LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112119\
Data File : BF117916.D
Acq On : 21 Nov 2019 17:00
Operator : JU
Sample : K5904-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-(6-8)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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	2.169	9	14	48	rVB	654442	1086683	24.42%	3.189%
2	5.122	511	516	527	rVB	431914	495512	11.14%	1.454%
3	5.528	580	585	588	rBV	3019578	2784187	62.58%	8.170%
4	6.534	751	756	759	rBV	3037602	2920975	65.65%	8.571%
5	6.681	777	781	785	rBV	3403781	3079838	69.22%	9.037%
6	6.916	817	821	824	rBV	1008390	798062	17.94%	2.342%
7	7.075	844	848	851	rBV	2787058	2407468	54.11%	7.064%
8	7.475	912	916	919	rBV	2174791	1882104	42.30%	5.523%
9	8.204	1036	1040	1043	rBV	1284438	1078314	24.24%	3.164%
10	9.280	1219	1223	1226	rBV	4325608	3525385	79.24%	10.345%
11	9.674	1286	1290	1299	rBV	510677	445073	10.00%	1.306%
12	9.963	1336	1339	1350	rVB	1504780	1374348	30.89%	4.033%
13	10.757	1470	1474	1487	rBV	2447582	2235312	50.24%	6.559%
14	11.457	1589	1593	1599	rBV	1792293	1467216	32.98%	4.305%
15	11.974	1678	1681	1692	rBV2	74393	100304	2.25%	0.294%
16	13.051	1859	1864	1871	rBV	4686334	4449244	100.00%	13.056%
17	13.951	2012	2017	2032	rBV4	142941	349800	7.86%	1.026%
18	14.104	2039	2043	2047	rBV	1466925	1288069	28.95%	3.780%
19	14.568	2119	2122	2125	rBV	69286	59380	1.33%	0.174%
20	14.886	2172	2176	2181	rBV	84591	100368	2.26%	0.295%
21	14.968	2186	2190	2194	rVB	392744	397791	8.94%	1.167%
22	15.239	2232	2236	2241	rBV	95209	110982	2.49%	0.326%
23	15.615	2294	2300	2309	rBV	1012866	1434402	32.24%	4.209%
24	16.098	2378	2382	2389	rVB	70732	116587	2.62%	0.342%
25	16.633	2469	2473	2481	rVB2	49774	91451	2.06%	0.268%

