LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051617\
Data File : BF095178.D
Acq On : 17 May 2017 2:56
Operator : SJ/MA
Sample : I3153-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-2-6

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-BF050217.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	5.119	538	541	559	rBV	139424	291554	14.63%	1.870%
2	5.743	644	647	679	rBV	792251	1756220	88.14%	11.261%
3	7.313	910	914	931	rBV	911530	1678090	84.22%	10.760%
4	7.437	931	935	950	rVB	1291737	1992508	100.00%	12.776%
5	7.772	988	992	1005	rVB	348947	432377	21.70%	2.772%
6	8.013	1028	1033	1051	rBV	1187627	1475897	74.07%	9.464%
7	8.672	1140	1145	1158	rBV	731427	1020251	51.20%	6.542%
8	9.789	1331	1335	1350	rBV	480386	649953	32.62%	4.168%
9	11.560	1631	1636	1647	rBV	1414514	1711439	85.89%	10.974%
10	11.660	1650	1653	1659	rVB3	25595	32170	1.61%	0.206%
11	11.854	1680	1686	1689	rBV7	17979	37912	1.90%	0.243%
12	12.254	1750	1754	1764	rBV	115955	226863	11.39%	1.455%
13	12.466	1787	1790	1795	rBV6	40411	61507	3.09%	0.394%
14	12.619	1809	1816	1823	rBV2	378887	600347	30.13%	3.850%
15	13.924	2033	2038	2046	rBV	472372	729547	36.61%	4.678%
16	15.030	2222	2226	2233	rVB	326115	412589	20.71%	2.646%
17	15.995	2387	2390	2393	rVB2	147527	183134	9.19%	1.174%
18	17.348	2615	2620	2628	rVB	1111137	1321271	66.31%	8.472%
19	18.695	2845	2849	2854	rBV	408722	440745	22.12%	2.826%
20	19.812	3036	3039	3042	rVB	53560	53190	2.67%	0.341%
21	20.371	3129	3134	3144	rBV	280386	403768	20.26%	2.589%
22	20.647	3178	3181	3187	rBV8	25349	59649	2.99%	0.382%
23	21.053	3247	3250	3253	rBV5	14942	24275	1.22%	0.156%

