LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088668.D
Acq On : 4 Jul 2016 1:16
Operator : UM/SJ
Sample : H3817-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BS-4A-9-9.5FT

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	1.850	21	23	35	rVB	41444	59618	1.94%	0.211%
2	2.021	35	38	41	rBV	64019	75320	2.45%	0.266%
3	3.027	123	126	135	rBV	78758	179608	5.84%	0.635%
4	4.959	292	295	300	rBB	187410	262566	8.53%	0.928%
5	5.382	329	332	334	rBV	2806656	2874623	93.41%	10.158%
6	6.422	420	423	425	rBV	2747232	3077445	100.00%	10.874%
7	6.547	431	434	437	rBV	2537931	3018786	98.09%	10.667%
8	6.787	452	455	456	rBV	571776	686465	22.31%	2.426%
9	6.936	466	468	471	rVB	1917995	2077079	67.49%	7.340%
10	7.347	501	504	506	rBV	1979333	1991619	64.72%	7.038%
11	7.782	538	542	545	rBV	30568	76384	2.48%	0.270%
12	8.068	564	567	569	rVB	1157121	994424	32.31%	3.514%
13	9.142	658	661	664	rBV	2716080	2854895	92.77%	10.088%
14	9.542	693	696	698	rBV	423683	477743	15.52%	1.688%
15	9.816	717	720	722	rVB	1300596	1105257	35.91%	3.906%
16	10.205	751	754	755	rBV	42299	50370	1.64%	0.178%
17	10.605	786	789	791	rBV	2037815	2190425	71.18%	7.740%
18	10.731	798	800	804	rVB	48454	51060	1.66%	0.180%
19	11.176	837	839	840	rBV	109762	92260	3.00%	0.326%
