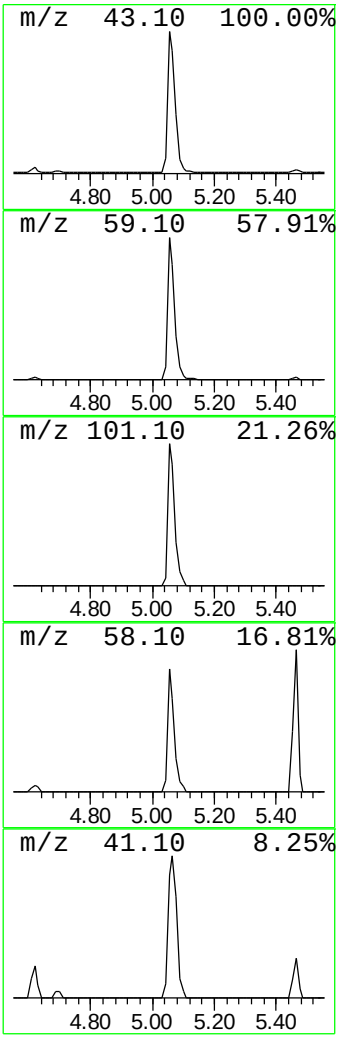
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	8.90 ng	363770	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	t-Butyl ethyl ether	102	C6H14O	1000118-18-4	17
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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ClientSampleId : GRID-8A-(0-10)

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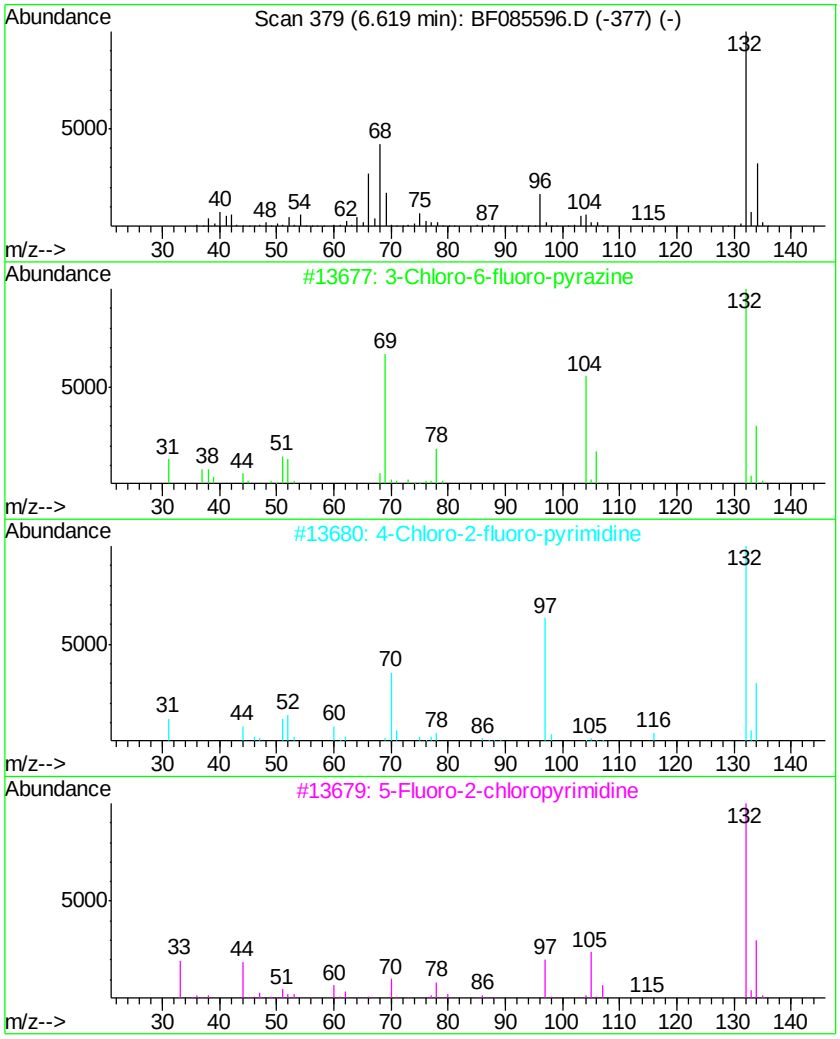
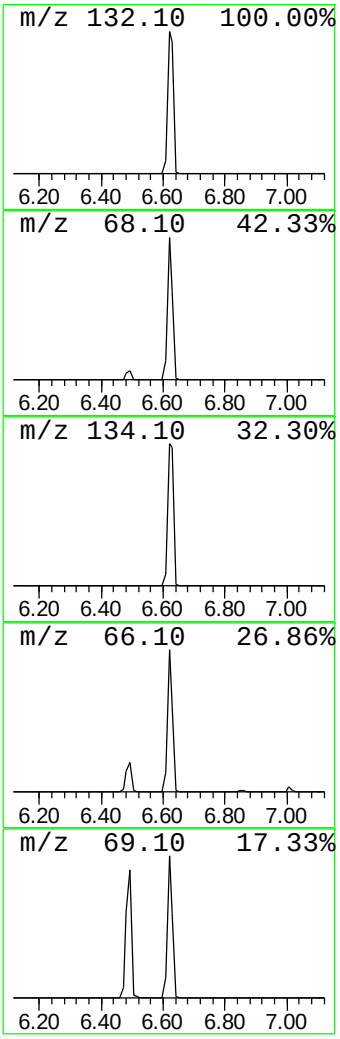
Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	79.79 ng	3261020	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





