LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100956.D
Acq On : 29 Nov 2017 2:09
Operator : SJ/JU
Sample : I6579-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(7-8)

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	5.093	507	511	523	rBV	173135	256108	14.38%	1.713%
2	5.487	573	578	581	rBV	1767882	1746972	98.09%	11.687%
3	6.493	744	749	752	rBV	1548865	1758096	98.72%	11.761%
4	6.634	768	773	776	rBV	1829153	1780977	100.00%	11.914%
5	6.857	808	811	815	rBV	483822	375621	21.09%	2.513%
6	7.016	834	838	841	rBV	1579589	1350178	75.81%	9.032%
7	7.422	902	907	910	rBV	1004881	1059404	59.48%	7.087%
8	8.139	1025	1029	1032	rBV	585053	455008	25.55%	3.044%
9	8.692	1120	1123	1127	rBV	84329	63698	3.58%	0.426%
10	9.216	1207	1212	1215	rBV	2005289	1699520	95.43%	11.369%
11	9.604	1275	1278	1283	rBV	56435	43792	2.46%	0.293%
12	9.892	1324	1327	1331	rBV	453996	427443	24.00%	2.860%
13	10.610	1445	1449	1452	rBV	262192	242053	13.59%	1.619%
14	10.686	1458	1462	1465	rBV	971582	885719	49.73%	5.925%
15	11.380	1577	1580	1583	rBV	461527	373882	20.99%	2.501%
16	11.898	1665	1668	1673	rBV	49737	44318	2.49%	0.296%
17	12.592	1783	1786	1791	rVB	27569	24377	1.37%	0.163%
18	12.822	1821	1825	1828	rVB	24827	22815	1.28%	0.153%