20	11.291	847	849	851	rVB	1289399	1082343	35.17%	3.825%
21	11.359	851	855	859	rVB4	30775	74043	2.41%	0.262%
22	11.599	874	876	879	rVB	68450	63734	2.07%	0.225%
23	12.879	985	988	990	rBV	2816893	2677088	86.99%	9.460%
24	13.359	1028	1030	1036	rBV	29550	62785	2.04%	0.222%
25	13.794	1066	1068	1076	rBV	118780	216084	7.02%	0.764%
26	13.920	1076	1079	1081	rVV	822585	930160	30.23%	3.287%
27	14.434	1123	1124	1131	rVB2	36216	62657	2.04%	0.221%
28	15.303	1197	1200	1203	rBV	534813	718616	23.35%	2.539%
29	15.840	1244	1247	1257	rVB4	13665	50087	1.63%	0.177%
30	19.063	1524	1529	1535	rVB3	56802	166355	5.41%	0.588%

Sum of corrected areas: 28299899

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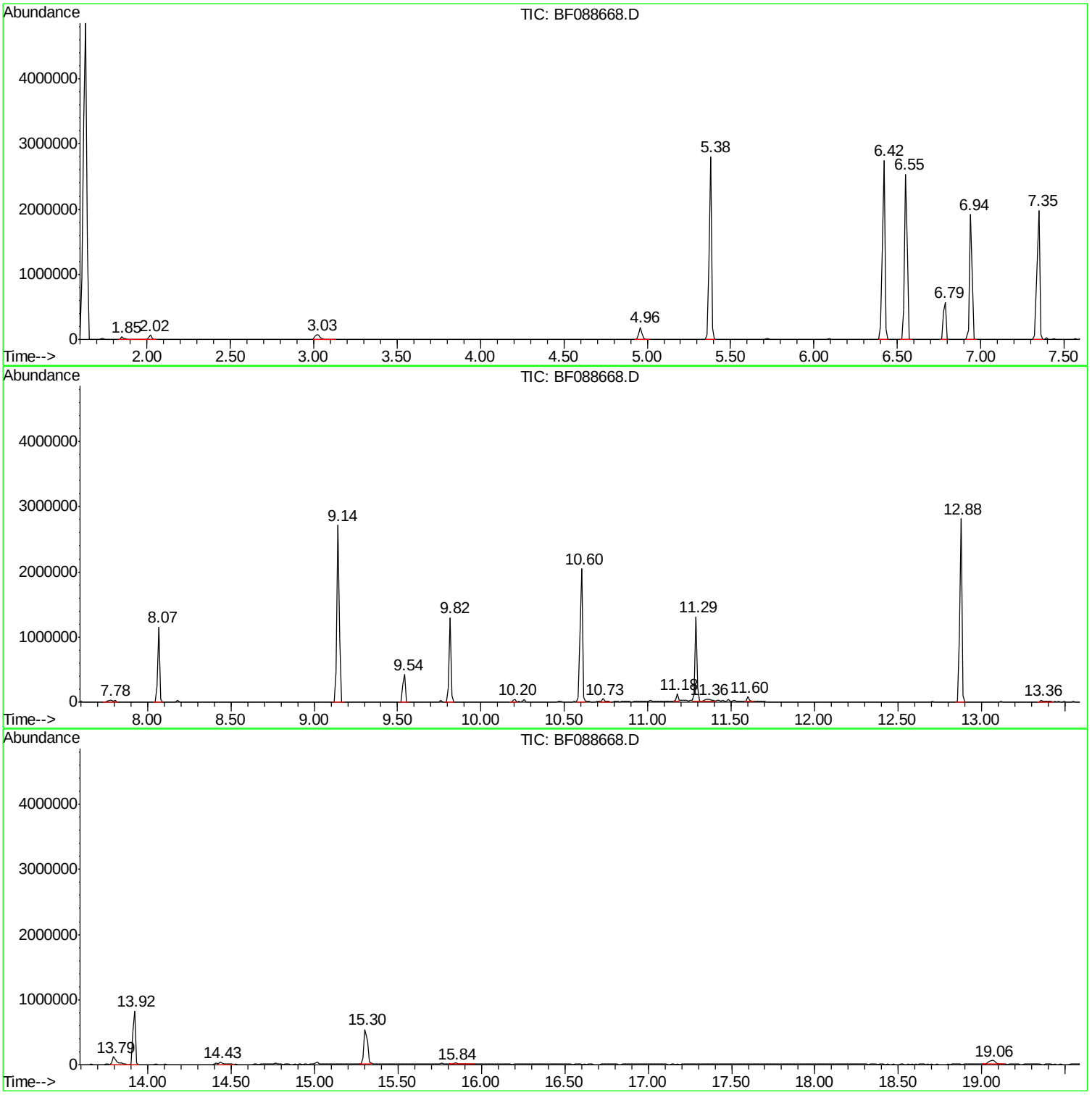
BS-4A-9-9.5FT

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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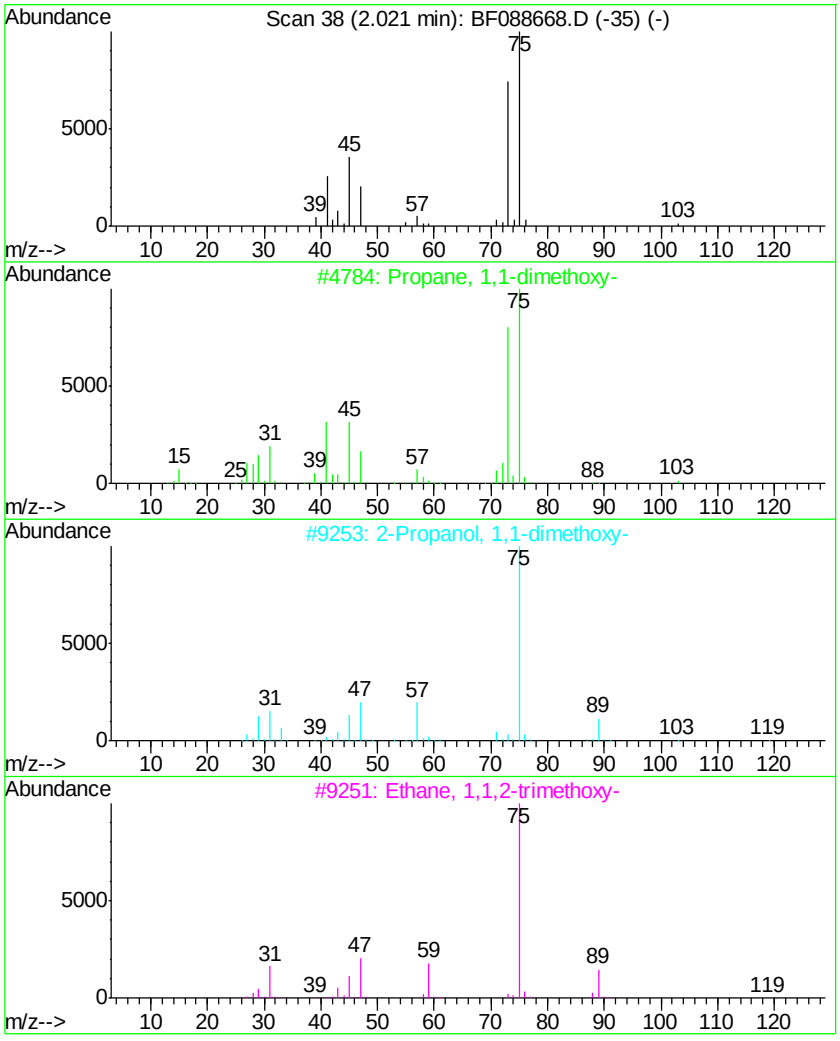
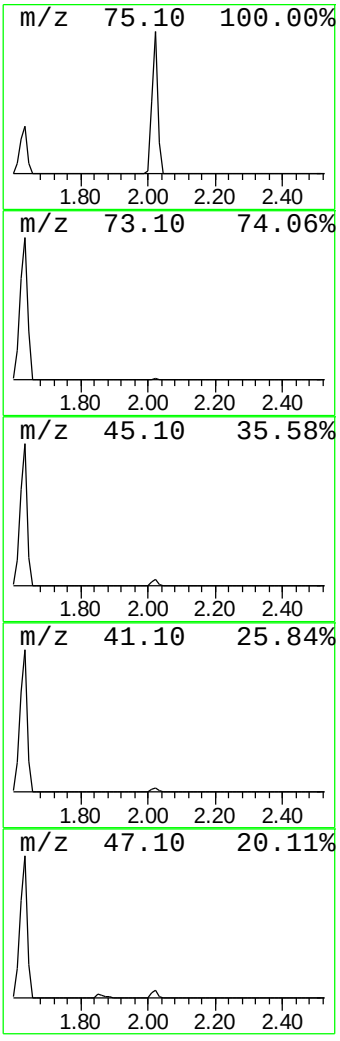
Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	2.19 ng	75320	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	38
3	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	36
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	14
5	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10