Sum of corrected areas: 15595256

LSC Report - Integrated Chromatogram

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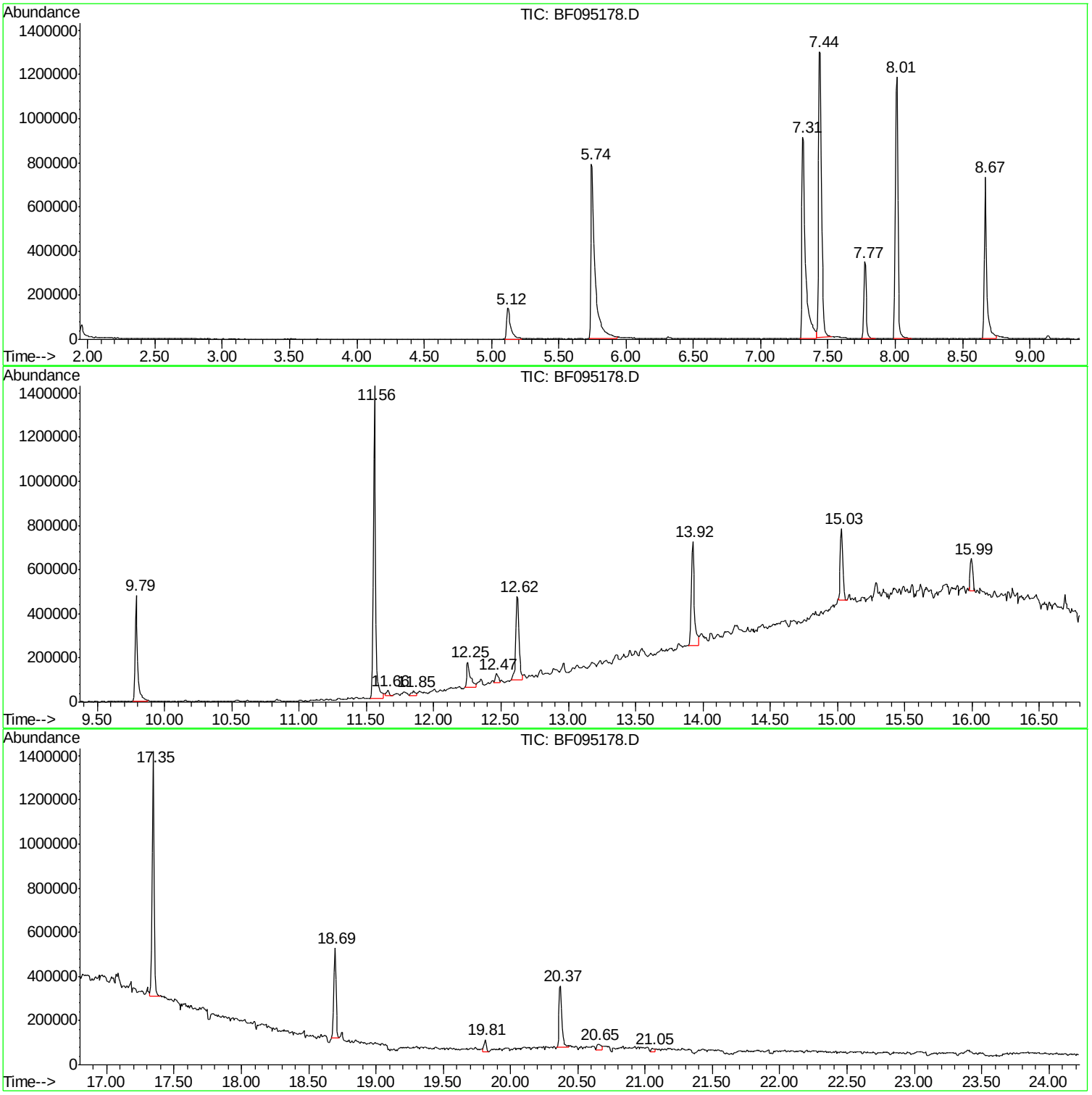
Instrument : BNA_F
ClientSampleId : DS-2-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051617\
Data File : BF095178.D
Acq On : 17 May 2017 2:56
Operator : SJ/MA
Sample : I3153-04
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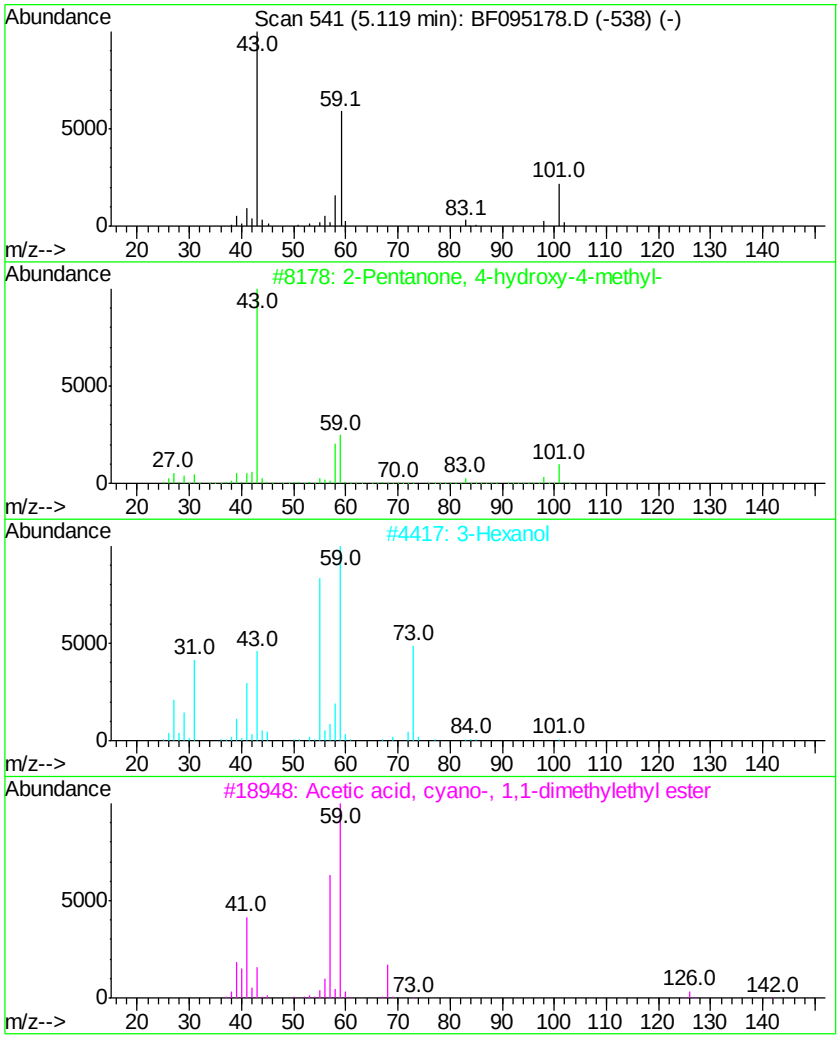
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

