LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
Data File : BF094277.D
Acq On : 7 Apr 2017 17:17
Operator : SJ/MA
Sample : I2585-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 22A

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-BF032217.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	3.975	351	355	361	rBV	244337	251383	4.91%	0.764%
2	4.375	419	423	427	rBV	1892425	1824533	35.62%	5.547%
3	4.698	475	478	484	rBV	144431	140478	2.74%	0.427%
4	5.445	601	605	613	rVB	1277297	1157657	22.60%	3.520%
5	5.592	624	630	633	rBV	3259172	3464301	67.63%	10.533%
6	5.845	668	673	676	rBV	963663	921553	17.99%	2.802%
7	6.022	698	703	707	rBV	3282816	3503956	68.40%	10.654%
8	6.498	777	784	787	rBV	2451167	2891286	56.44%	8.791%
9	7.345	923	928	932	rBV	1338871	1269277	24.78%	3.859%
10	7.416	936	940	948	rVB5	35142	57889	1.13%	0.176%
11	8.586	1136	1139	1143	rBV2	56321	75909	1.48%	0.231%
12	8.675	1147	1154	1157	rVB	4519221	5122373	100.00%	15.574%
13	9.163	1234	1237	1243	rBV	85949	98843	1.93%	0.301%
14	9.486	1286	1292	1296	rBV	1310760	1349262	26.34%	4.102%
15	9.810	1341	1347	1350	rBV3	61688	85927	1.68%	0.261%
16	10.039	1382	1386	1389	rVB2	62320	63569	1.24%	0.193%
17	10.463	1451	1458	1461	rBV	2349257	2700855	52.73%	8.212%
18	11.310	1597	1602	1606	rBV	1297748	1275088	24.89%	3.877%
19	12.045	1723	1727	1732	rBV2	207671	246268	4.81%	0.749%