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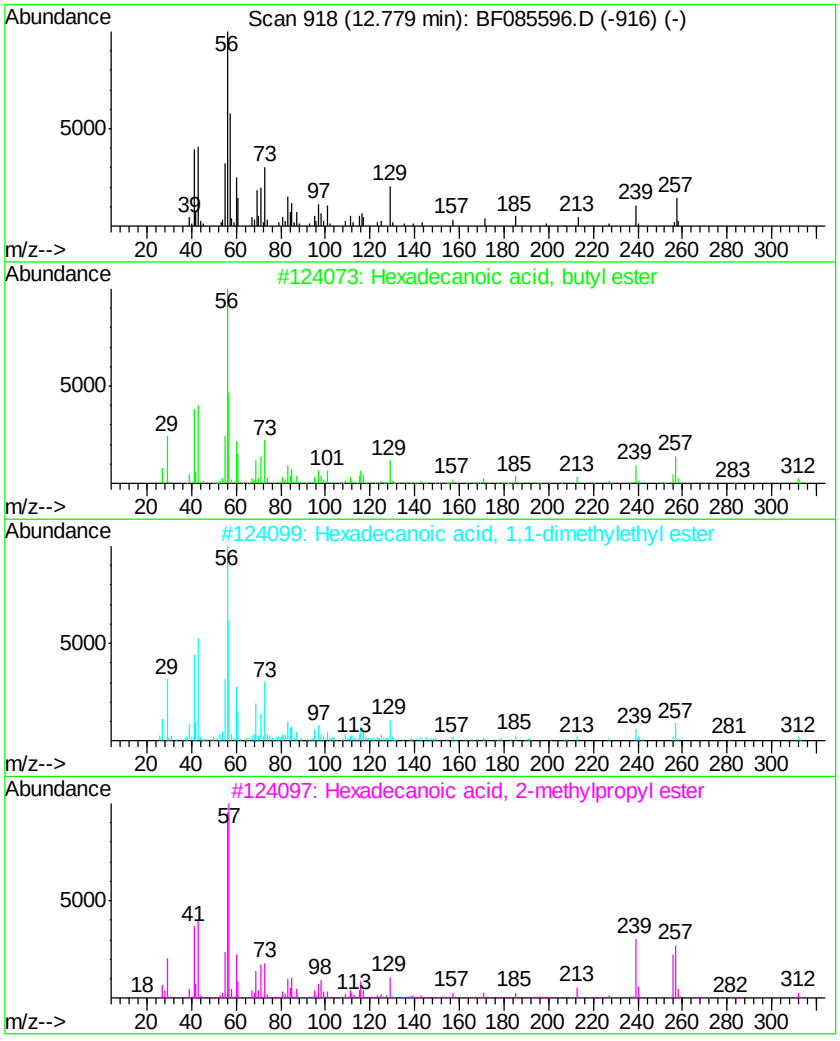
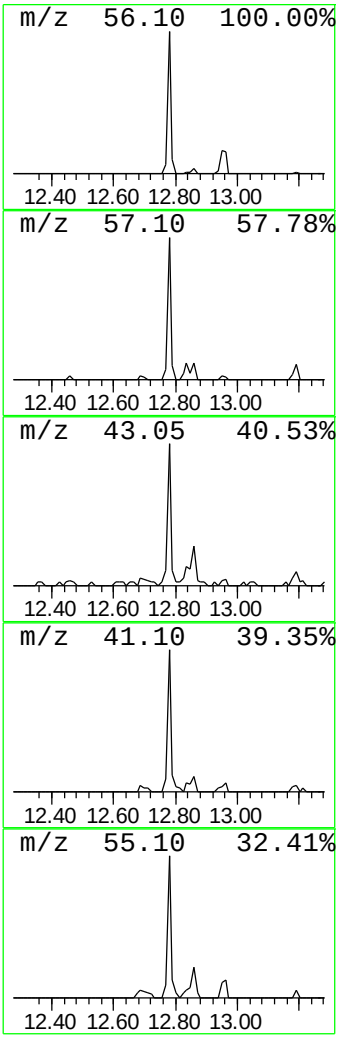
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	4.60 ng	155859	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	40
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32





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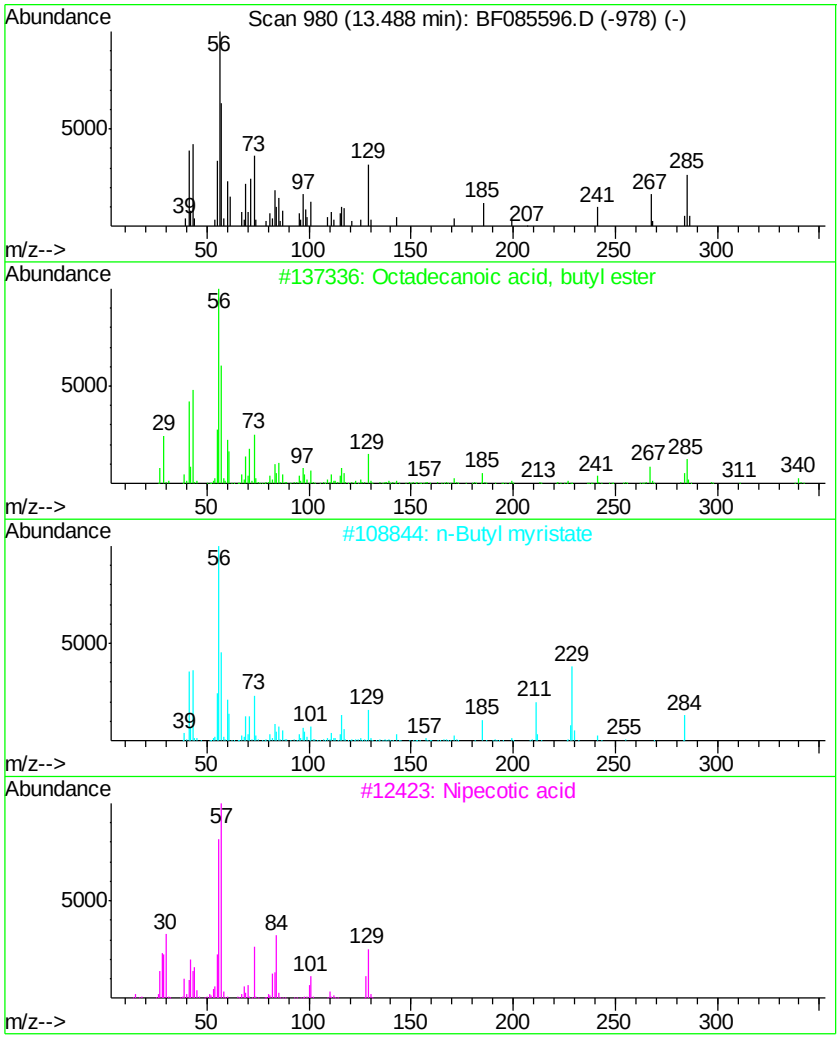
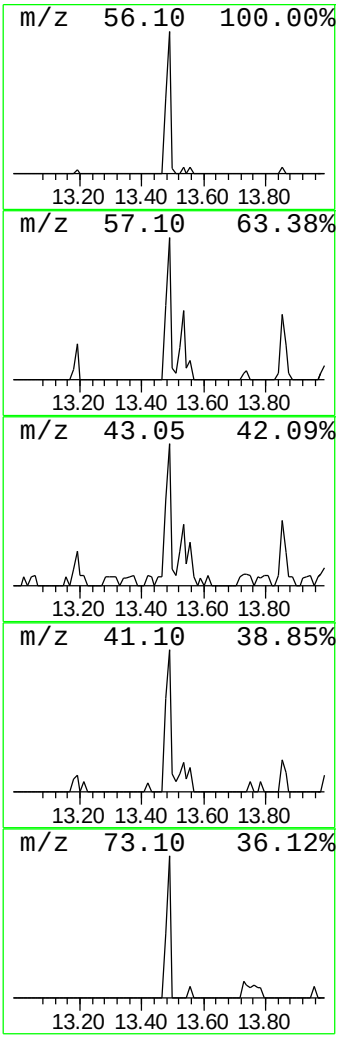
Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.59 ng	87607	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	n-Butyl myristate	284	C18H36O2	000110-36-1	53