Sum of corrected areas: 34078855

LSC Report - Integrated Chromatogram

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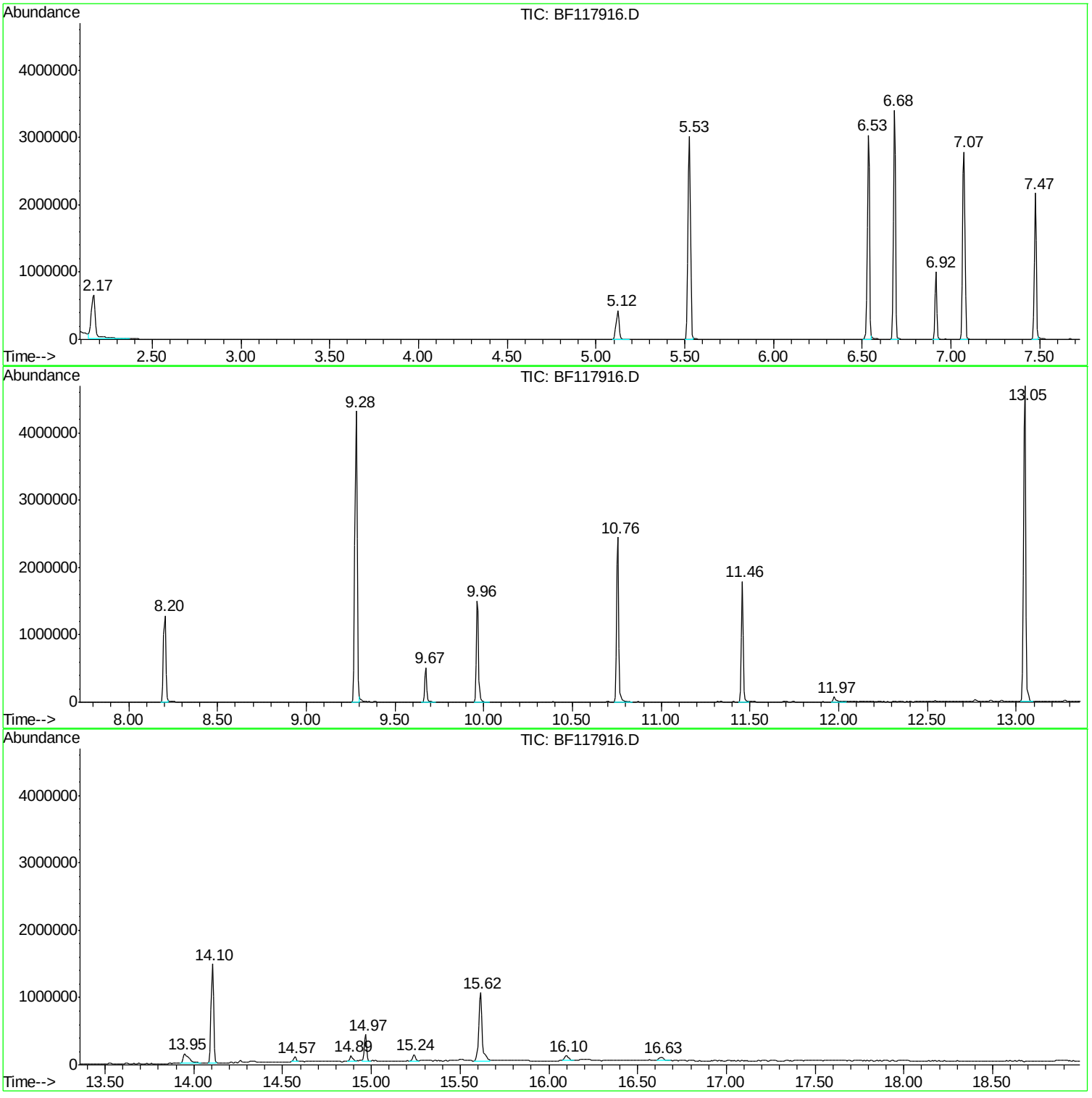
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Acq On : 21 Nov 2019 17:00
Operator : JU
Sample : K5904-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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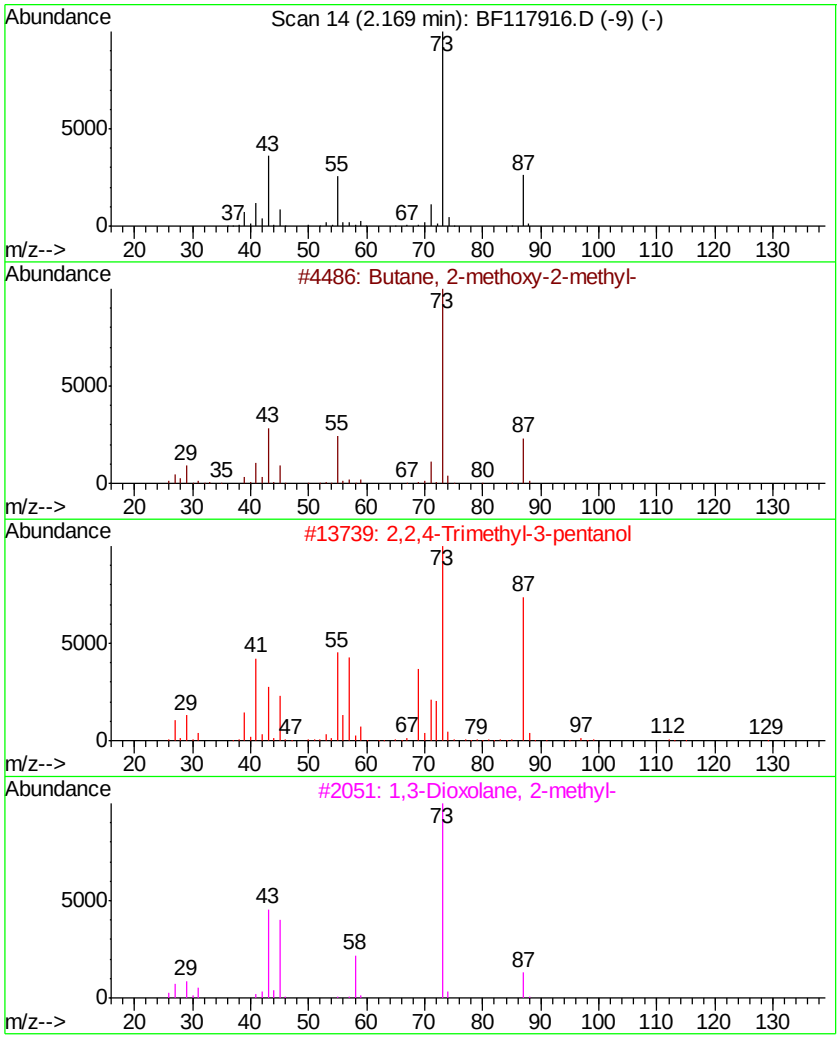
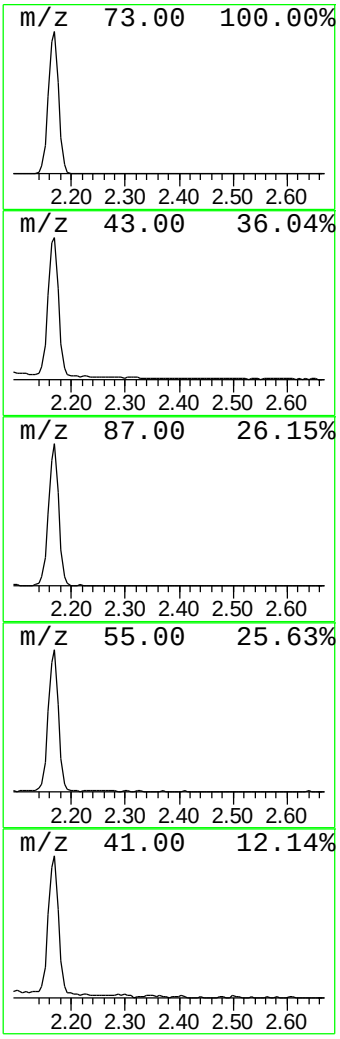
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	27.23 ng	1086680	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Operator : JU
Sample : K5904-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

