LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090253.D
Acq On : 27 Sep 2016 15:55
Operator : UM/SJ
Sample : H4954-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-GRID-20B

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-BF092016.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	1.644	4	5	55	rVB	3263754	9493639	100.00%	21.800%
2	4.558	257	260	273	rVB	403691	689729	7.27%	1.584%
3	5.039	298	302	304	rBV	2176427	3217005	33.89%	7.387%
4	6.136	394	398	400	rBV	2289157	3454355	36.39%	7.932%
5	6.239	404	407	409	rBV	3091745	3195379	33.66%	7.337%
6	6.467	425	427	430	rBV	842644	794909	8.37%	1.825%
7	6.627	438	441	443	rBV	2769446	2589374	27.27%	5.946%
8	7.039	475	477	480	rBV	1502679	1940394	20.44%	4.456%
9	7.759	537	540	542	rBV	1166051	1086239	11.44%	2.494%
10	8.845	632	635	637	rBV	3529381	4120833	43.41%	9.463%
11	9.245	667	670	672	rBV	931677	1011324	10.65%	2.322%
12	9.496	690	692	695	rVB	1273454	1242514	13.09%	2.853%
13	10.285	758	761	764	rBV	2124871	2312669	24.36%	5.311%
14	10.433	772	774	778	rBV	113252	136645	1.44%	0.314%
15	10.971	818	821	823	rBV	1348378	1317197	13.87%	3.025%