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Acetamide, N-2-propenyl-	99	C5H9NO	000692-33-1	27
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27





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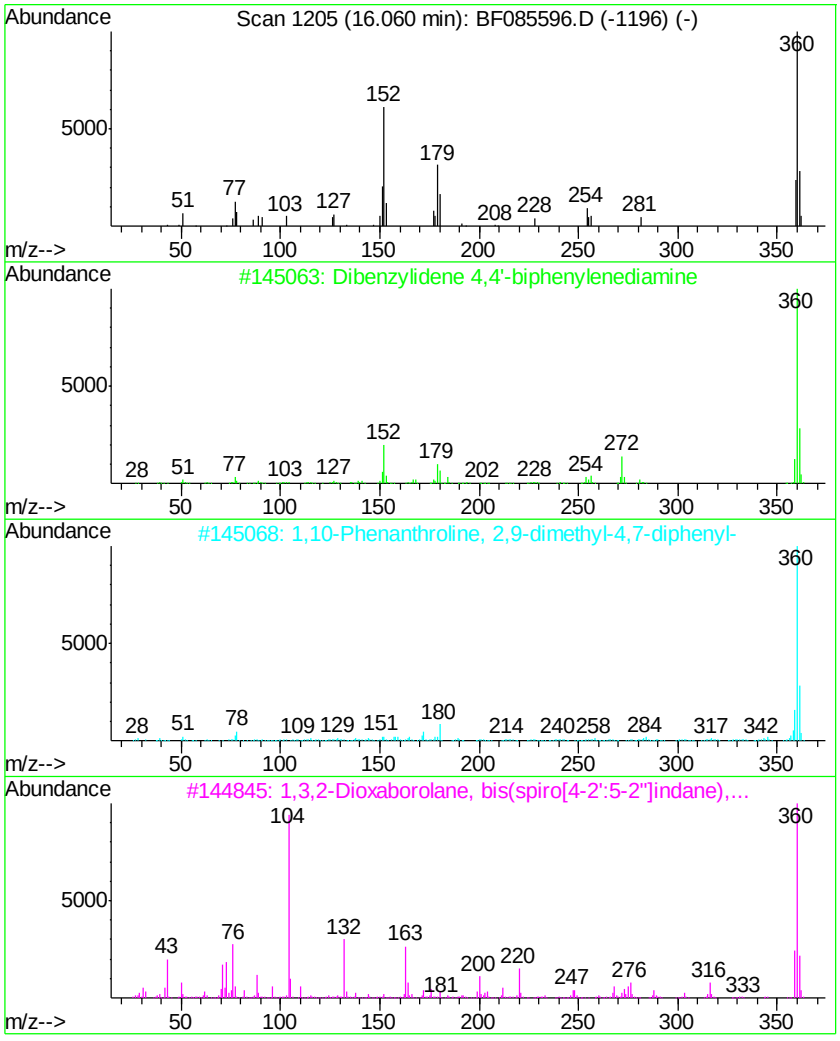
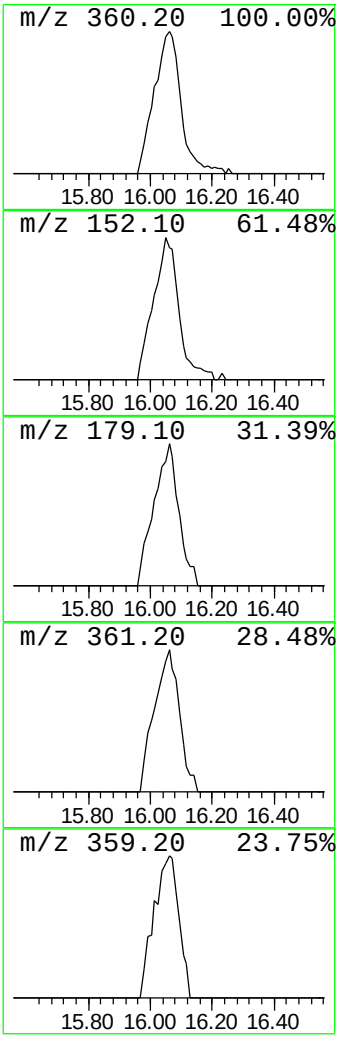
Peak Number 7 Dibenzylidene 4,4'-biphenyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	6.06 ng	212877	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	93
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43
3	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	43
4	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
5	Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	38





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
n-Propyl acetate	2.70	4.1	ng	169204	1	6.86	817376	20.0
2-Pentanone, 4-hy...	5.05	8.9	ng	363770	1	6.86	817376	20.0
unknown6.62	6.62	79.8	ng	3261020	1	6.86	817376	20.0
Hexadecanoic acid...	12.78	4.6	ng	155859	5	14.00	677238	20.0
Octadecanoic acid...	13.49	2.6	ng	87607	5	14.00	677238	20.0
Dibenzylidene 4,4...	16.06	6.1	ng	212877	6	15.43	702013	20.0