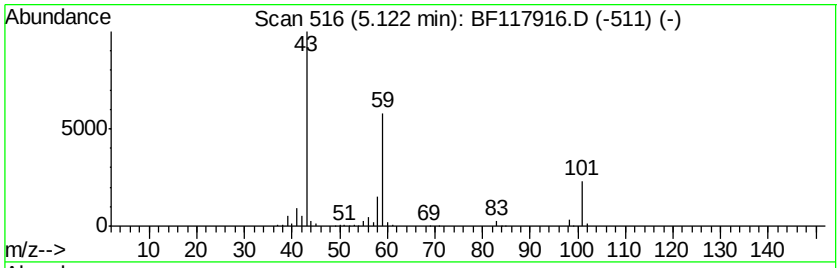
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

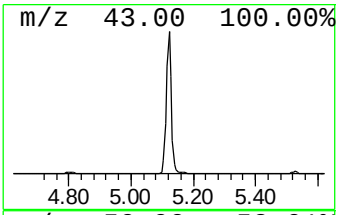
****

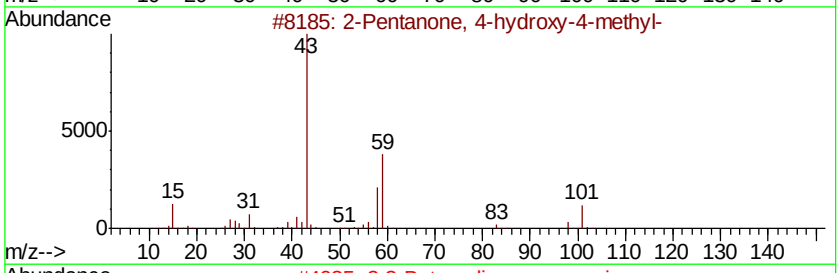
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