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ClientSampleId : BS-4A-9-9.5FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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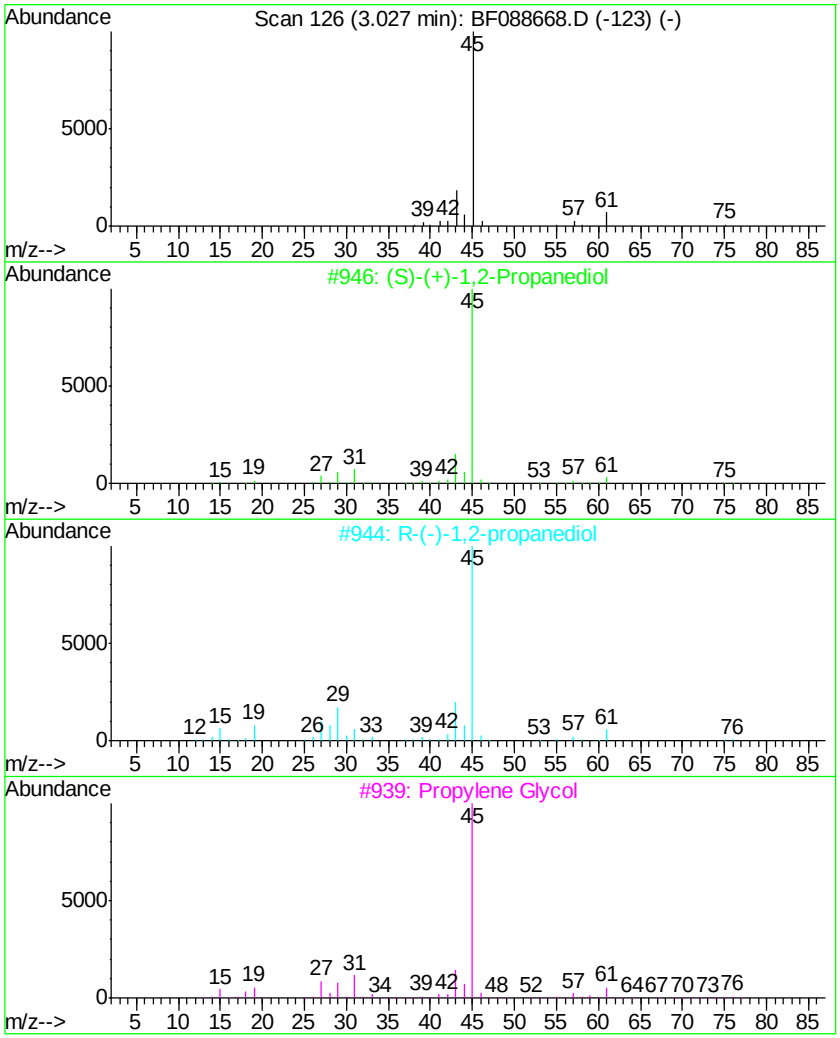
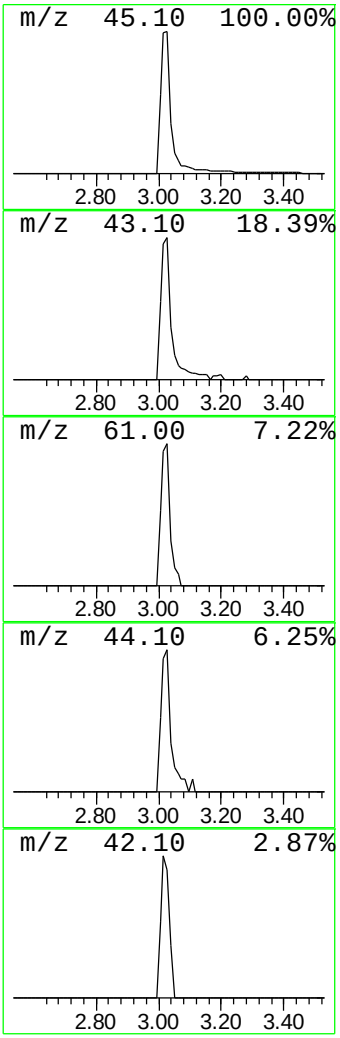
Peak Number 2 unknown3.03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.03	5.23 ng	179608	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	L-Lactic acid	90	C3H6O3	000079-33-4	9
5	2-Pentanol	88	C5H12O	006032-29-7	9





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Instrument : BNA_F