20	13.027	1890	1894	1897	rBV	162387	167830	3.28%	0.510%
21	13.110	1905	1908	1915	rVB	271490	280412	5.47%	0.853%
22	13.292	1933	1939	1943	rBV2	3279550	4028218	78.64%	12.248%
23	14.557	2150	2154	2159	rBV	943218	1025303	20.02%	3.117%
24	15.415	2297	2300	2305	rVB	129945	137866	2.69%	0.419%
25	16.192	2427	2432	2438	rVB	627637	749452	14.63%	2.279%

Sum of corrected areas: 32889488

LSC Report - Integrated Chromatogram

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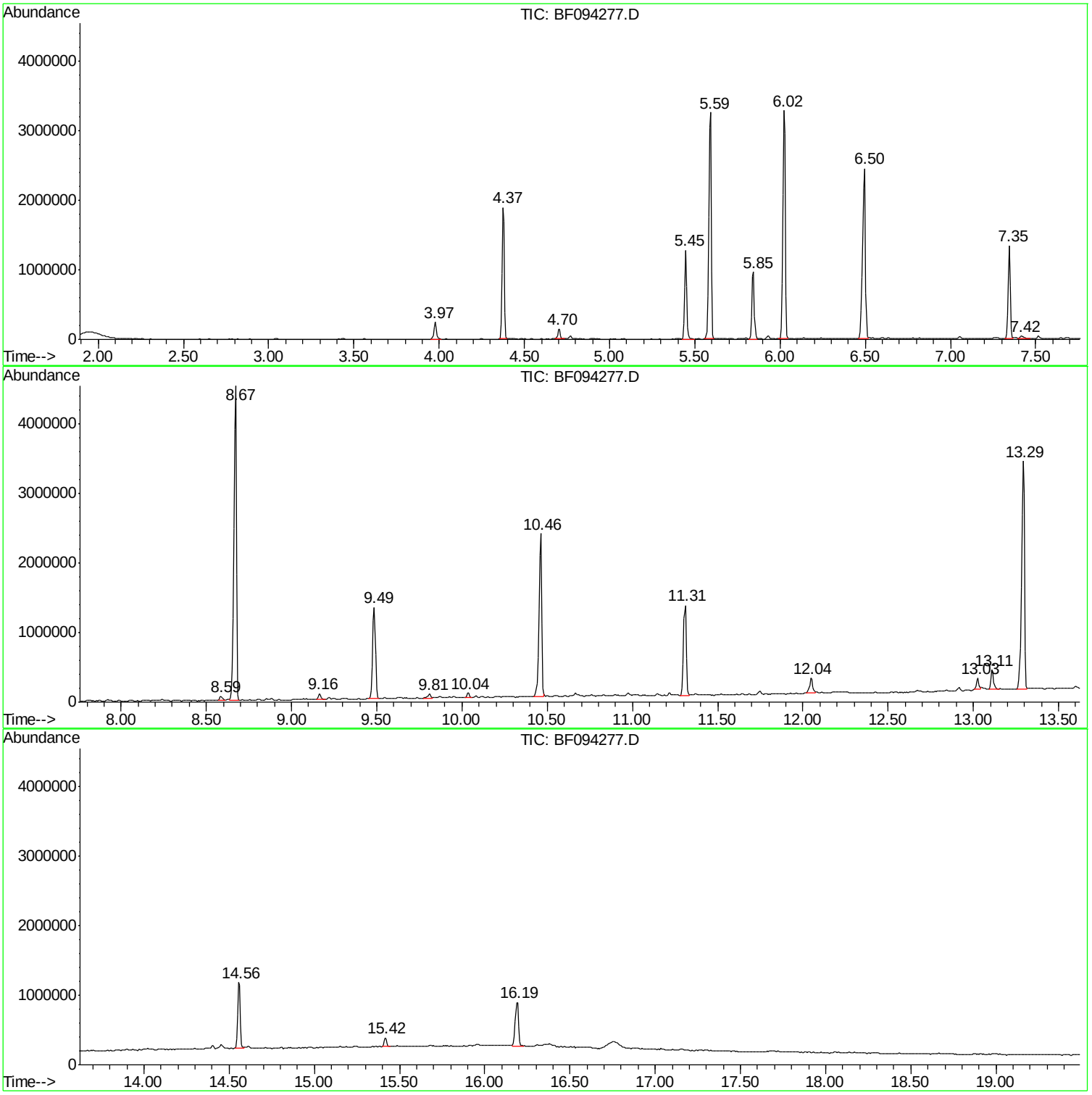
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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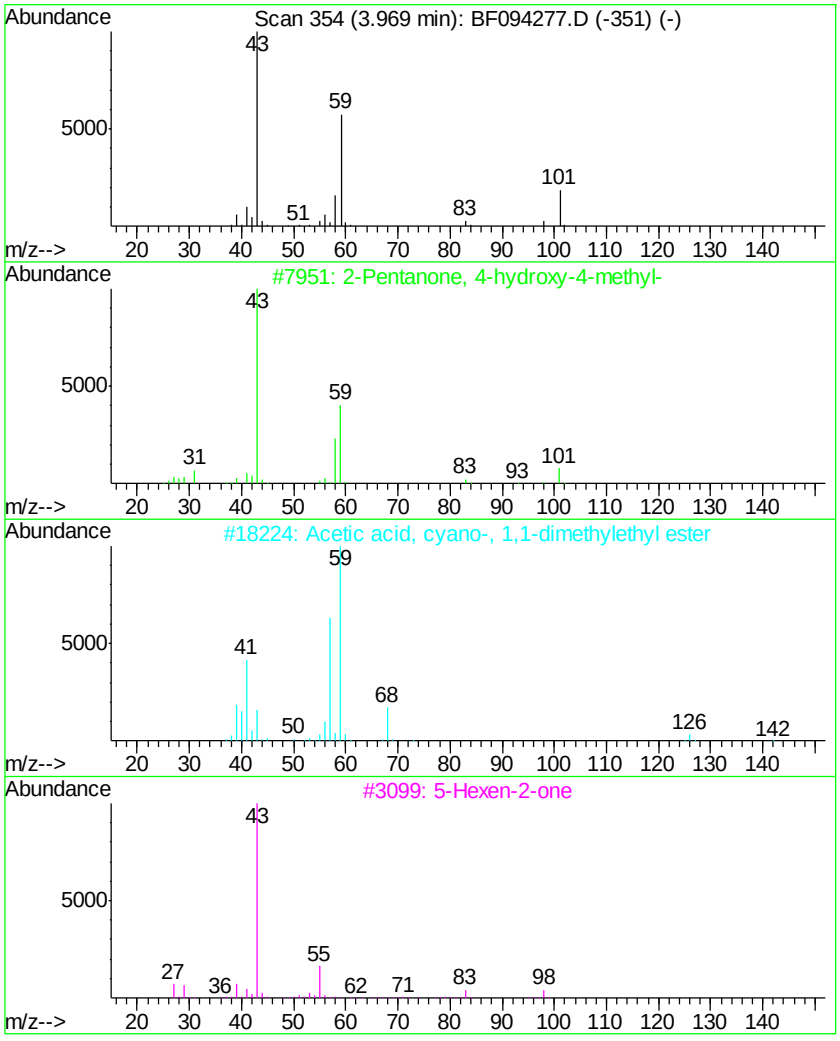
