LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080216\
Data File : BF089558.D
Acq On : 2 Aug 2016 20:40
Operator : UM/SJ
Sample : H4269-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-56-17.0-18.0

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-BF072716.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	36	rVB	530788	1113228	87.10%	9.265%
2	4.559	257	260	270	rBV	252387	433538	33.92%	3.608%
3	5.039	300	302	318	rBV	974545	1168670	91.44%	9.727%
4	5.450	336	338	343	rBV	17296	19268	1.51%	0.160%
5	6.136	396	398	405	rBV	1089919	1278033	100.00%	10.637%
6	6.239	405	407	409	rBV	1273312	1238686	96.92%	10.309%
7	6.467	426	427	438	rBV	193253	240280	18.80%	2.000%
8	6.627	438	441	443	rBV	818747	925762	72.44%	7.705%
9	7.050	475	478	488	rBV	479644	752704	58.90%	6.265%
10	7.187	488	490	496	rVB	18159	27193	2.13%	0.226%
11	7.759	538	540	550	rBV	262545	298220	23.33%	2.482%
12	8.833	632	634	637	rBV	1118011	1166052	91.24%	9.705%
13	9.233	667	669	672	rBV	247599	267199	20.91%	2.224%
14	9.496	690	692	695	rBV	368857	328879	25.73%	2.737%
15	9.953	730	732	734	rVB	20792	17790	1.39%	0.148%
16	10.285	759	761	763	rBV	692164	703730	55.06%	5.857%
17	10.422	771	773	779	rVB	28240	36121	2.83%	0.301%
18	10.868	809	812	813	rBV	19107	17018	1.33%	0.142%
19	10.971	819	821	826	rBV	249209	263212	20.60%	2.191%
20	11.222	841	843	848	rBV	117876	172885	13.53%	1.439%