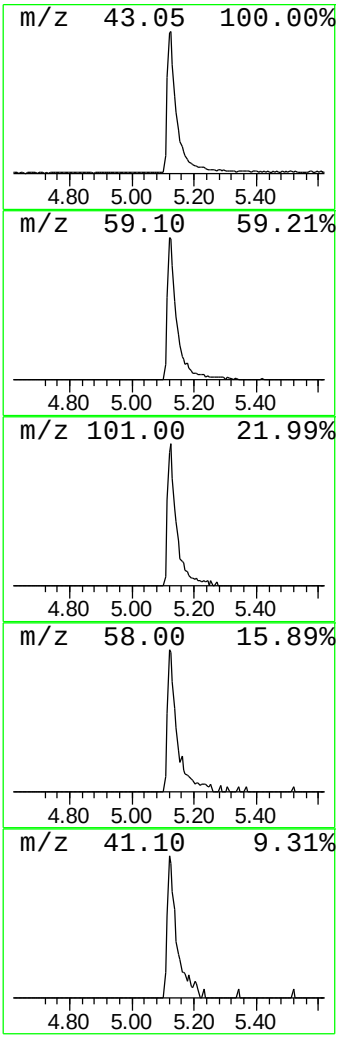
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	13.49 ng	291554	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol	102	C6H14O	000623-37-0	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Sample : I3153-04
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Instrument : BNA_F
ClientSampleId : DS-2-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

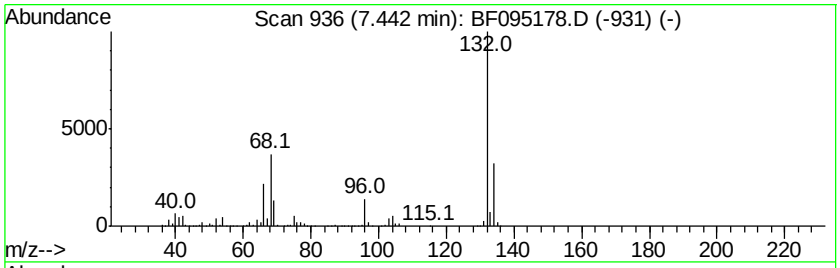
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

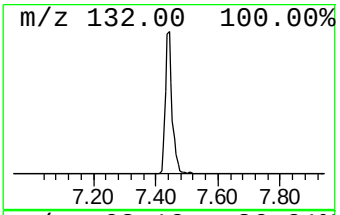
****

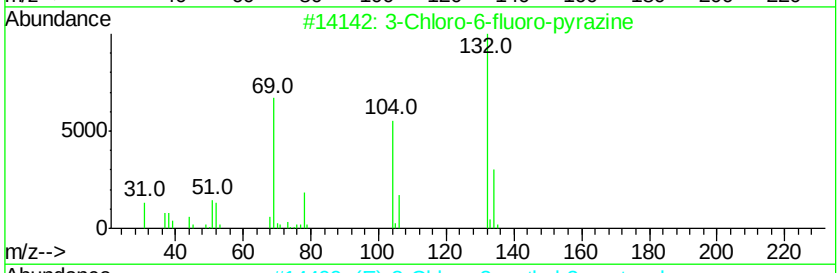
Peak Number 2 unknown7.44 Concentration Rank 1