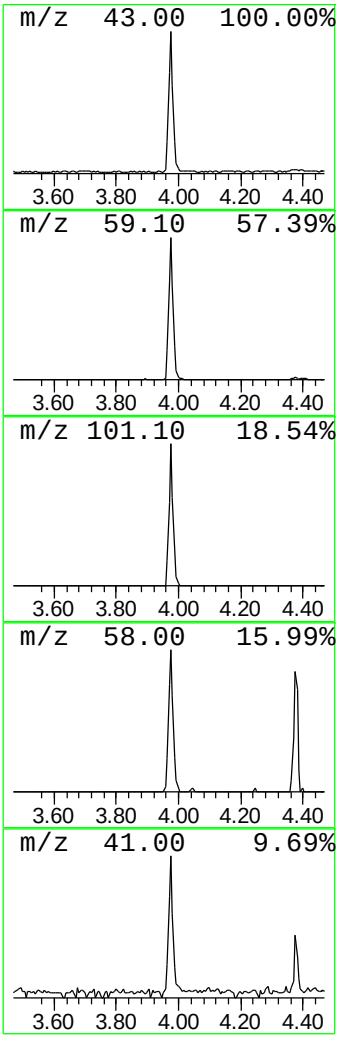
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.97	5.46 ng	251383	1,4-Dichlorobenzene-d4	5.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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ClientSampleId : 22A

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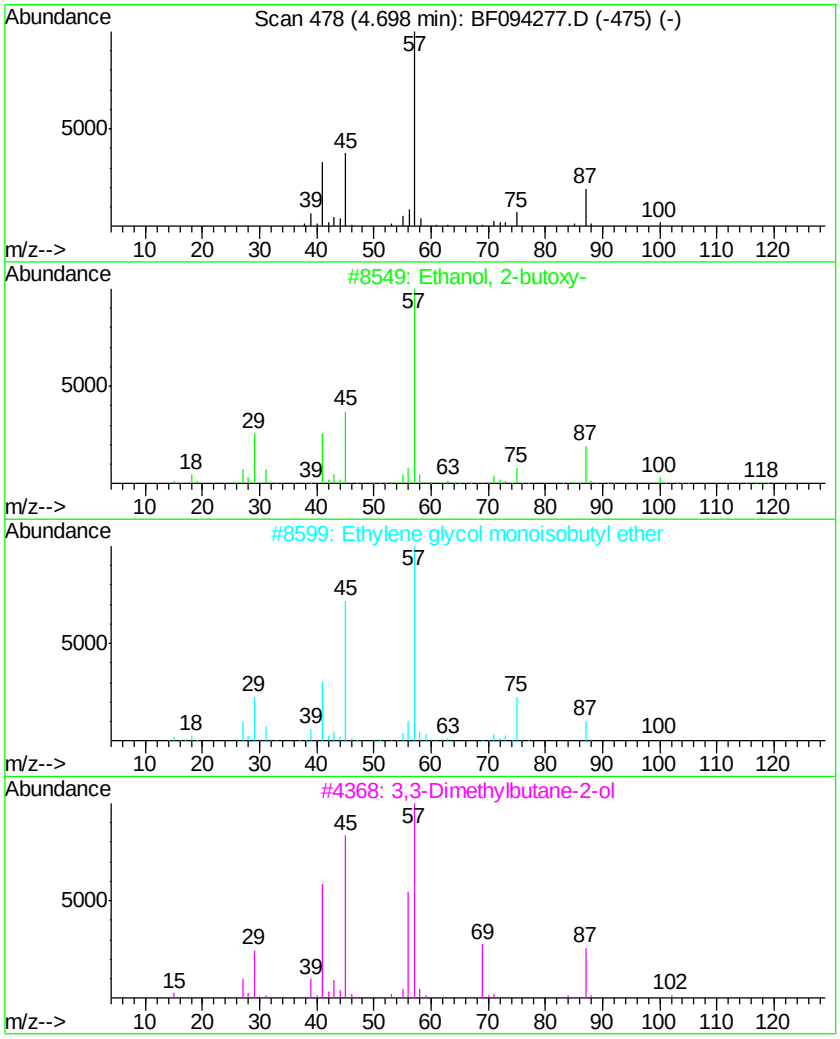
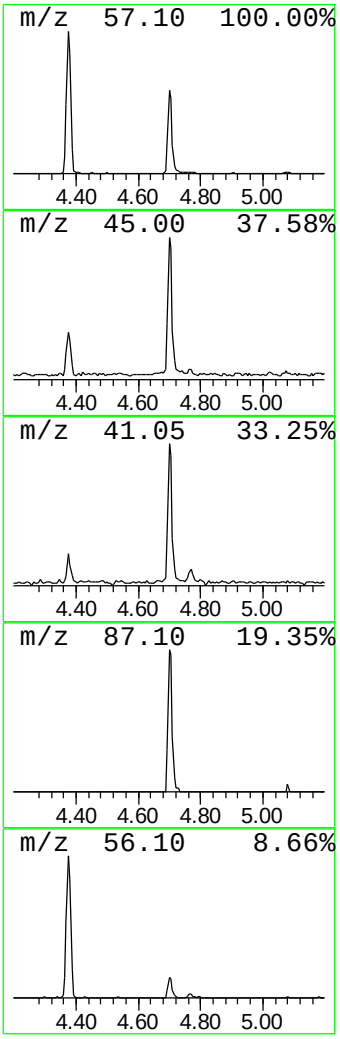
Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	3.05 ng	140478	1,4-Dichlorobenzene-d4	5.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	23
4	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	16
5	1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	12