19	12.969	1845	1850	1853	rBV	1440237	1342095	75.36%	8.978%
20	13.422	1924	1927	1934	rBV4	21669	30927	1.74%	0.207%
21	13.857	1998	2001	2008	rBV2	36789	47955	2.69%	0.321%
22	14.021	2024	2029	2032	rBV	471218	432372	24.28%	2.892%
23	15.063	2202	2206	2208	rBV3	18311	25457	1.43%	0.170%
24	15.492	2274	2279	2289	rBV	276820	357724	20.09%	2.393%
25	16.439	2434	2440	2446	rBV5	22758	45454	2.55%	0.304%
26	17.557	2622	2630	2636	rBV8	10750	29765	1.67%	0.199%
27	18.045	2709	2713	2723	rVB9	9747	26429	1.48%	0.177%

Sum of corrected areas: 14948159

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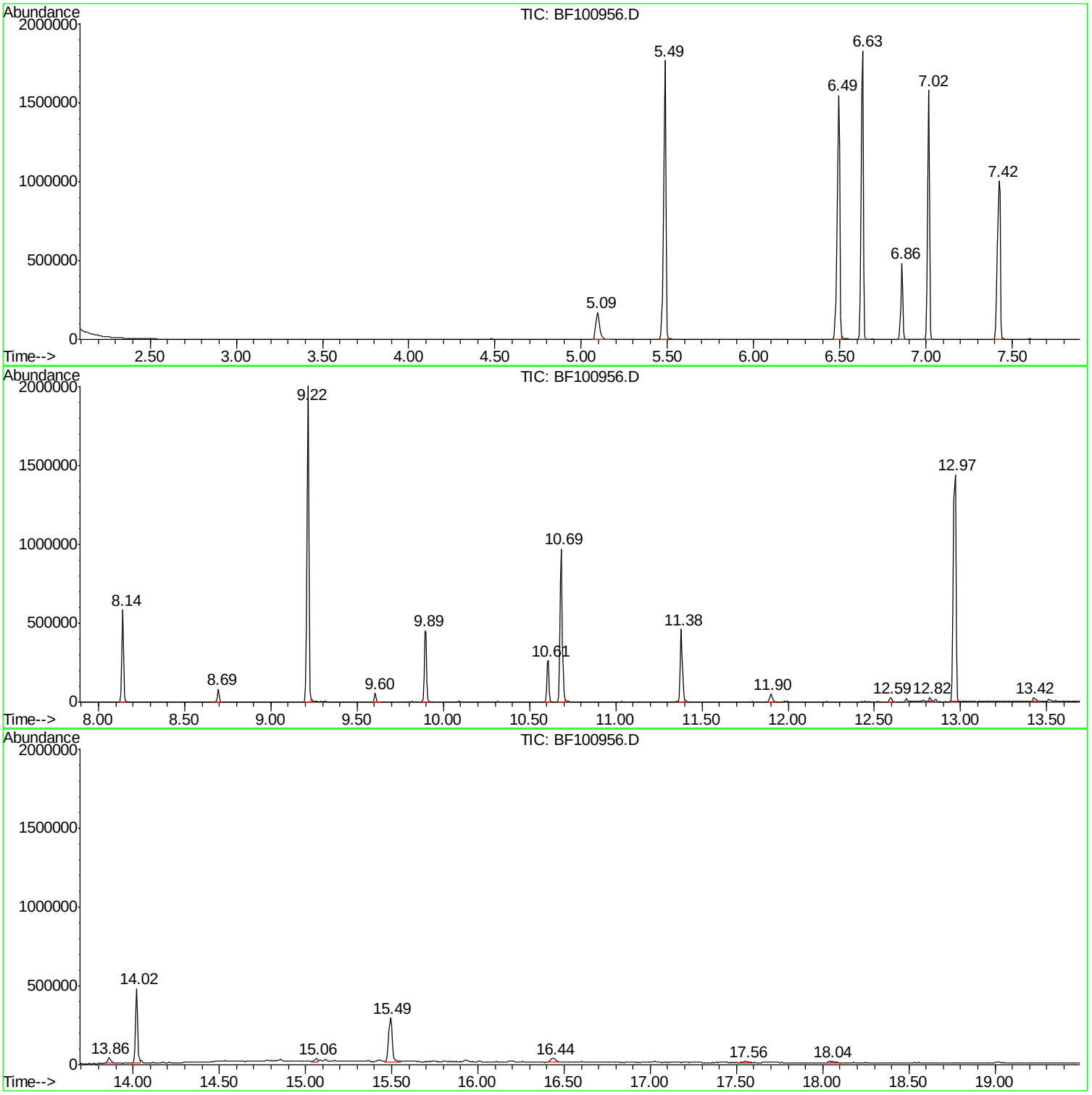