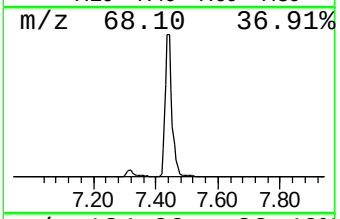
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	92.17 ng	1992510	1,4-Dichlorobenzene-d4	7.77

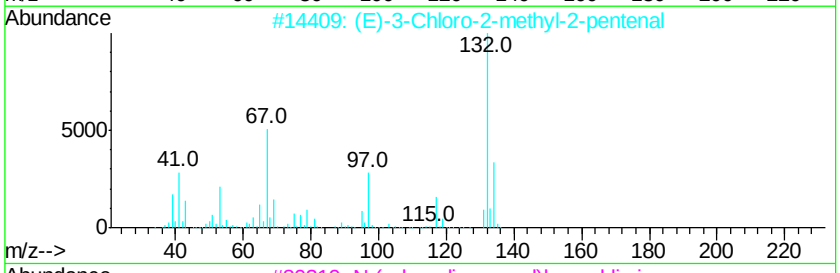
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	12

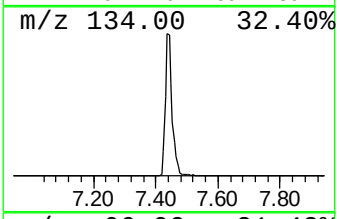


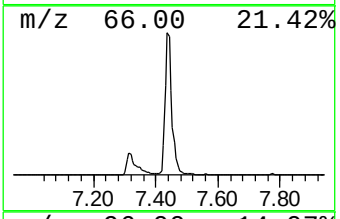


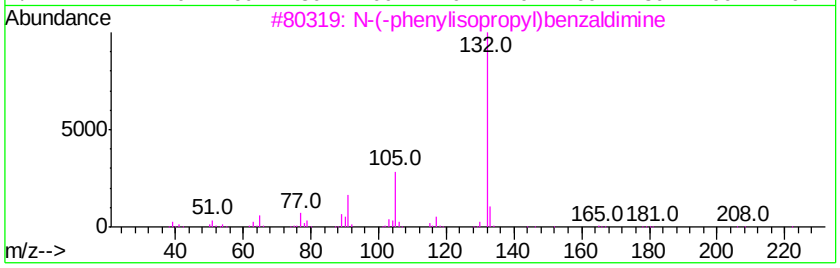


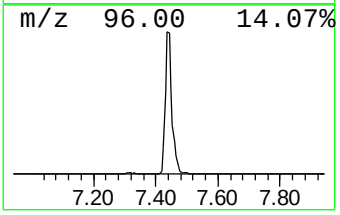












Library Search Compound Report

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Operator : SJ/MA
Sample : I3153-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-2-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

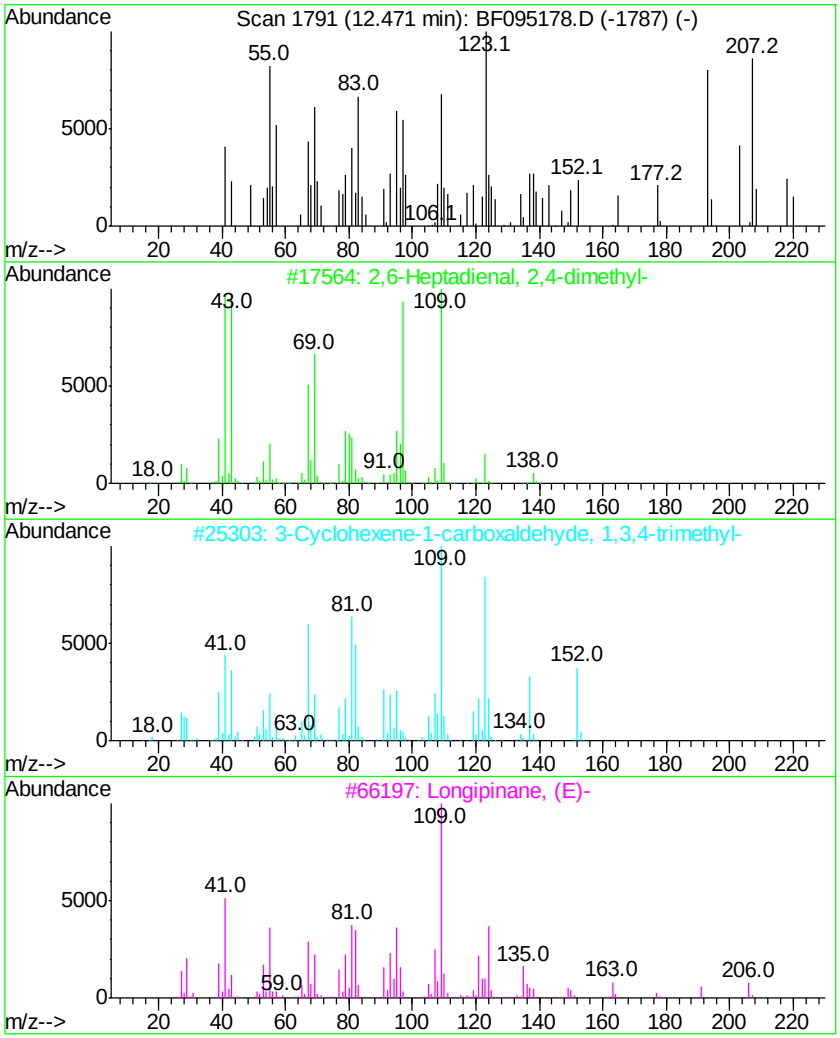
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