21	11.291	848	849	855	rVB	13848	14417	1.13%	0.120%
22	11.531	868	870	874	rBV	17163	21391	1.67%	0.178%
23	12.034	912	914	922	rBV	98076	192100	15.03%	1.599%
24	12.548	957	959	962	rBV	823735	836297	65.44%	6.960%
25	13.474	1038	1040	1048	rVB	29271	49768	3.89%	0.414%
26	13.588	1048	1050	1058	rBV	201478	222591	17.42%	1.853%
27	14.914	1163	1166	1173	rBV	178356	210015	16.43%	1.748%

Sum of corrected areas: 12015047

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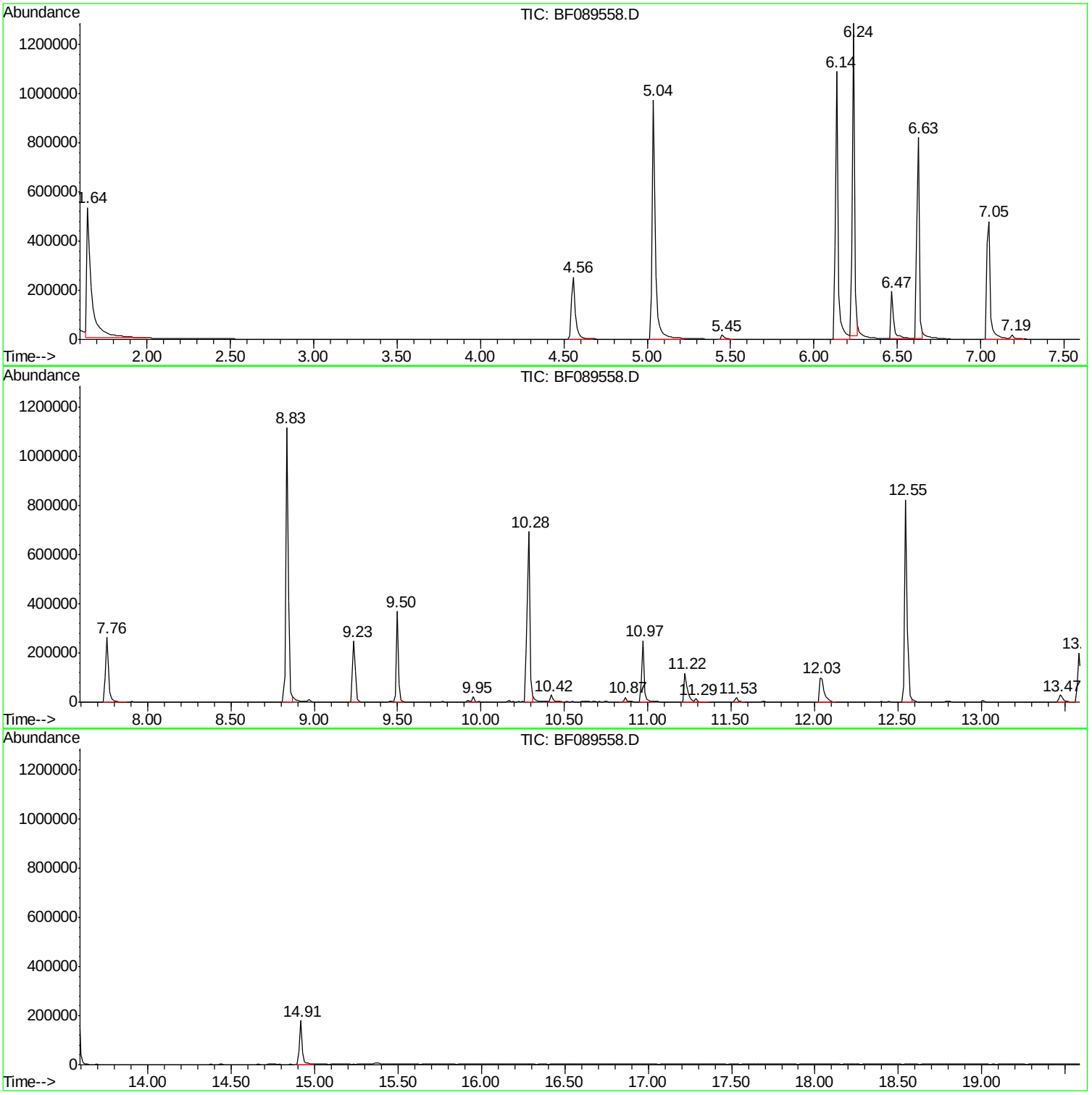
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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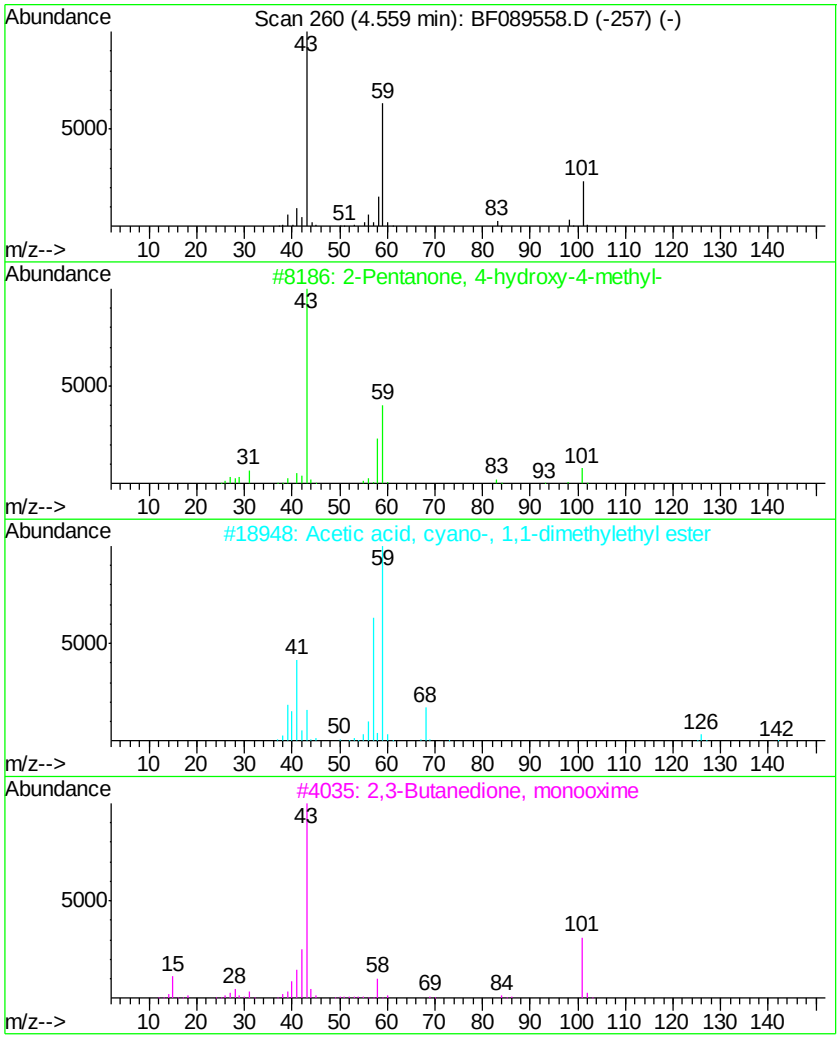