16	11.233	841	844	848	rBV	158333	201007	2.12%	0.462%
17	11.531	868	870	874	rBV2	56120	105024	1.11%	0.241%
18	12.559	957	960	962	rBV	3452308	3771346	39.72%	8.660%
19	13.474	1037	1040	1047	rBV	300130	446337	4.70%	1.025%
20	13.576	1047	1049	1052	rBV	1132095	1206115	12.70%	2.770%
21	14.365	1115	1118	1120	rBV	174845	244722	2.58%	0.562%
22	14.902	1162	1165	1167	rBV	884386	971921	10.24%	2.232%

Sum of corrected areas: 43548677

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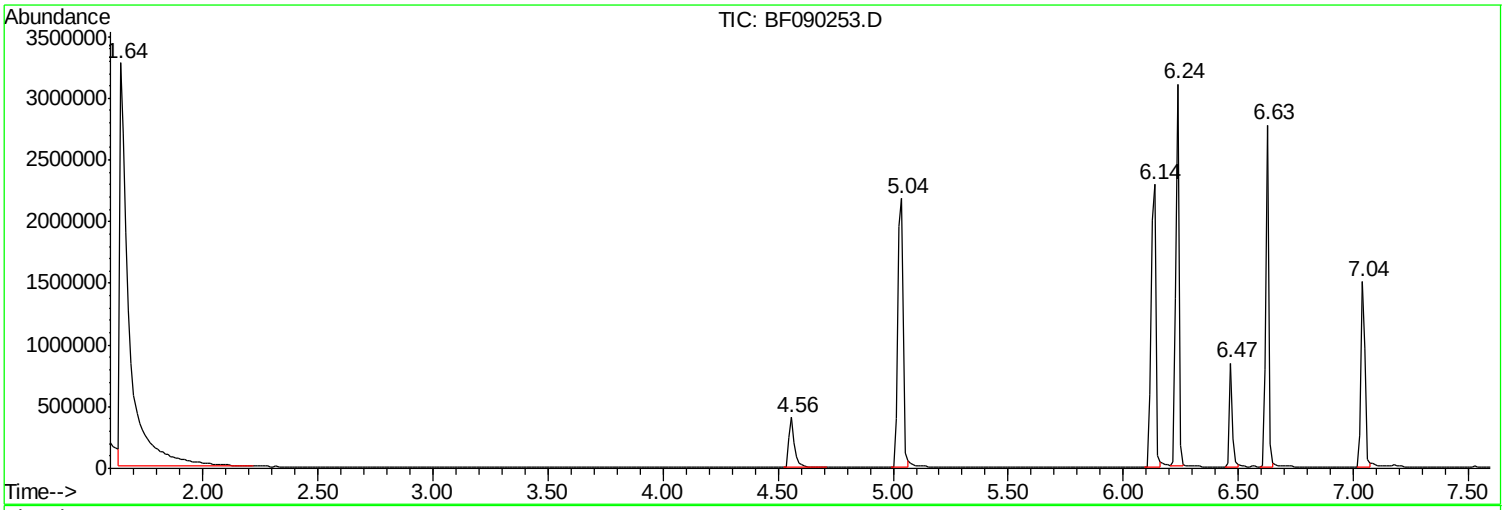
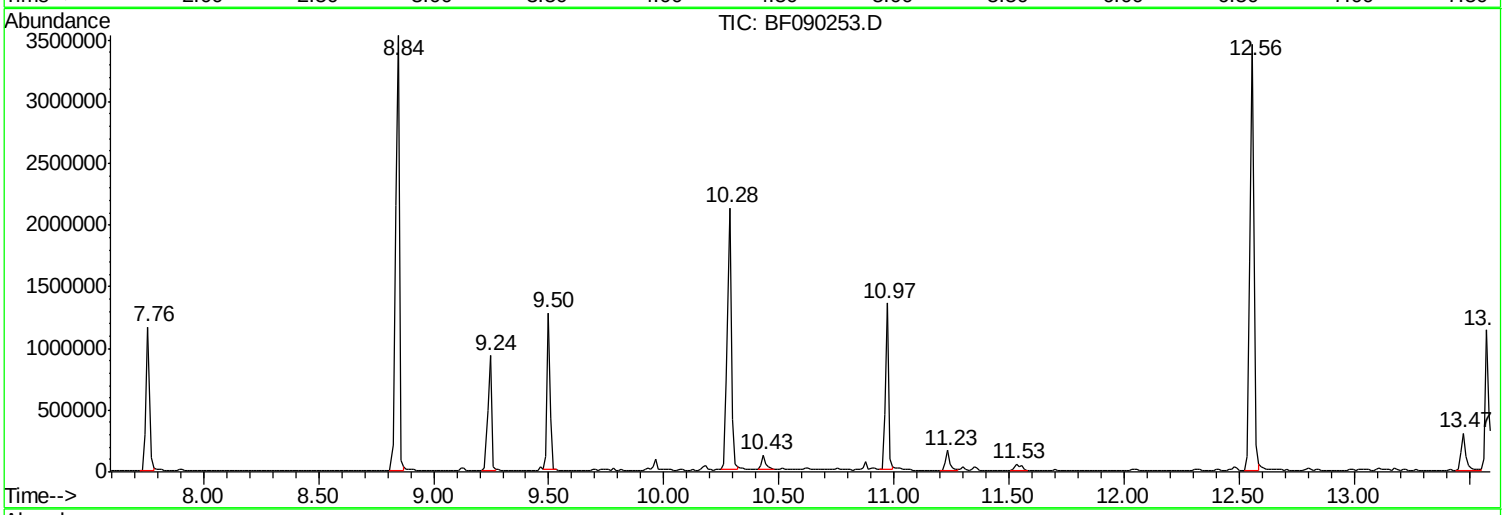