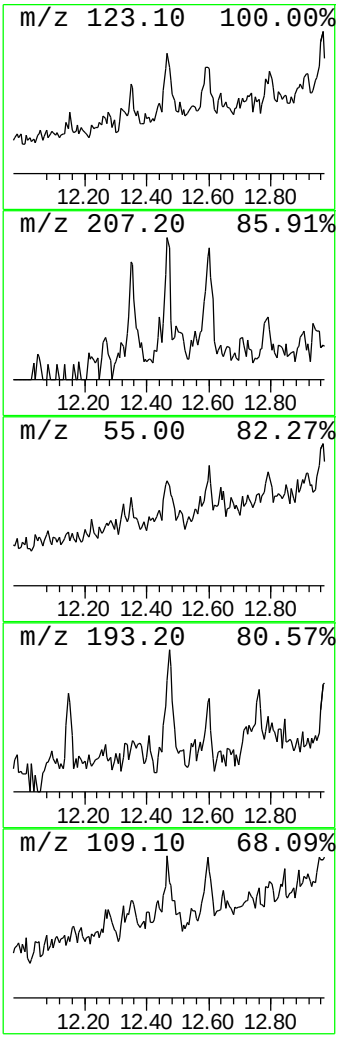
****

Peak Number 4 unknown12.47 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	2.05 ng	61507	Acenaphthene-d10	12.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	38
2	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	35
3	Longipinane, (E)-	206	C15H26	1000156-14-5	25
4	Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	15
5	1a,2,5,5-Tetramethyl-cis-1a,4a,5...	194	C13H22O	1000215-77-7	14