HAR-3-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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Instrument : BNA_F
ClientSampleId : HAR-3-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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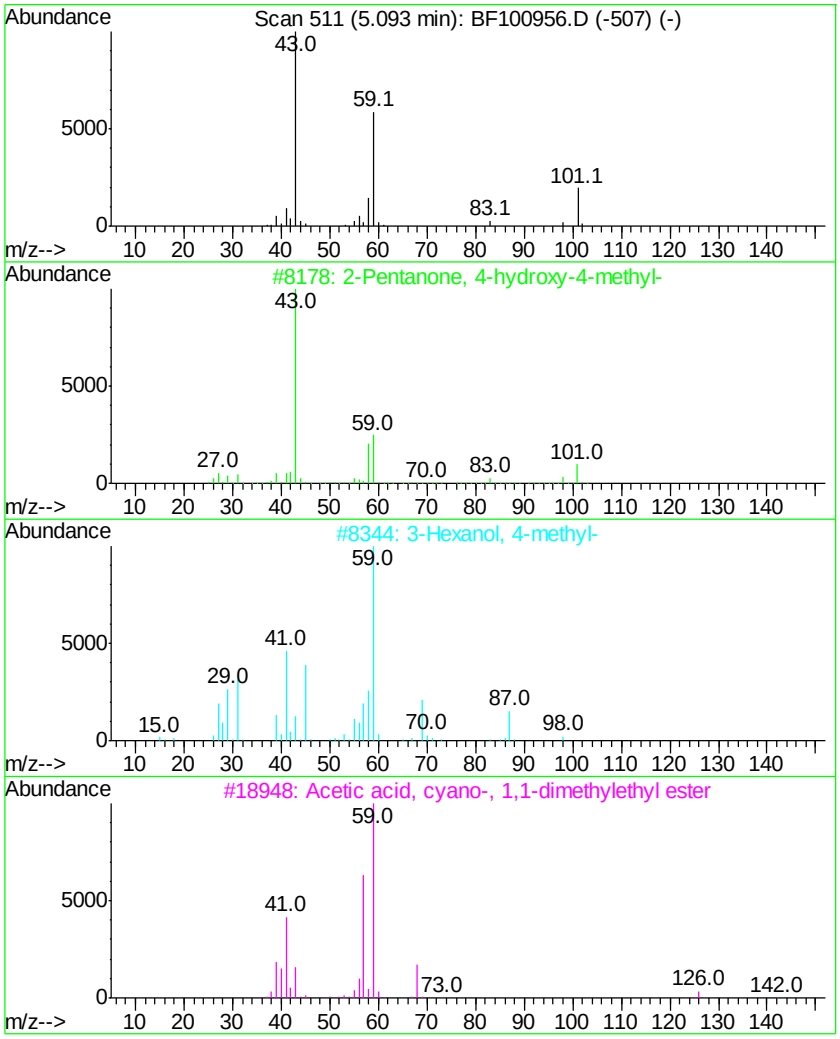
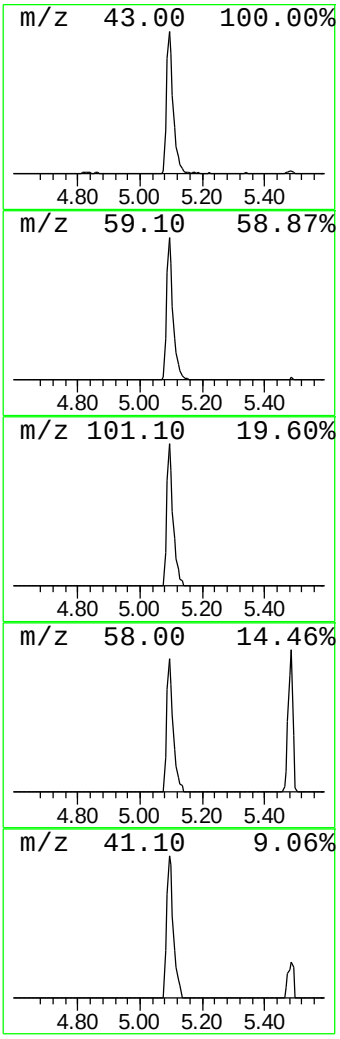
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	13.64 ng	256108	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	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butane	58	C4H10	000106-97-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument : BNA_F