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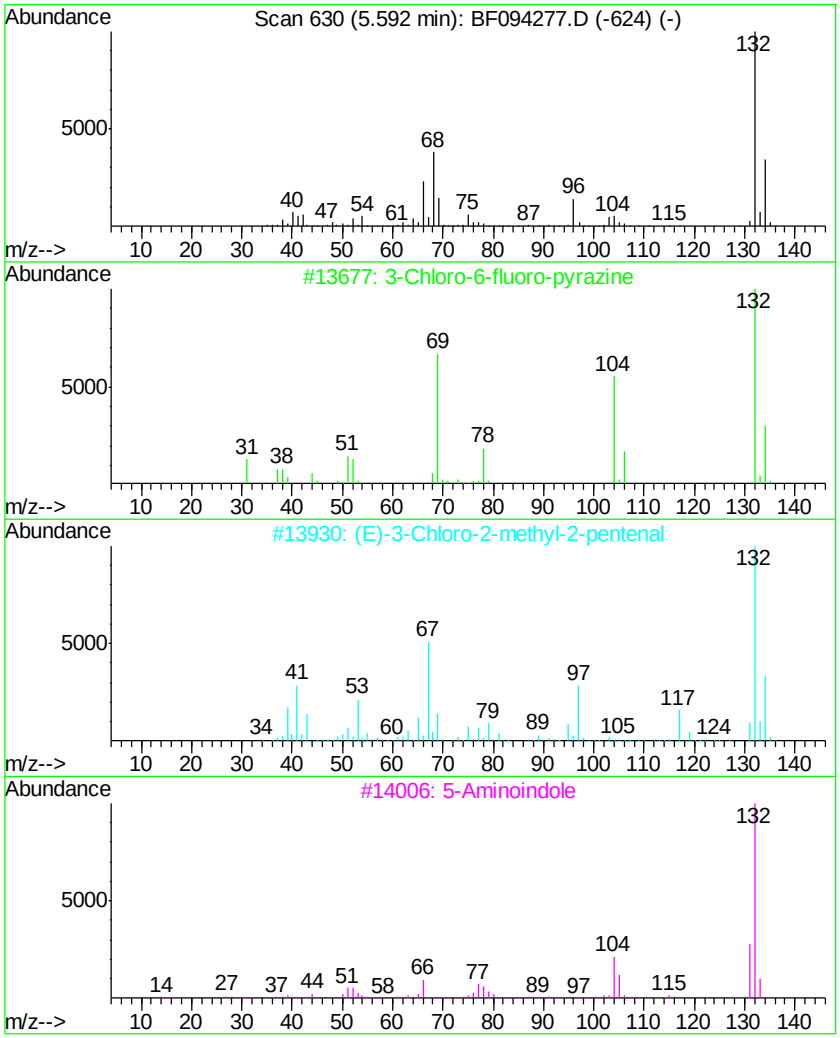
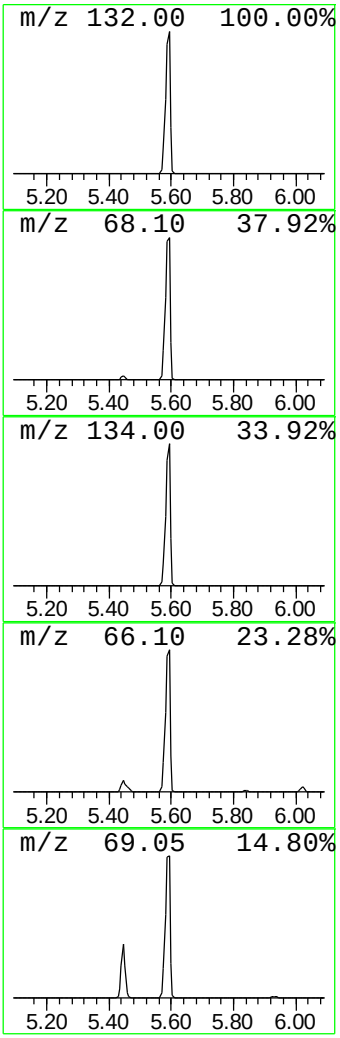
Peak Number 3 unknown5.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	75.18 ng	3464300	1,4-Dichlorobenzene-d4	5.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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Instrument : BNA_F
ClientSampleId : 22A

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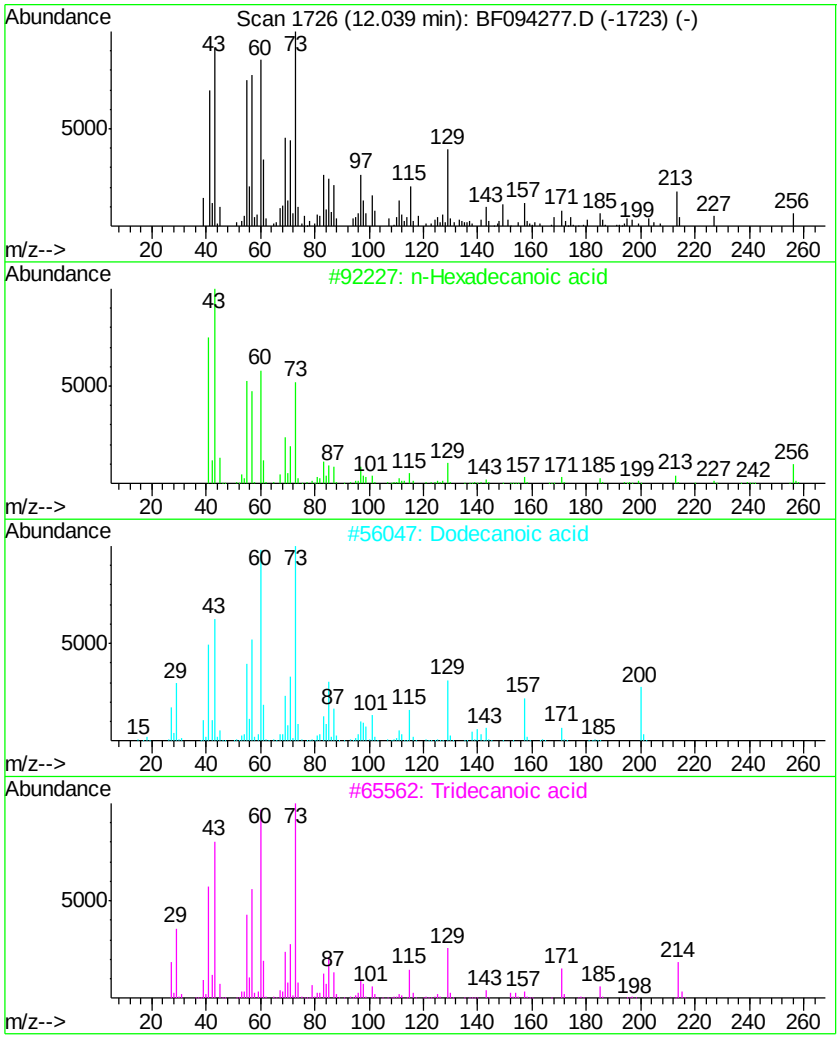
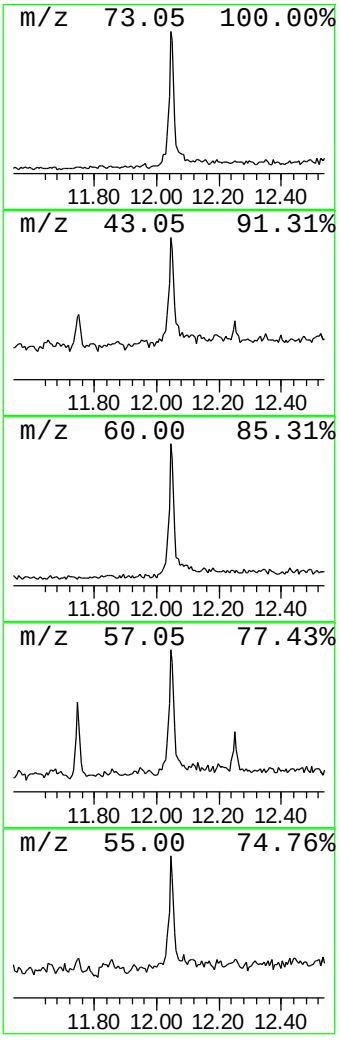
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	3.86 ng	246268	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Dodecanoic acid	200	C12H24O2	000143-07-7	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50