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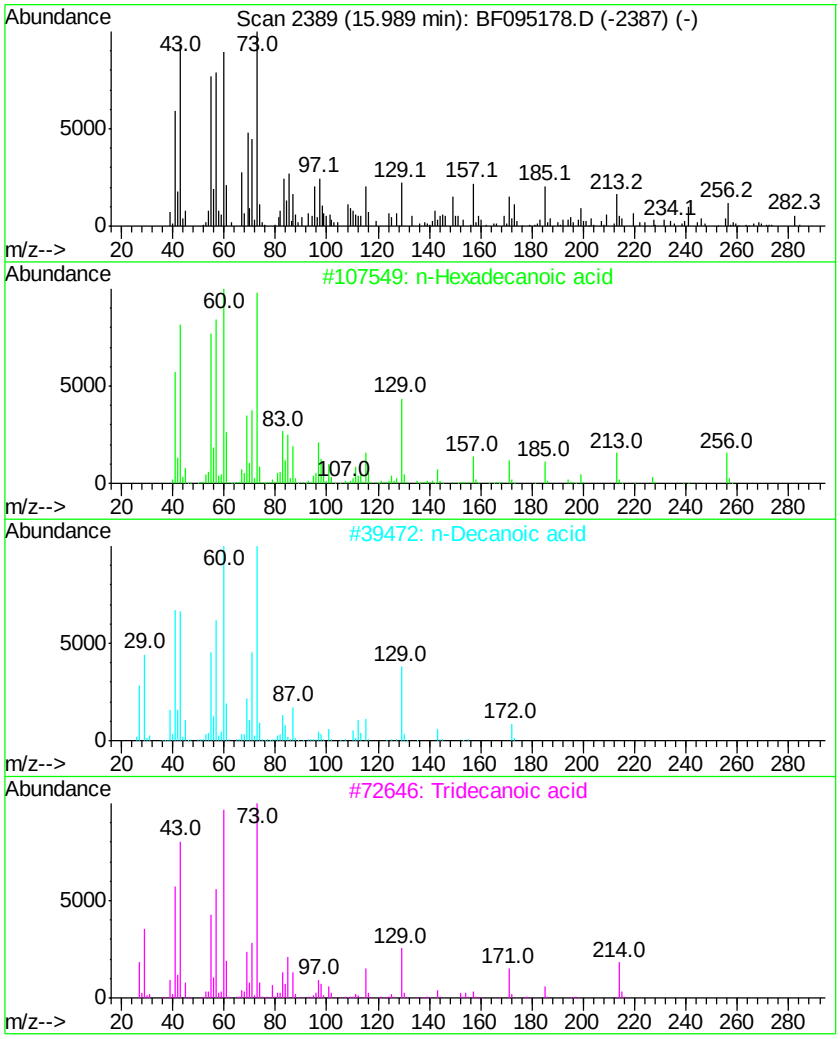
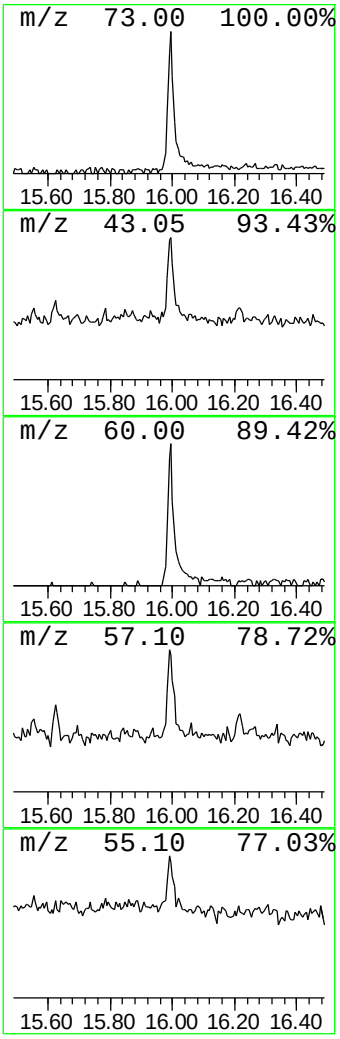
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	8.88 ng	183134	Phenanthrene-d10	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	n-Decanoic acid	172	C10H20O2	000334-48-5	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	60
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	49