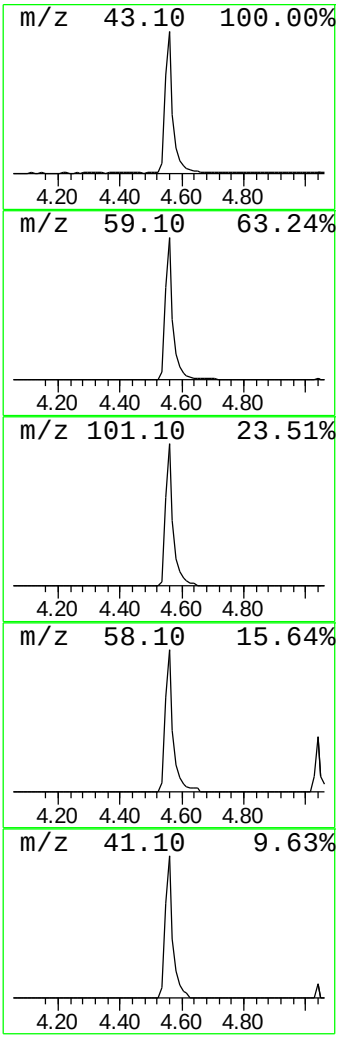
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	36.09 ng	433538	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	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetone	58	C3H6O	000067-64-1	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument : BNA_F
ClientSampleId : SB-56-17.0-18.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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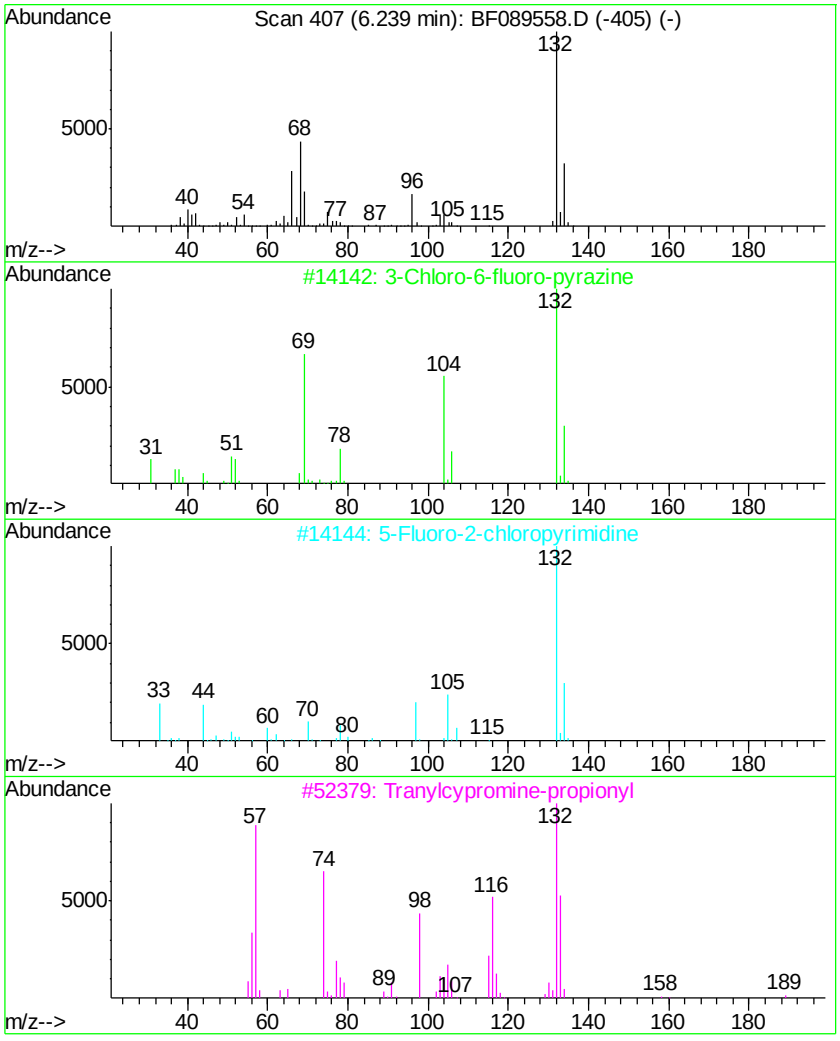
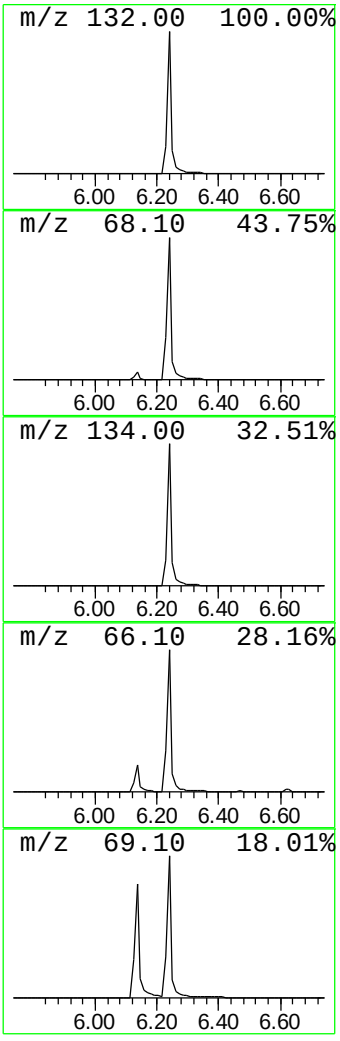
Peak Number 3 unknown6.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	103.10 ng	1238690	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	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-56-17.0-18.0