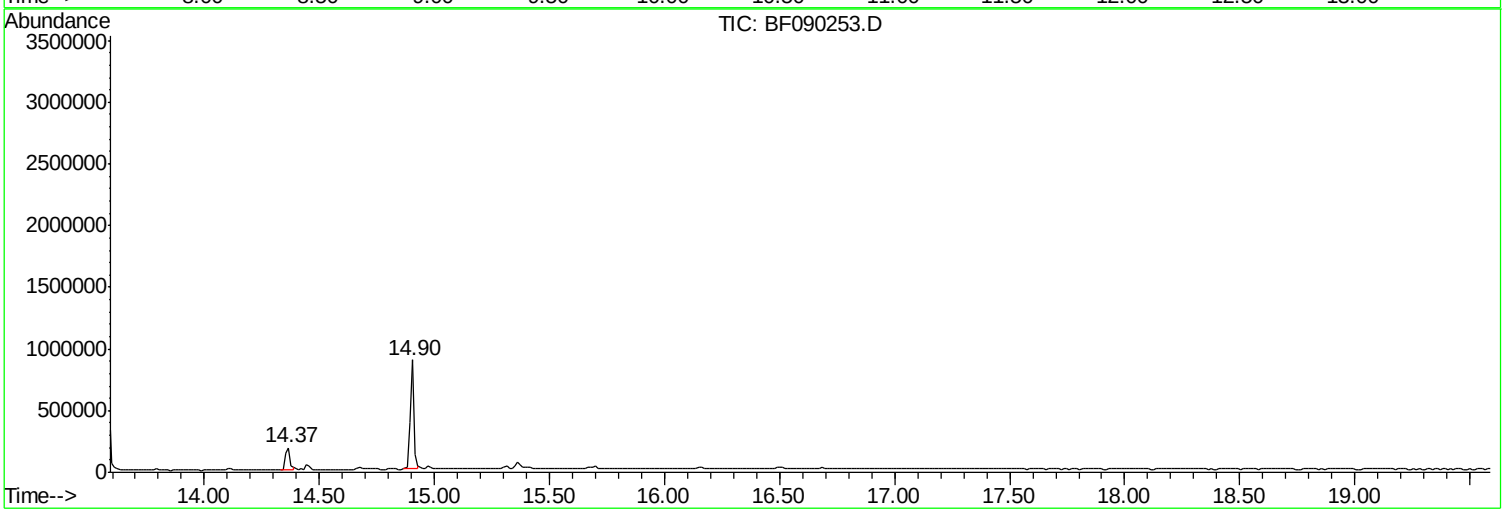
TRACK-D-GRID-20B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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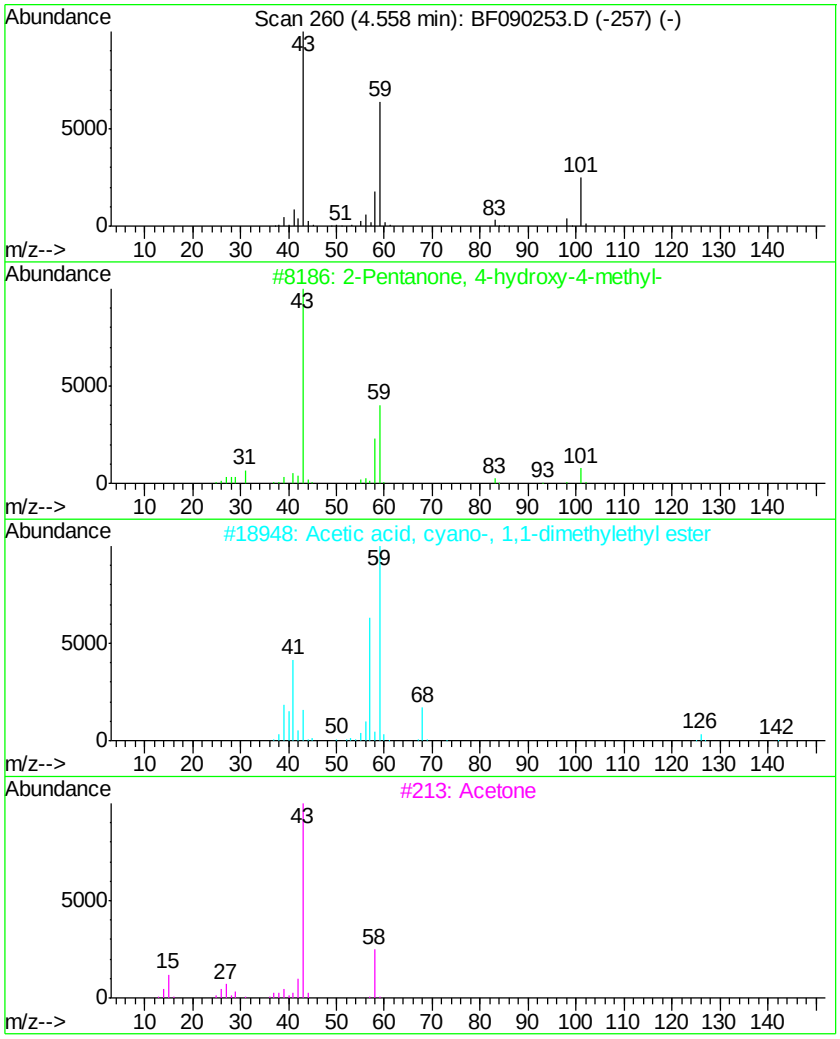
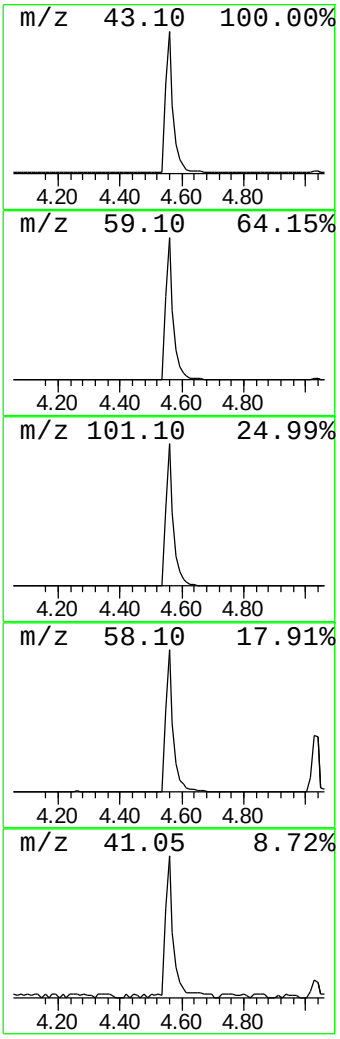
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	17.35 ng	689729	1,4-Dichlorobenzene-d4	6.47

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	17
3	Acetone	58	C3H6O	000067-64-1	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
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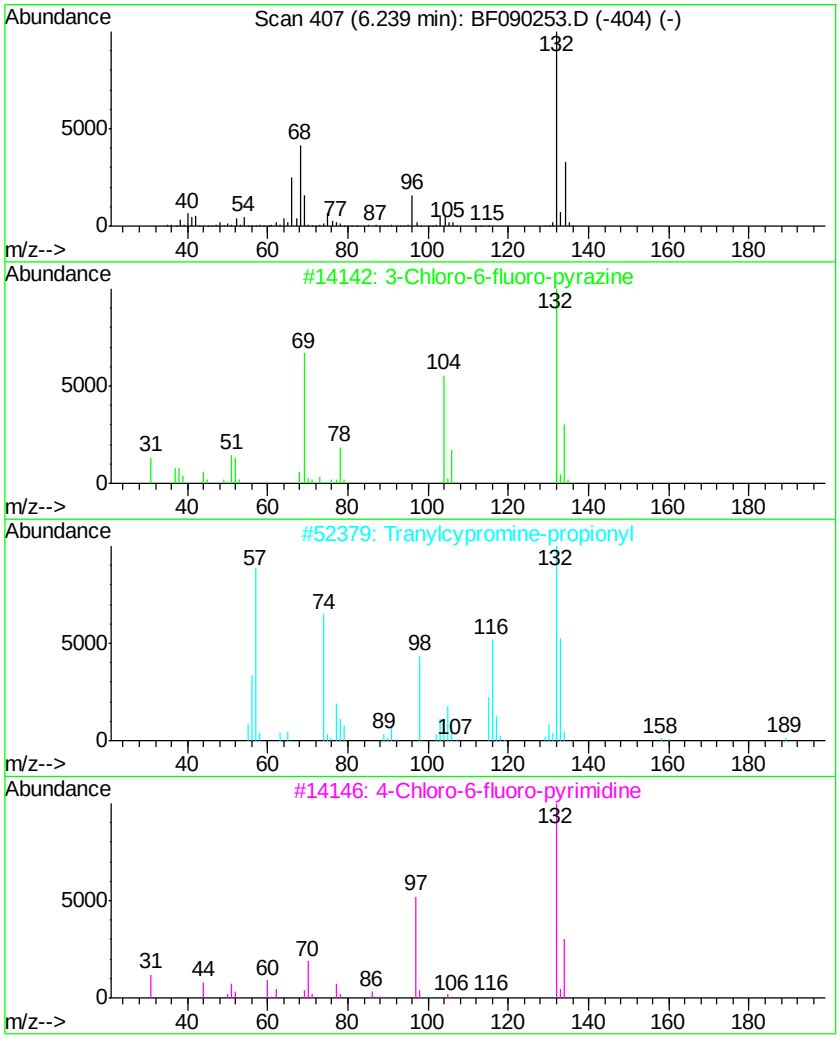