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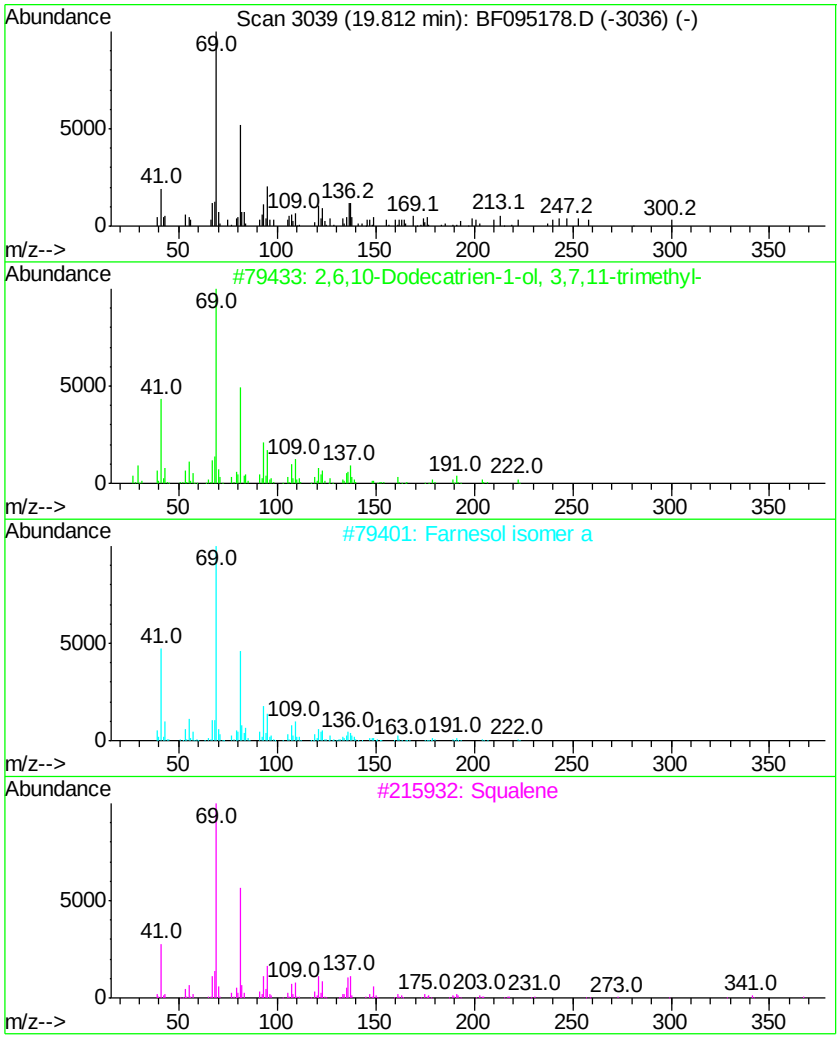
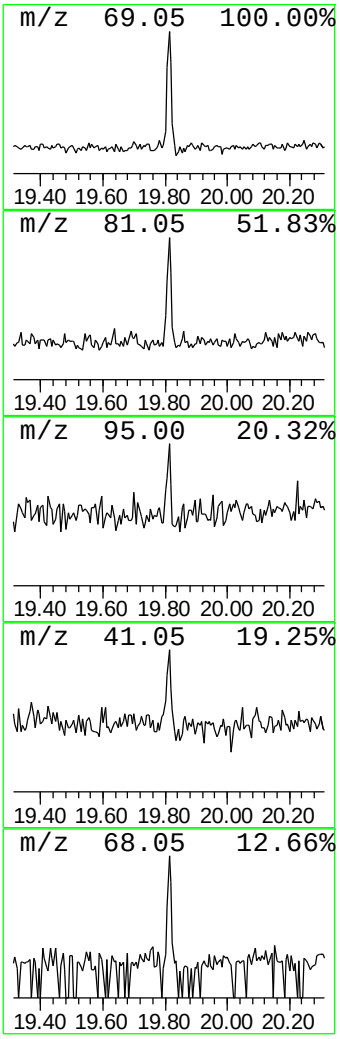
****

Peak Number 6 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.81	2.63 ng	53190	Perylene-d12	20.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	86
2	Farnesol isomer a	222	C15H26O	1000108-92-4	86
3	Squalene	410	C30H50	000111-02-4	81
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72