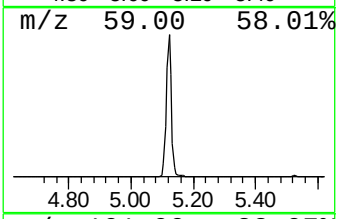
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	12.42 ng	495512	1,4-Dichlorobenzene-d4	6.92

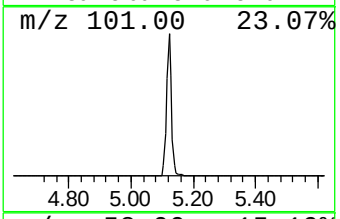
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9

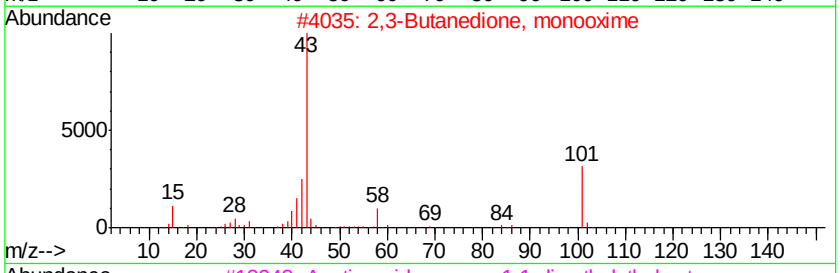


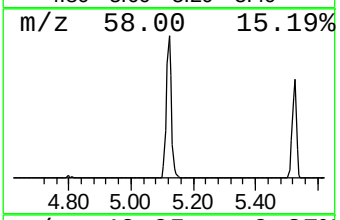


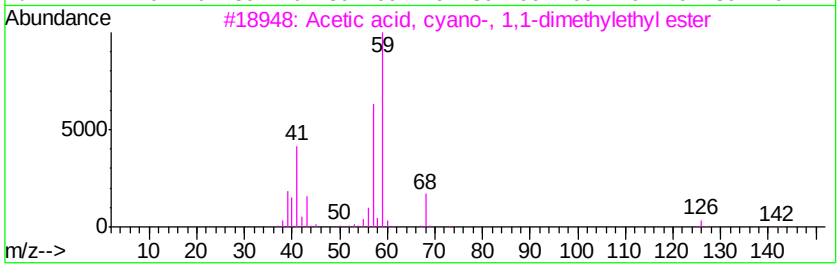


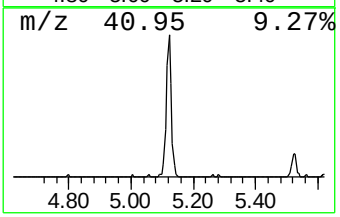












Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : 1-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