ClientSampleId : HAR-3-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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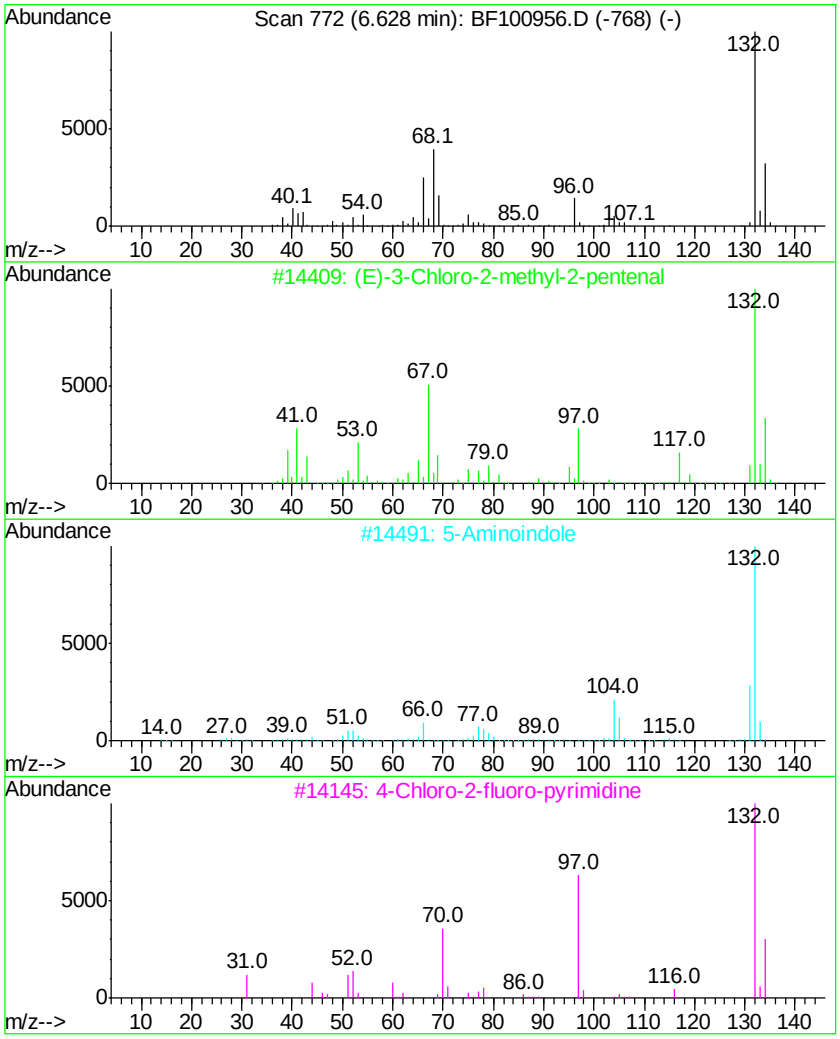
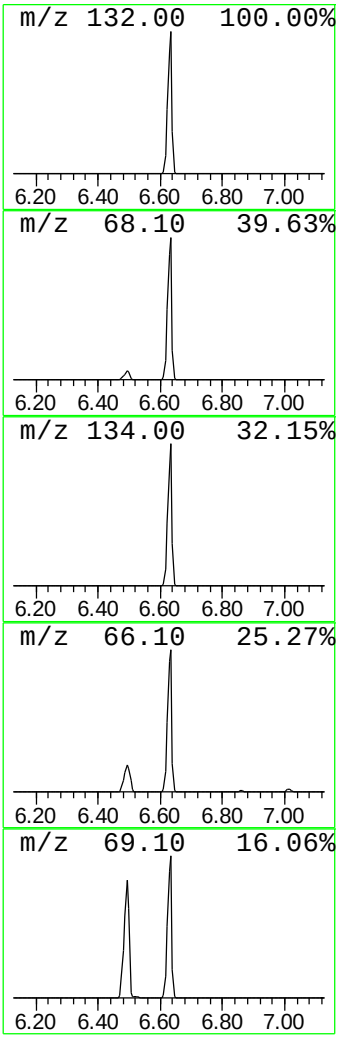
Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	94.83 ng	1780980	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Sample : I6579-08
Misc :
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Instrument : BNA_F
ClientSampleId : HAR-3-E(7-8)

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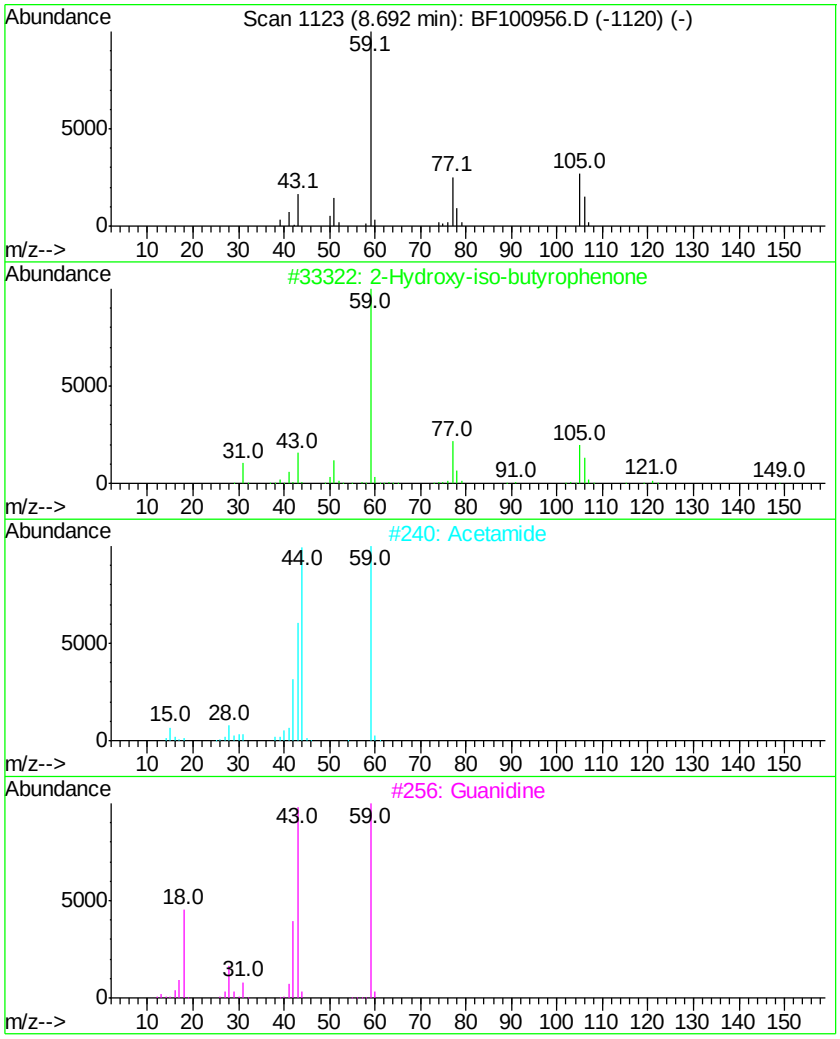