ClientSampleId : BS-4A-9-9.5FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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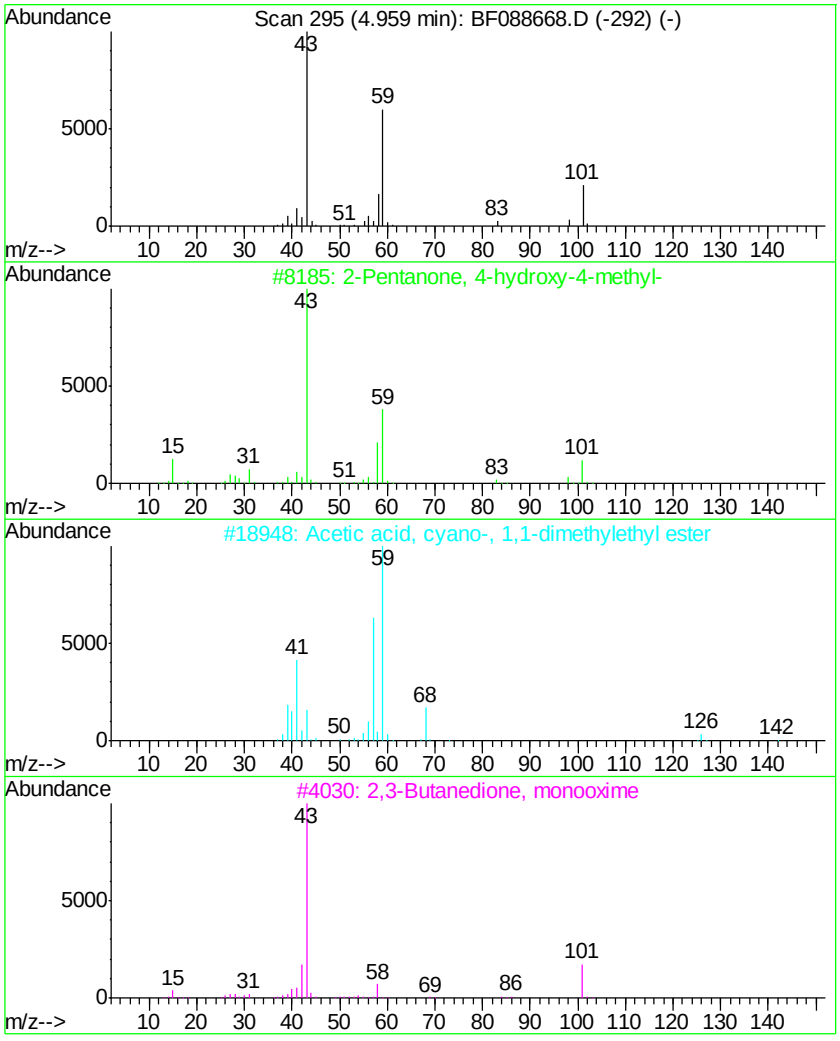
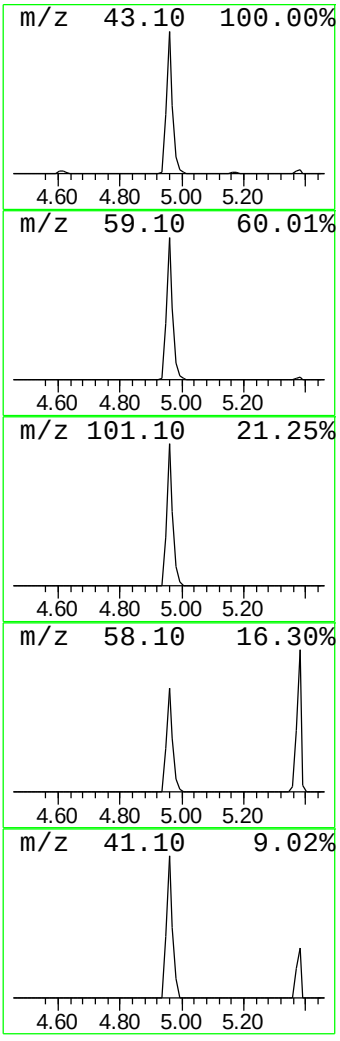
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	7.65 ng	262566	1,4-Dichlorobenzene-d4	6.79

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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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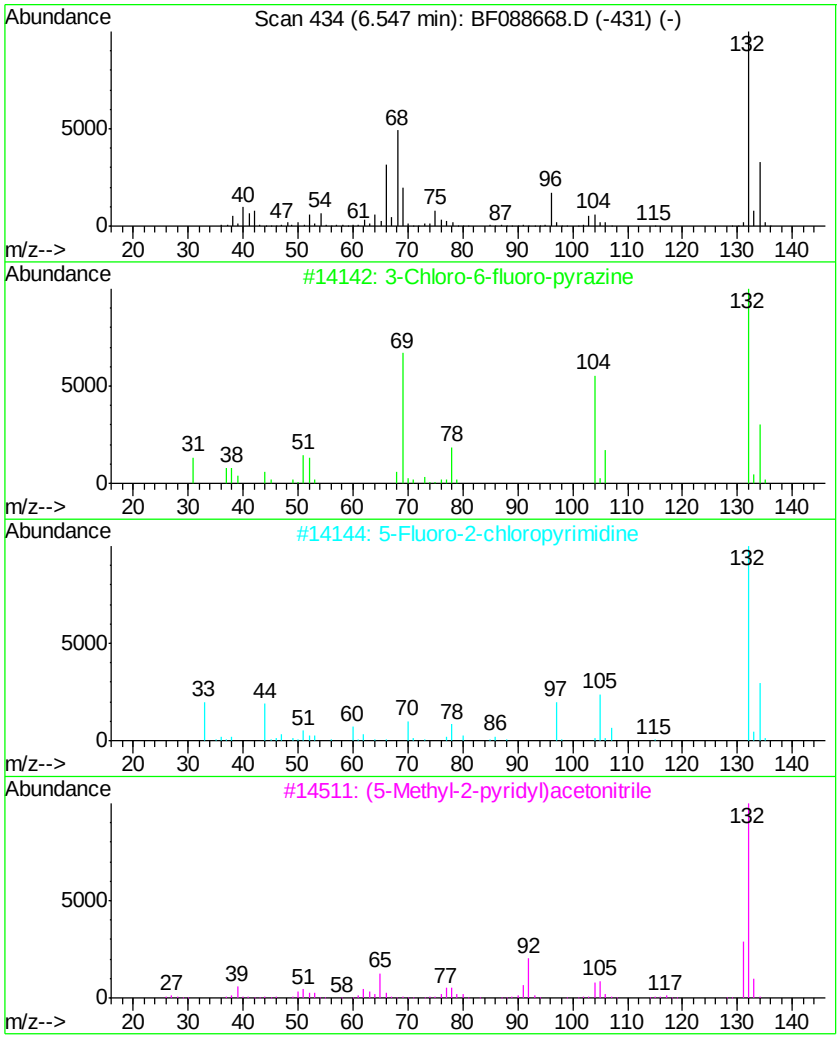
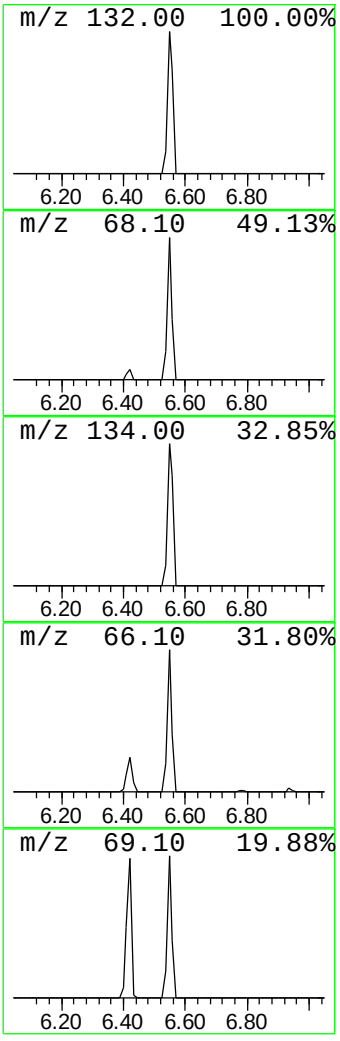
Peak Number 4 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	87.95 ng	3018790	1,4-Dichlorobenzene-d4	6.79