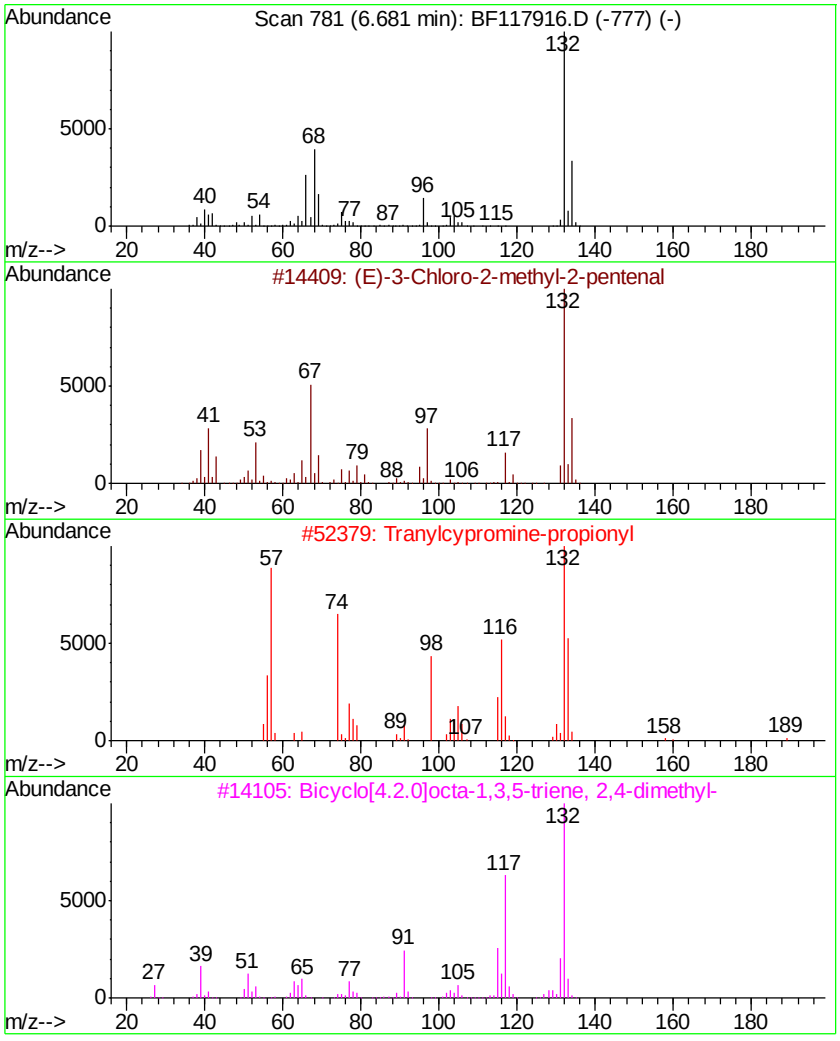
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