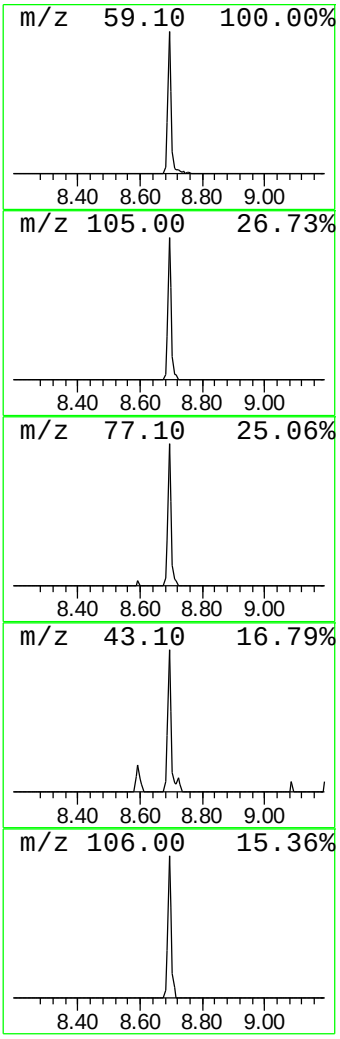
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	2.80 ng	63698	Naphthalene-d8	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Acetamide	59	C2H5NO	000060-35-5	5
3	Guanidine	59	CH5N3	000113-00-8	5
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	4
5	Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	4





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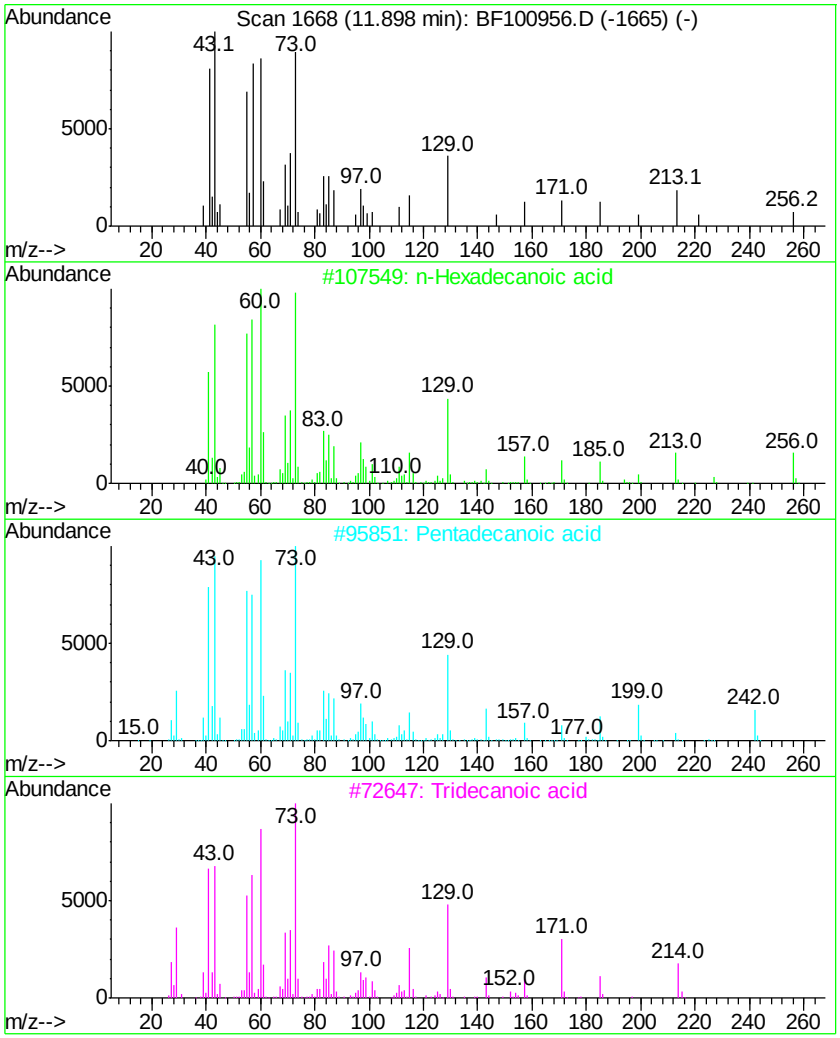
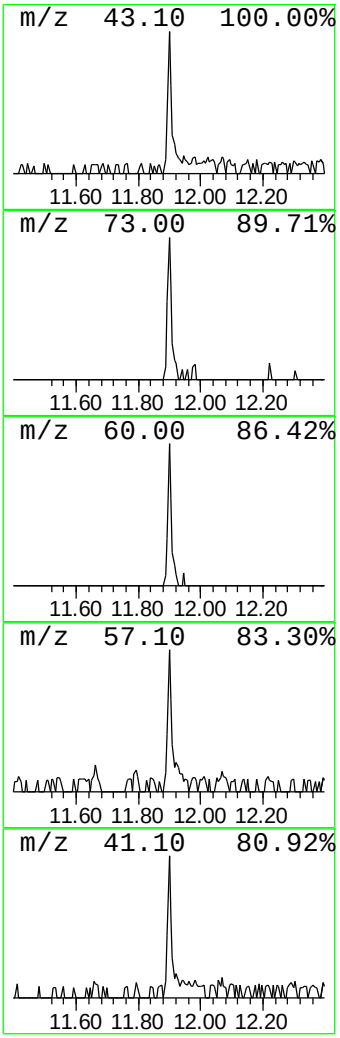
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.37 ng	44318	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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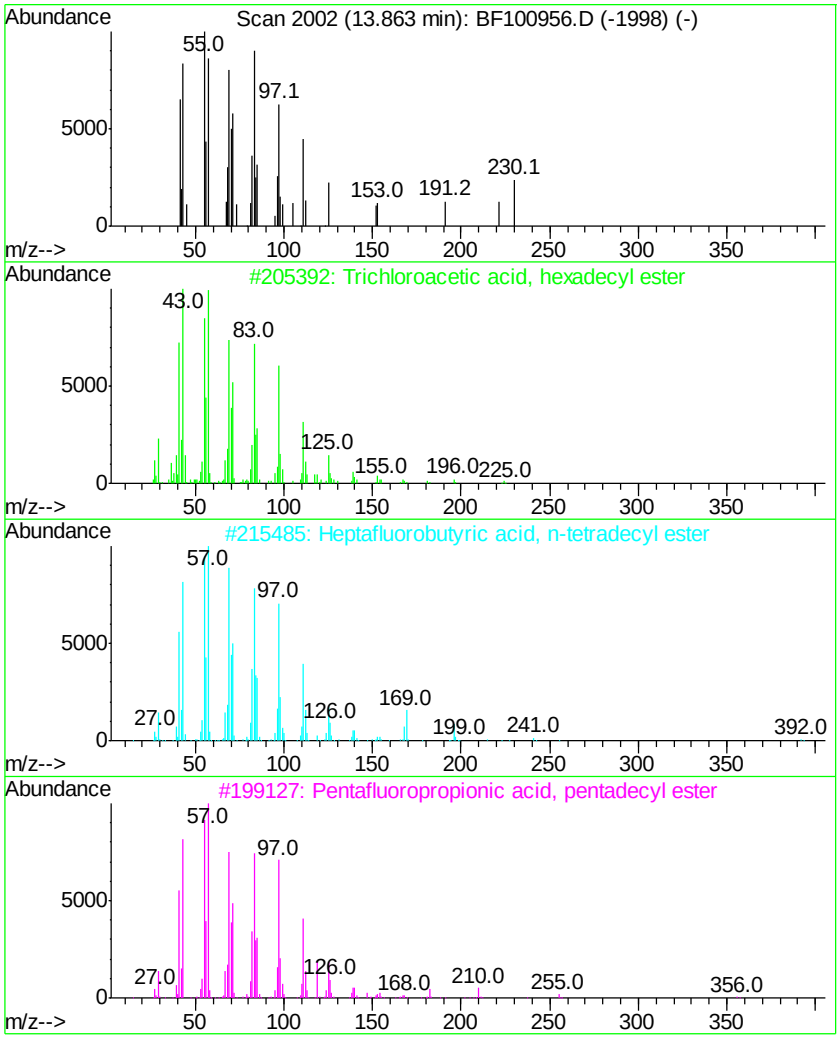