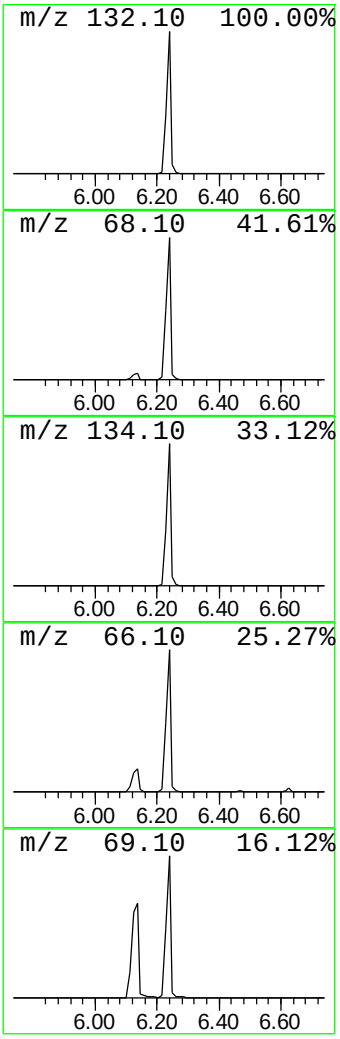
****
Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	80.40 ng	3195380	1,4-Dichlorobenzene-d4	6.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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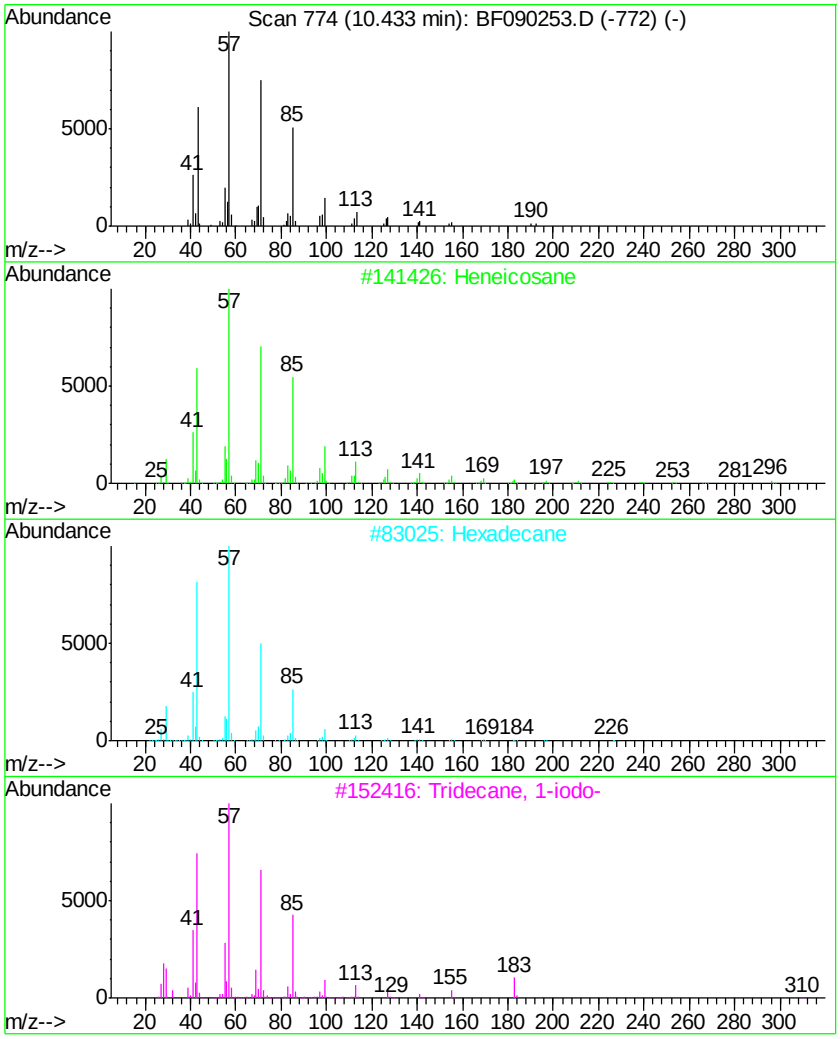
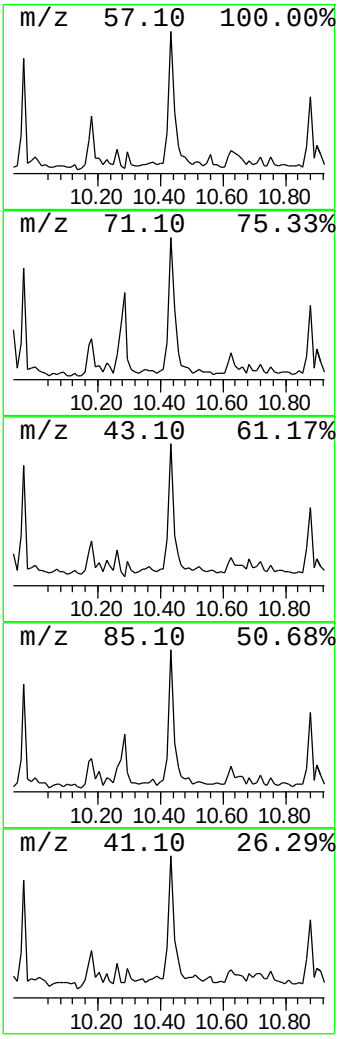
****
Peak Number 5 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	2.07 ng	136645	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4	Pentadecane	212	C15H32	000629-62-9	72
5	Heptacosane	380	C27H56	000593-49-7	72