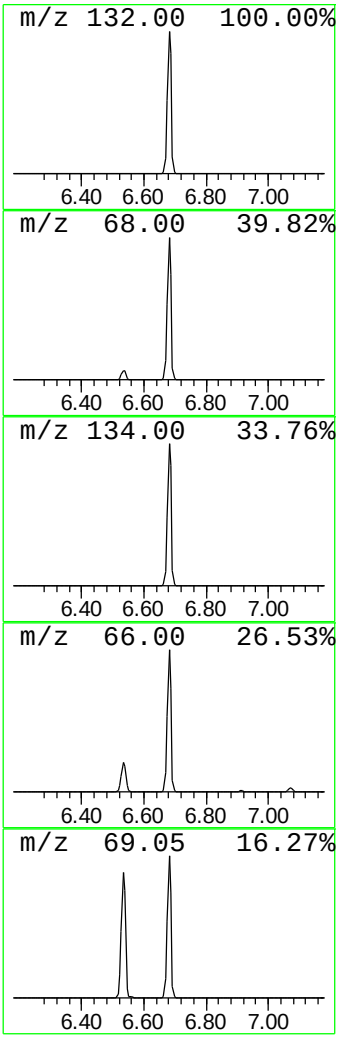
****

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	77.18 ng	3079840	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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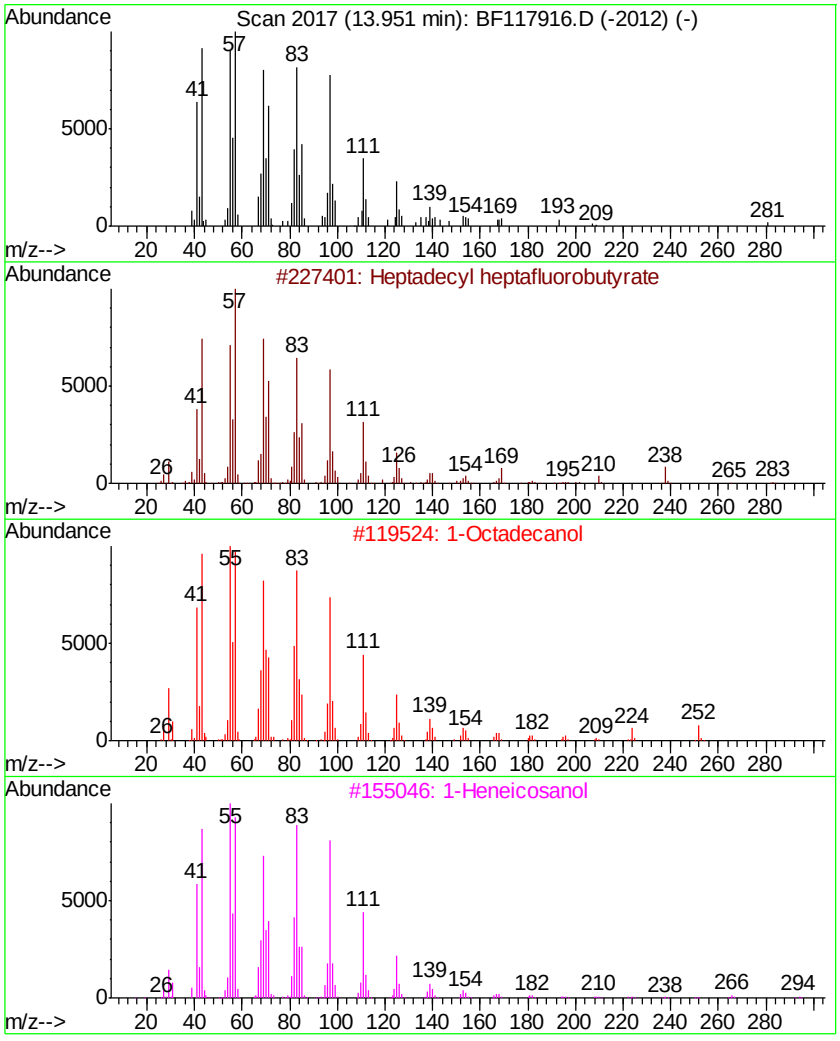
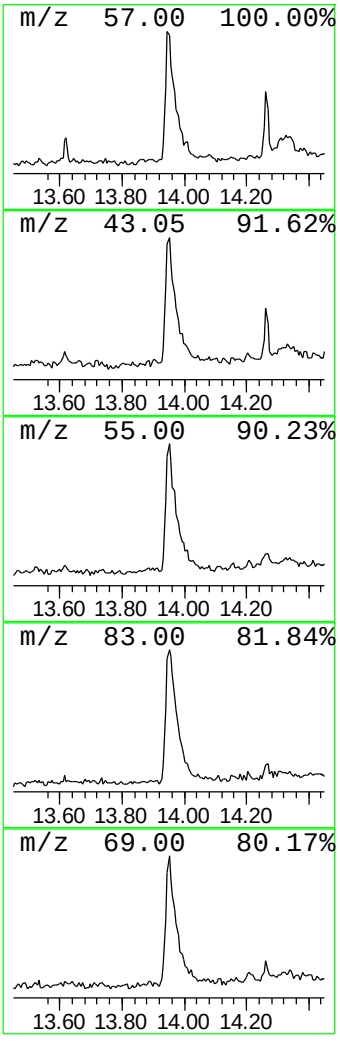
****

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	5.43 ng	349800	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Octadecanol	270	C18H38O	000112-92-5	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90