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Instrument : BNA_F
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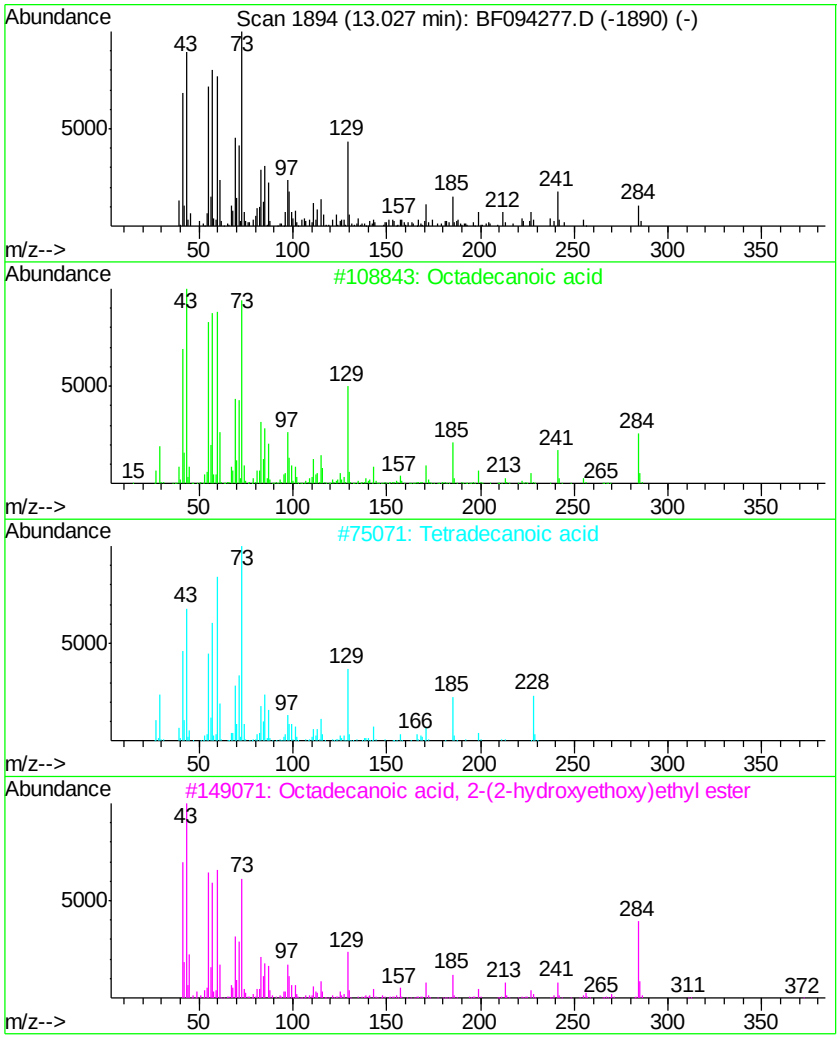
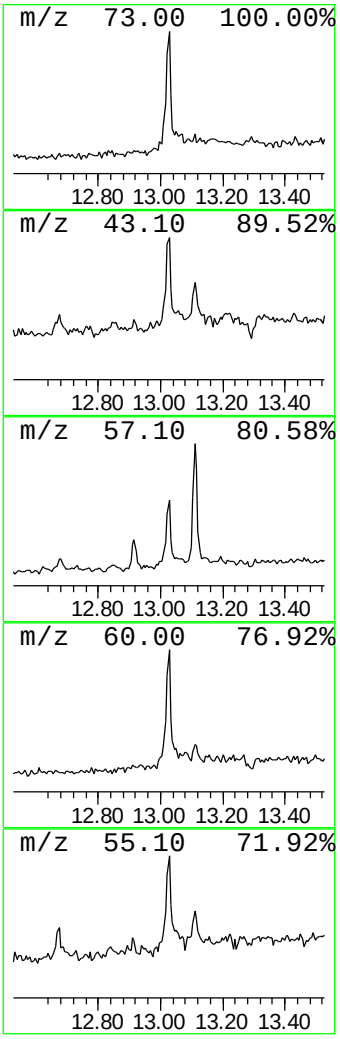
Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.03	3.27 ng	167830	Chrysene-d12	14.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Pentadecane	212	C15H32	000629-62-9	53





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TIC Library : C:\DATABASE\NIST02.L
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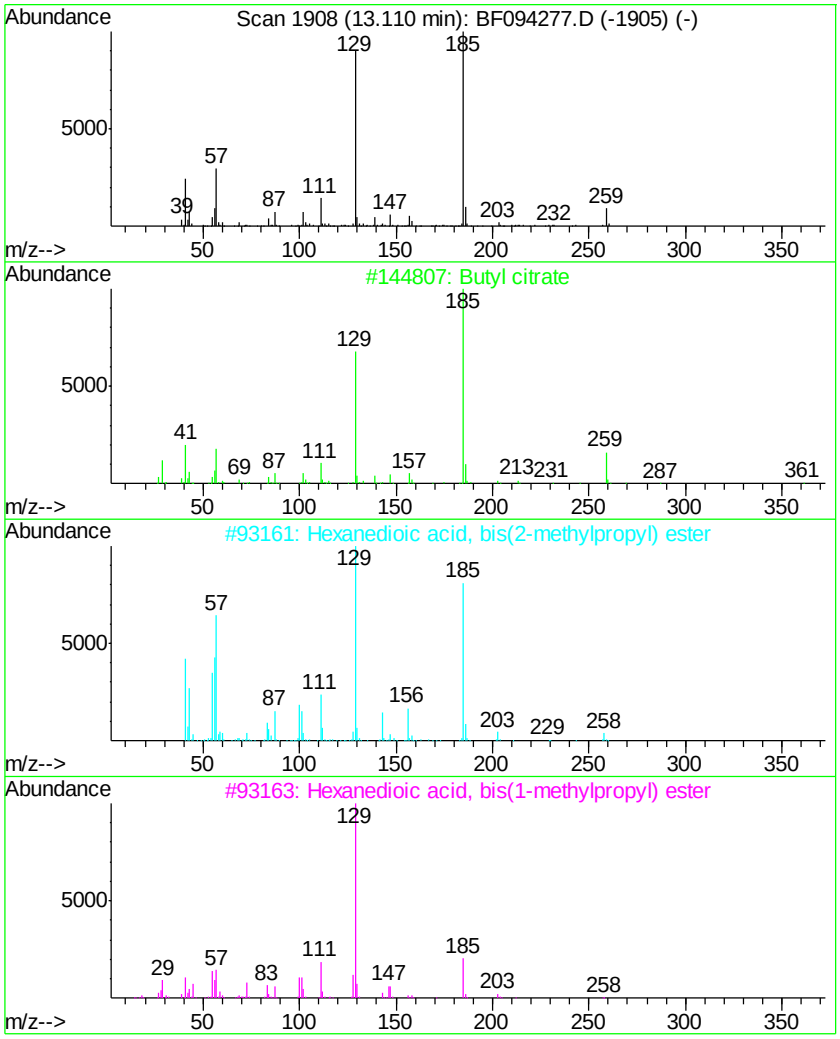
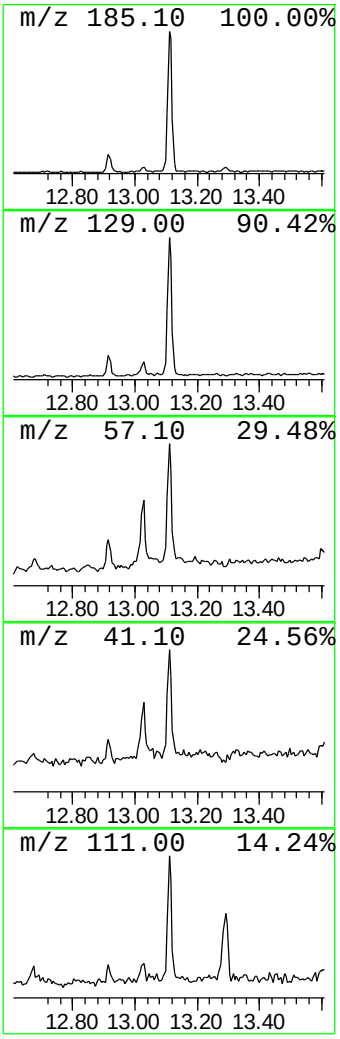