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TIC Library : C:\DATABASE\NIST11.L
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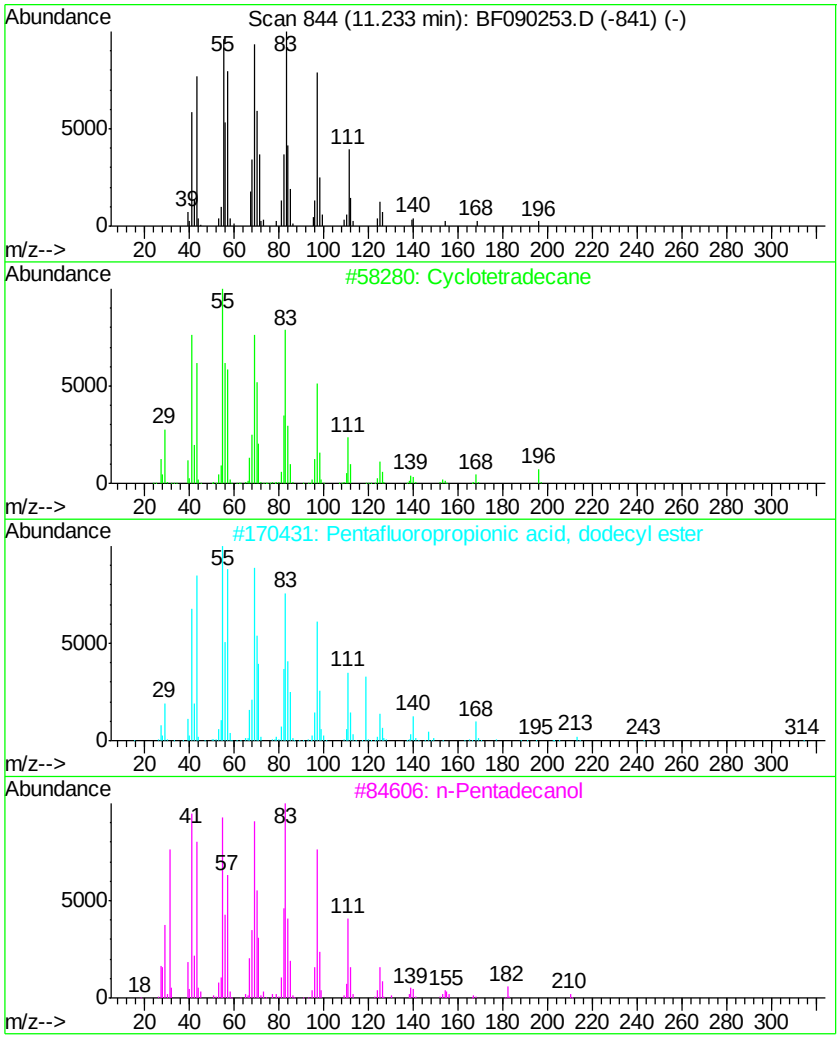
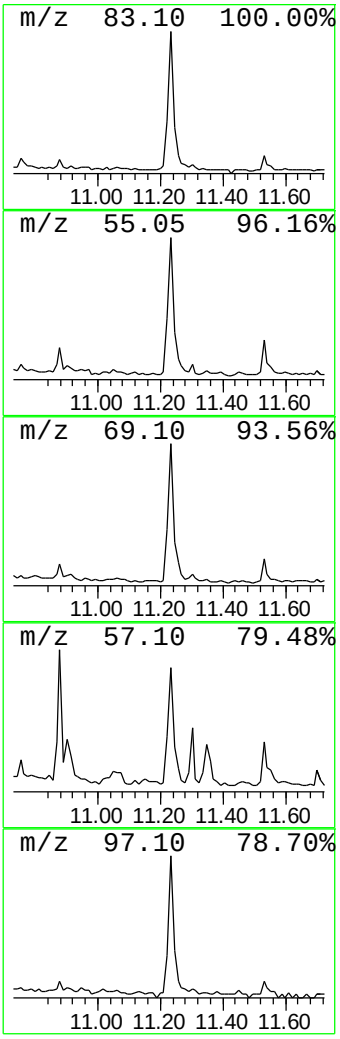
****

Peak Number 6 Cyclotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.23	3.05 ng	201007	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	94
2	Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	91
3	n-Pentadecanol	228	C15H32O	000629-76-5	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	Cyclododecane	168	C12H24	000294-62-2	91