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	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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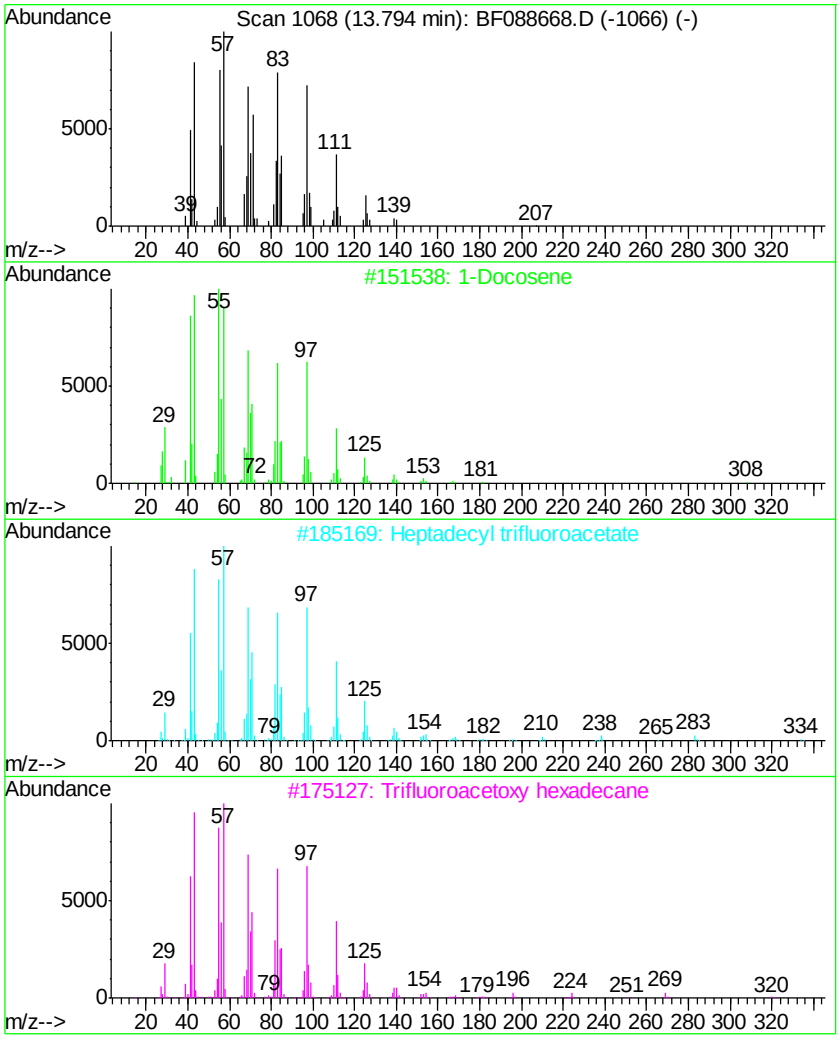
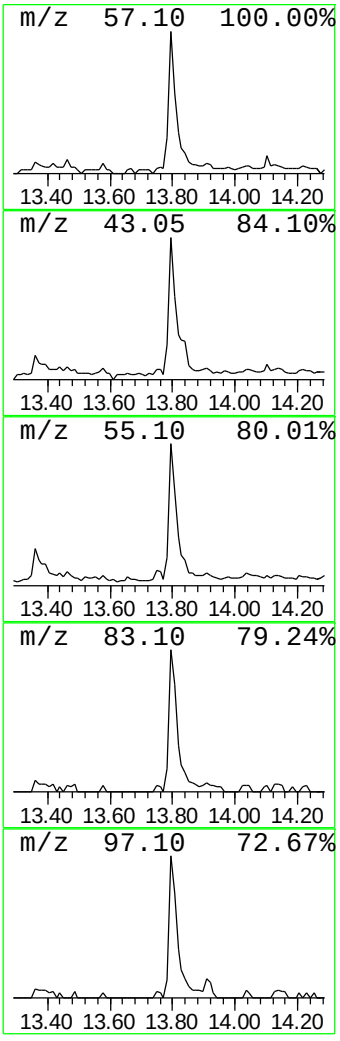
Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	4.65 ng	216084	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	87





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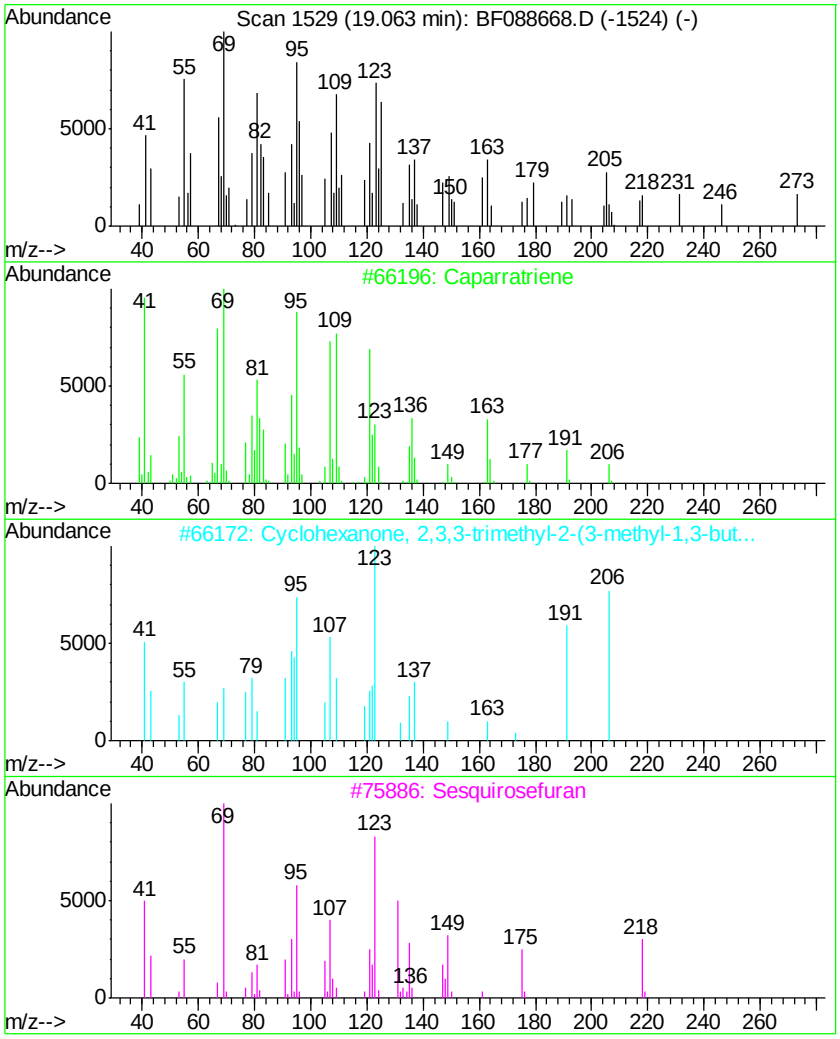
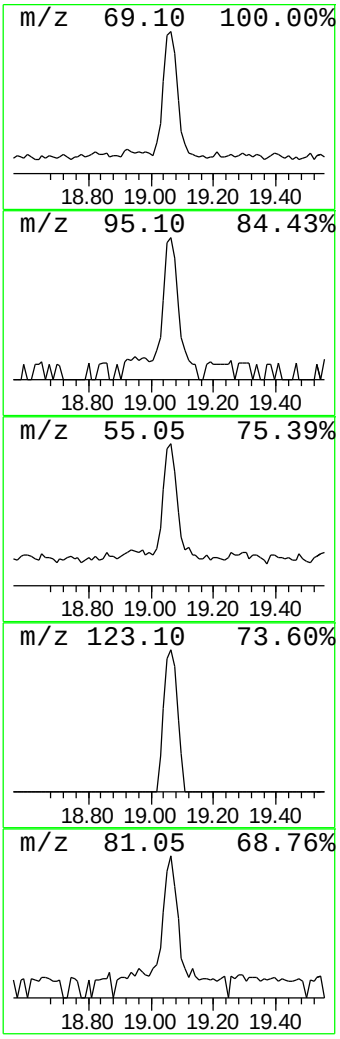
Peak Number 7 Caparratriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.06	4.63 ng	166355	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caparratriene	206	C15H26	1000374-08-7	56
2	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-91-9	45
3	Sesquirosefuran	218	C15H22O	039007-93-7	43
4	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	42
5	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	38





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	2.02	2.2	ng	75320	1	6.79	686465	20.0
unknown3.03	3.03	5.2	ng	179608	1	6.79	686465	20.0
2-Pentanone, 4-hy...	4.96	7.7	ng	262566	1	6.79	686465	20.0
unknown6.55	6.55	88.0	ng	3018790	1	6.79	686465	20.0
1-Docosene	13.79	4.7	ng	216084	5	13.92	930160	20.0
Caparratriene	19.06	4.6	ng	166355	6	15.30	718616	20.0