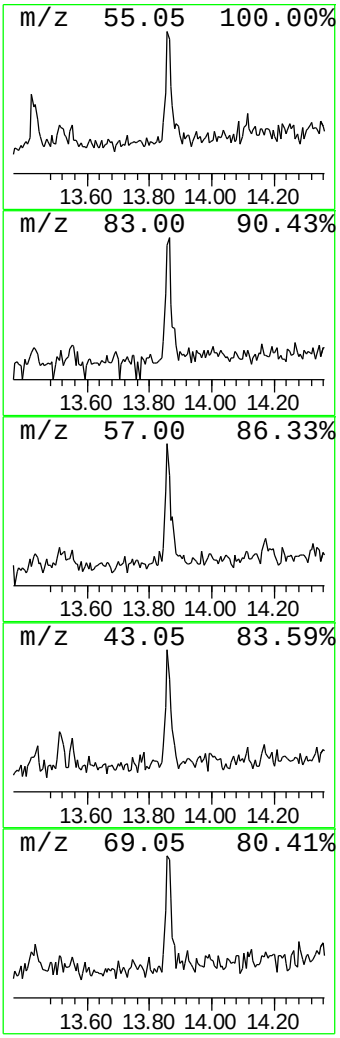
Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.22 ng	47955	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





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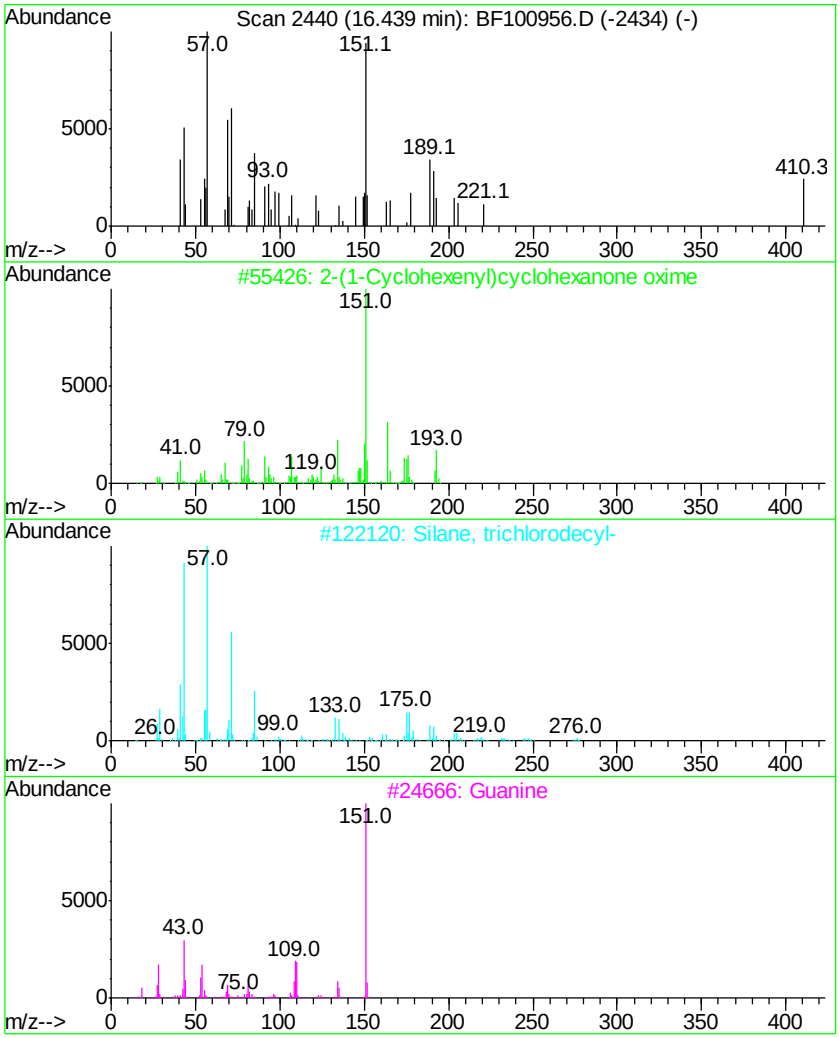
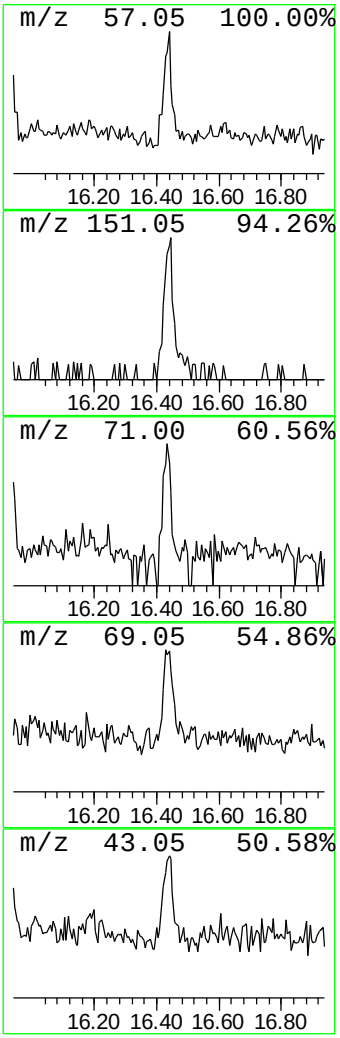
Peak Number 8 unknown16.44 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	2.54 ng	45454	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(1-Cyclohexenyl)cyclohexanone ...	193	C12H19NO	037575-86-3	22
2	Silane, trichlorodecyl-	274	C10H21Cl3Si	013829-21-5	22
3	Guanine	151	C5H5N5O	000073-40-5	14
4	Benzene, 1,1'-[1,2-ethanediylbis...	274	C16H18O4	000553-45-7	14
5	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	14





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
2-Pentanone, 4-hy...	5.09	13.6	ng	256108	1	6.86	375621	20.0
unknown6.63	6.63	94.8	ng	1780980	1	6.86	375621	20.0
2-Hydroxy-iso-but...	8.69	2.8	ng	63698	2	8.14	455008	20.0
n-Hexadecanoic acid	11.90	2.4	ng	44318	4	11.38	373882	20.0
Trichloroacetic a...	13.86	2.2	ng	47955	5	14.02	432372	20.0
unknown16.44	16.44	2.5	ng	45454	6	15.49	357724	20.0