Peak Number 7 Butyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.11	5.47 ng	280412	Chrysene-d12	14.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	56
3	Hexanedioic acid, bis(1-methylpr...	258	C14H26O4	038447-22-2	56
4	Hexanedioic acid, dibutyl ester	258	C14H26O4	000105-99-7	39
5	Butanedioic acid, 2,3-dimethyl-,...	258	C14H26O4	056051-57-1	39





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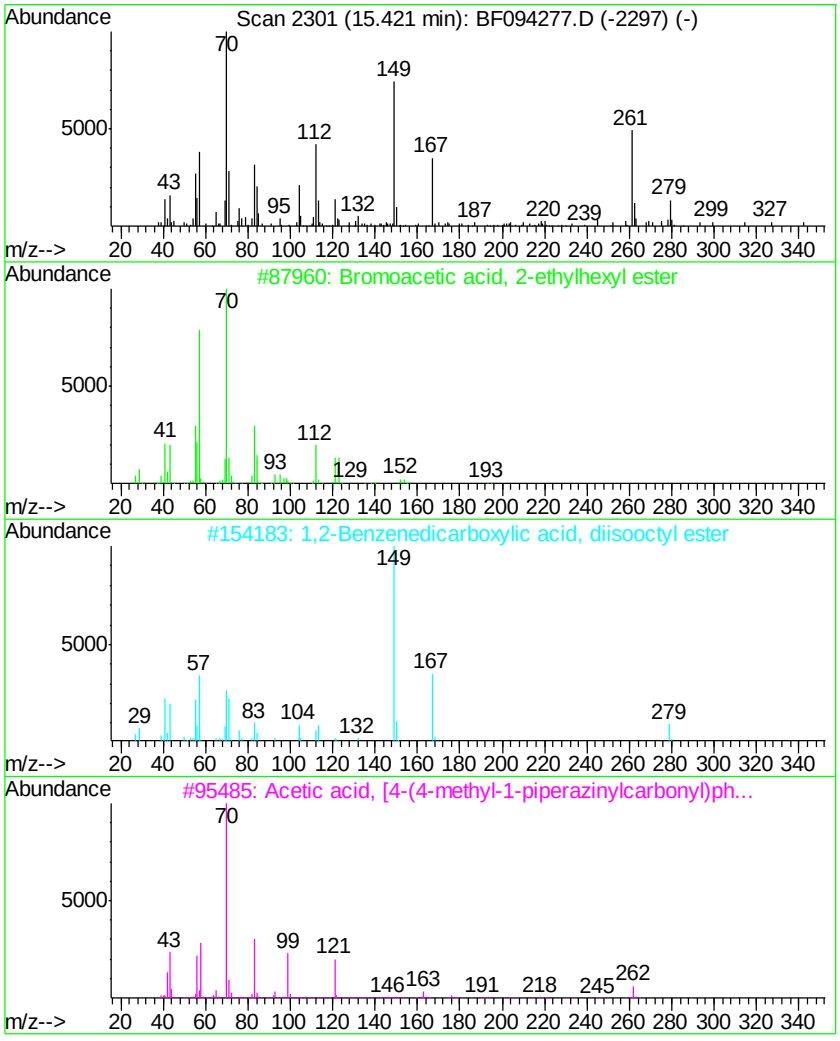
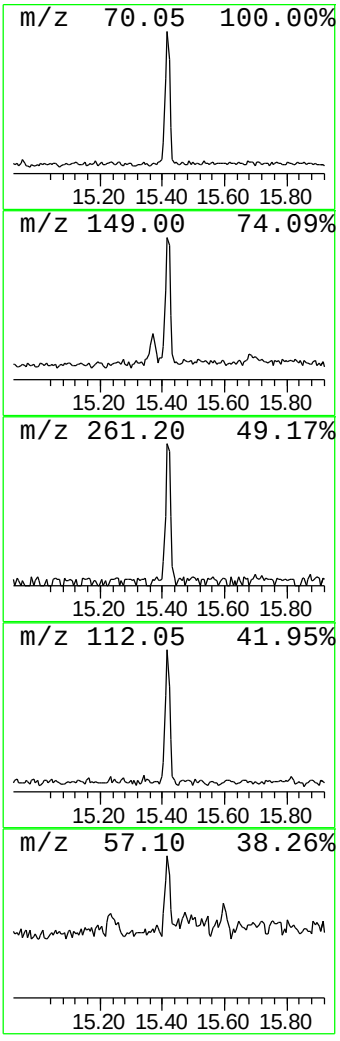
Peak Number 8 unknown15.42 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	3.68 ng	137866	Perylene-d12	16.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	38
2	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	32
3	Acetic acid, [4-(4-methyl-1-pipe...	262	C14H18N2O3	346699-90-9	22
4	1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	17
5	Undecane, 3-methylene-	168	C12H24	071138-64-2	14





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...	3.97	5.5	ng	251383	1	5.85	921553	20.0
Ethanol, 2-butoxy-	4.70	3.0	ng	140478	1	5.85	921553	20.0
unknown5.59	5.59	75.2	ng	3464300	1	5.85	921553	20.0
n-Hexadecanoic acid	12.04	3.9	ng	246268	4	11.31	1275090	20.0
Octadecanoic acid	13.03	3.3	ng	167830	5	14.56	1025300	20.0
Butyl citrate	13.11	5.5	ng	280412	5	14.56	1025300	20.0
unknown15.42	15.42	3.7	ng	137866	6	16.19	749452	20.0