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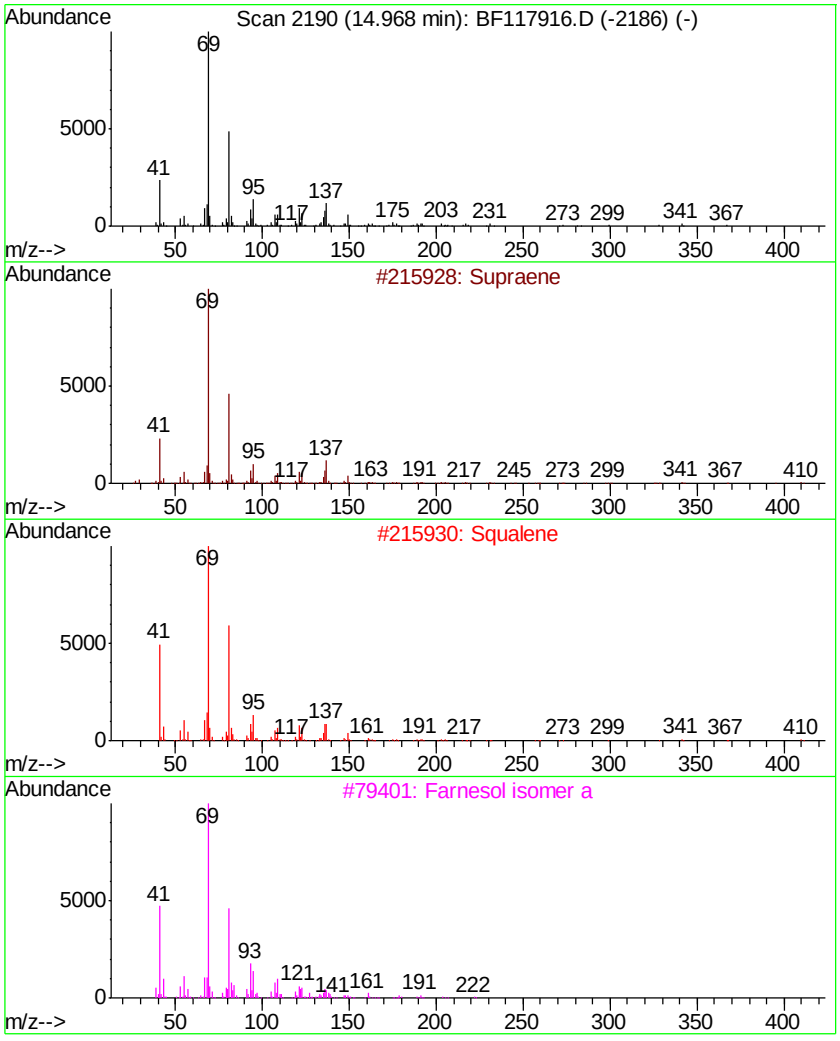
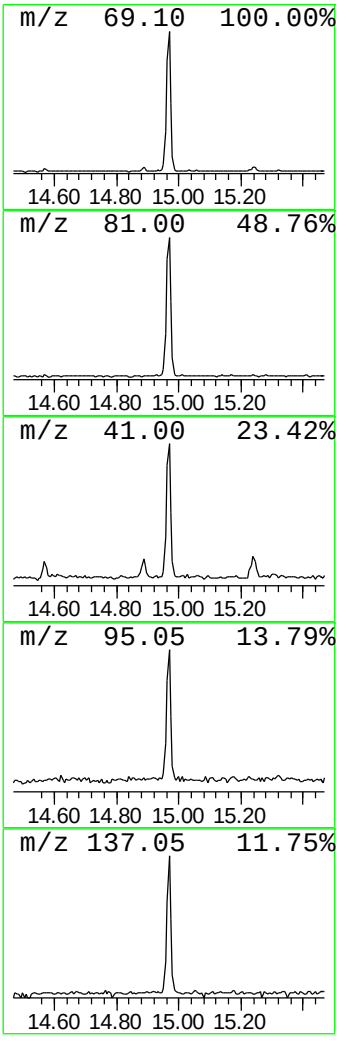
****

Peak Number 6 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	5.55 ng	397791	Perylene-d12	15.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	Farnesol isomer a	222	C15H26O	1000108-92-4	72
4	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.17	27.2	ng	1086680	1	6.92	798062	20.0
2-Pentanone, 4-hy...	5.12	12.4	ng	495512	1	6.92	798062	20.0
unknown6.68	6.68	77.2	ng	3079840	1	6.92	798062	20.0
Heptadecyl heptaf...	13.95	5.4	ng	349800	5	14.10	1288070	20.0
Supraene	14.97	5.5	ng	397791	6	15.62	1434400	20.0