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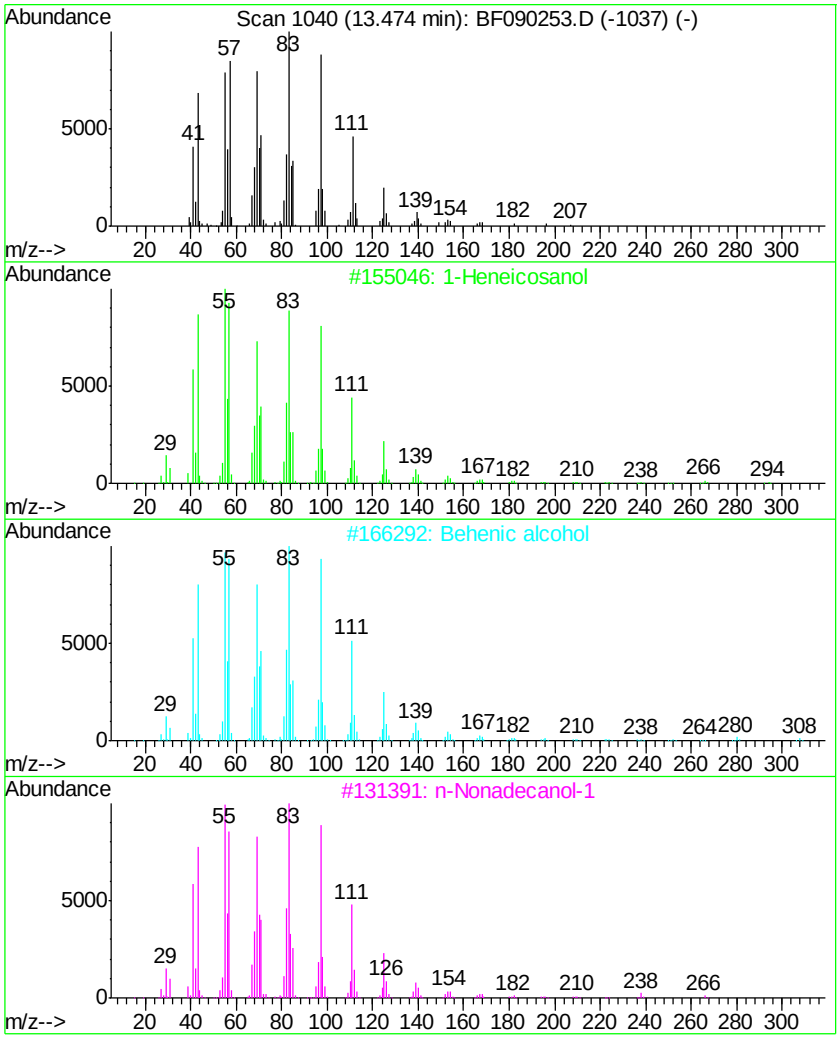
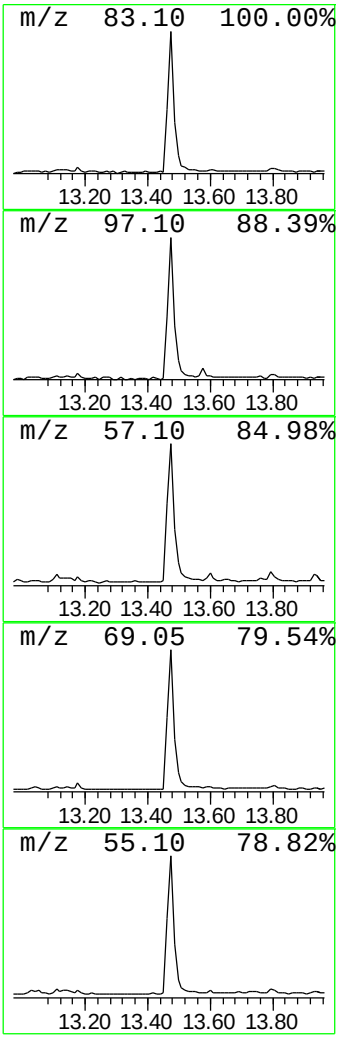
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	7.40 ng	446337	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





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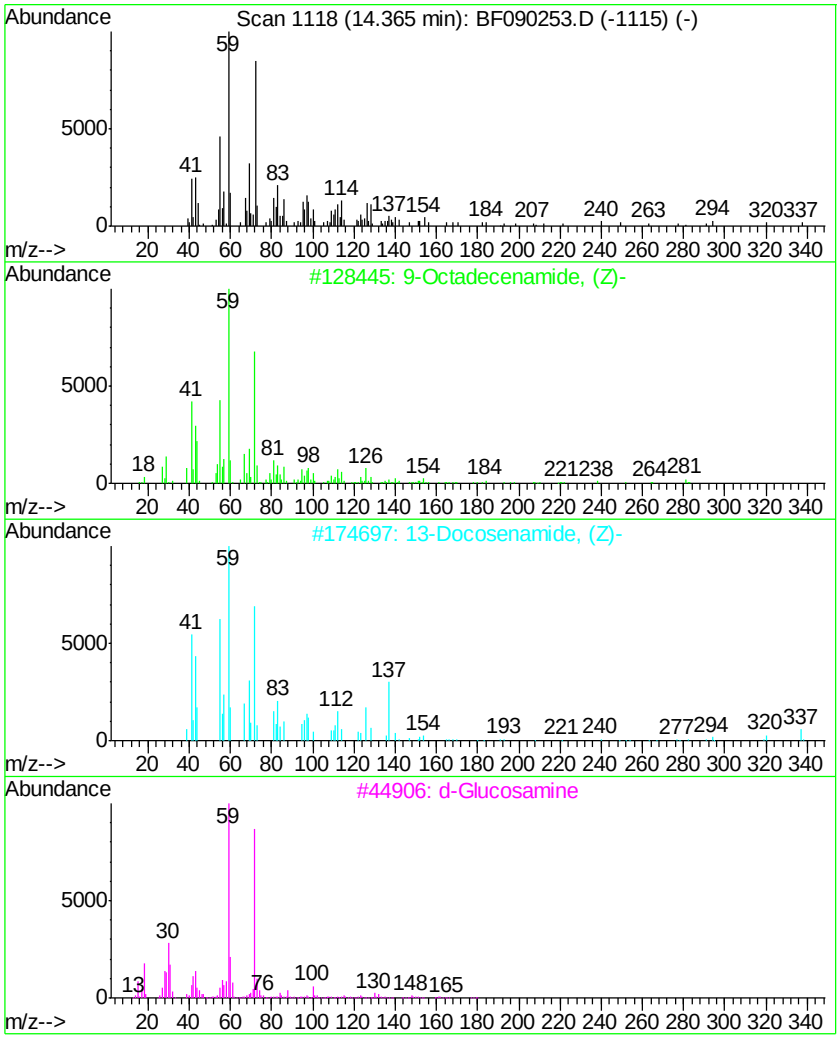
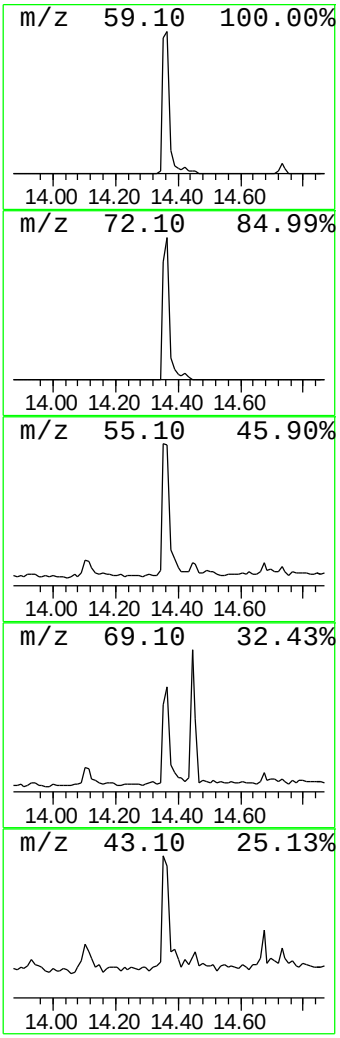
****
Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	5.04 ng	244722	Perylene-d12	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	53
3	d-Glucosamine	179	C6H13NO5	000090-77-7	50
4	Octadecanamide	283	C18H37NO	000124-26-5	47
5	d,l-trans-4-Methyl-5-methoxy-1-(...	184	C11H20O2	1000101-22-2	30





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.56	17.4	ng	689729	1	6.47	794909	20.0
unknown6.24	6.24	80.4	ng	3195380	1	6.47	794909	20.0
Heneicosane	10.43	2.1	ng	136645	4	10.97	1317200	20.0
Cyclotetradecane	11.23	3.0	ng	201007	4	10.97	1317200	20.0
1-Heneicosanol	13.47	7.4	ng	446337	5	13.58	1206120	20.0
9-Octadecenamide,...	14.37	5.0	ng	244722	6	14.90	971921	20.0