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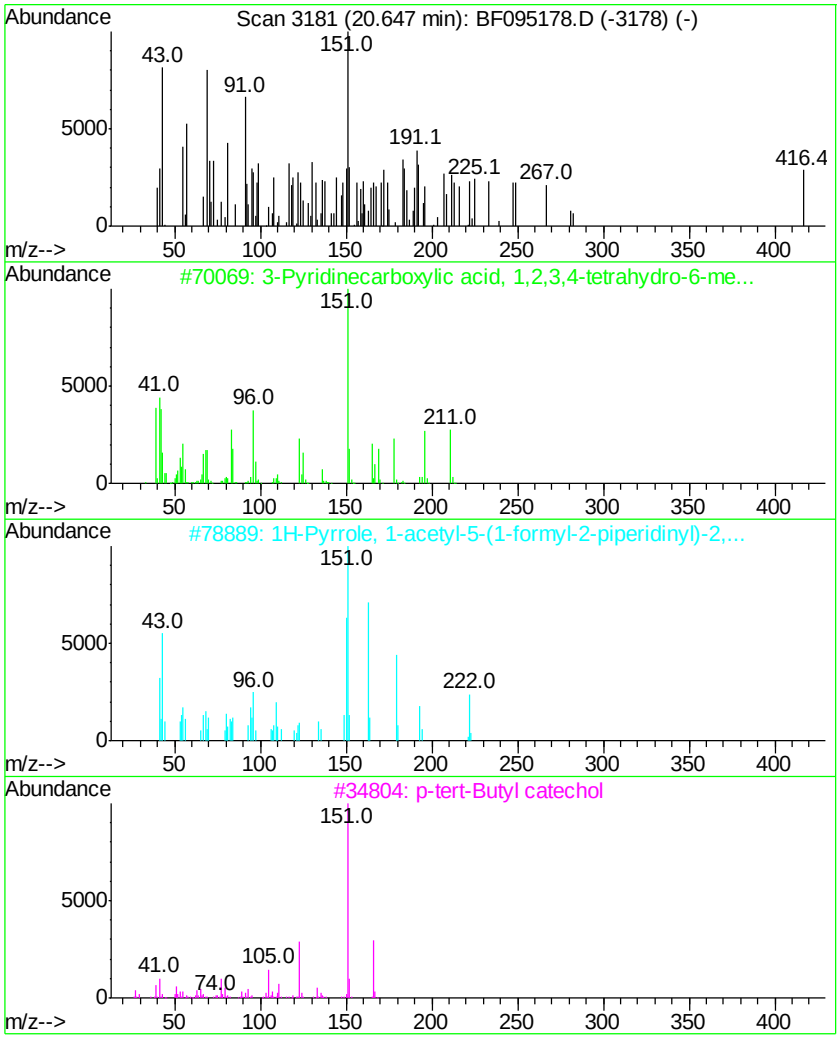
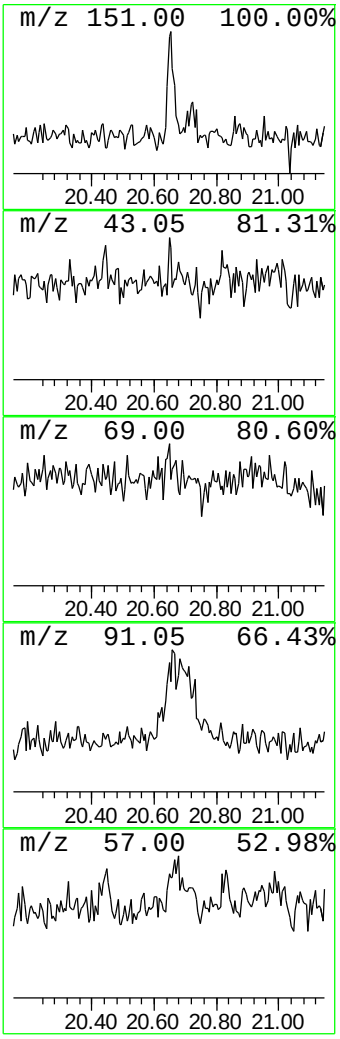
****

Peak Number 7 unknown20.65 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.65	2.95 ng	59649	Perylene-d12	20.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pyridinecarboxylic acid, 1,2,3...	211	C10H13NO4	1000318-75-3	25
2	1H-Pyrrole, 1-acetyl-5-(1-formyl...	222	C12H18N2O2	055028-85-8	12
3	p-tert-Butyl catechol	166	C10H14O2	000098-29-3	11
4	1H-Benzocyclohepten-7-ol, 2,3,4,...	222	C15H26O	006892-80-4	11
5	Benzenemethanol, 2-(dimethylamino)-	151	C9H13NO	004707-56-6	10





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	13.5	ng	291554	1	7.77	432377	20.0
unknown7.44	7.44	92.2	ng	1992510	1	7.77	432377	20.0
unknown12.47	12.47	2.0	ng	61507	3	12.62	600347	20.0
n-Hexadecanoic acid	15.99	8.9	ng	183134	4	15.03	412589	20.0
2,6,10-Dodecatrie...	19.81	2.6	ng	53190	6	20.37	403768	20.0
unknown20.65	20.65	3.0	ng	59649	6	20.37	403768	20.0