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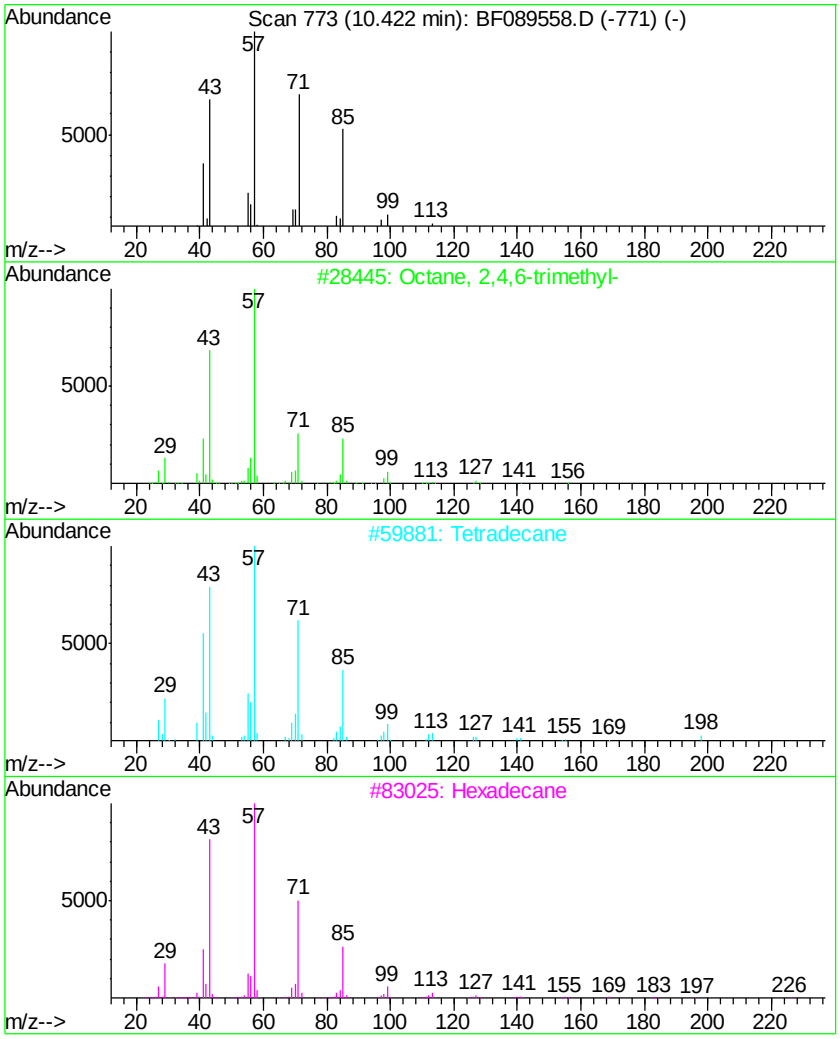
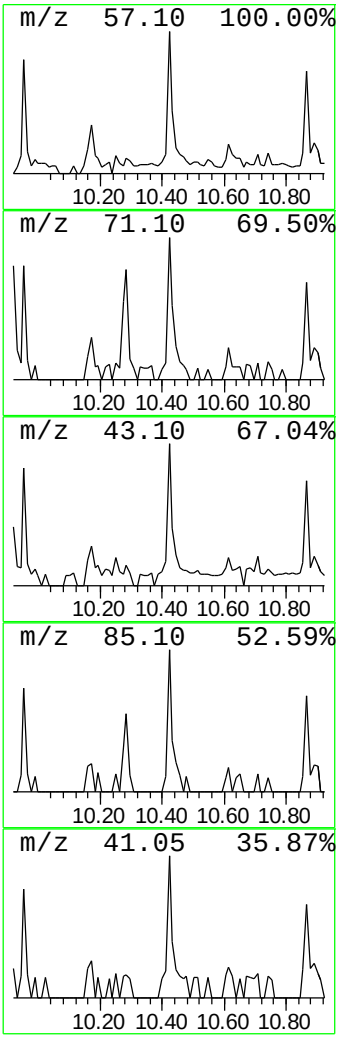
Peak Number 5 Octane, 2,4,6-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.42	2.74 ng	36121	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80
2	Tetradecane	198	C14H30	000629-59-4	78
3	Hexadecane	226	C16H34	000544-76-3	78
4	Pentadecane	212	C15H32	000629-62-9	72
5	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	59





Library Search Compound Report

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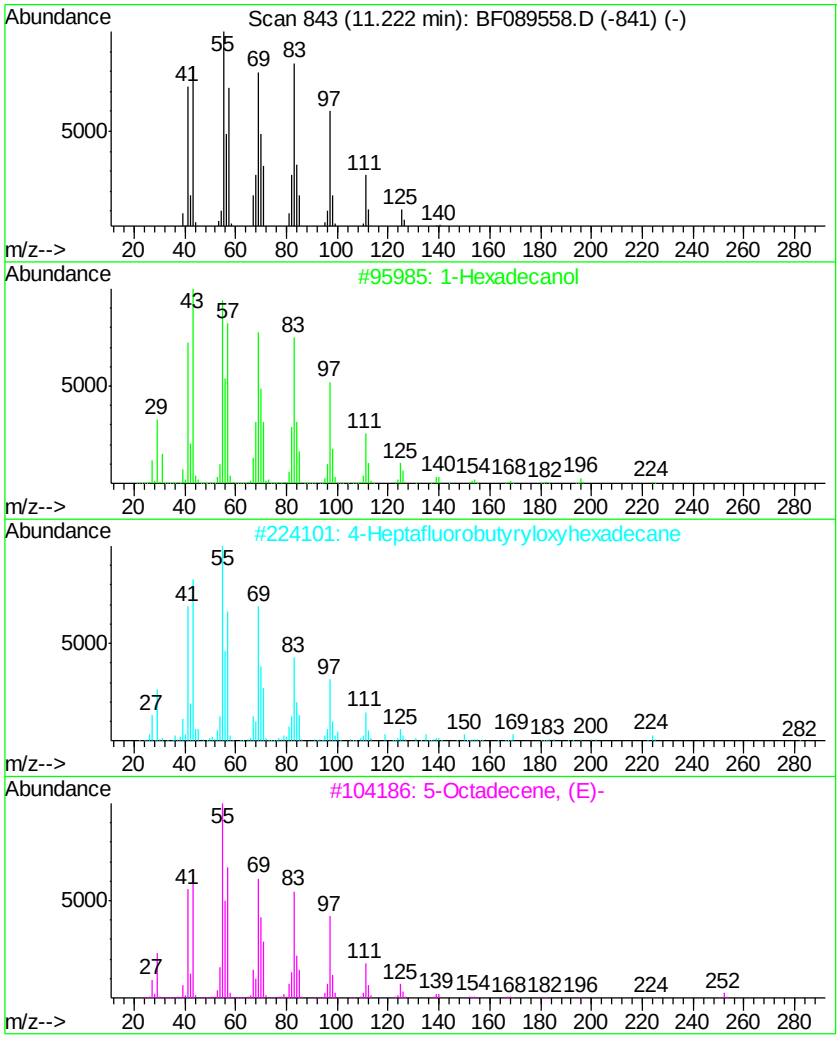
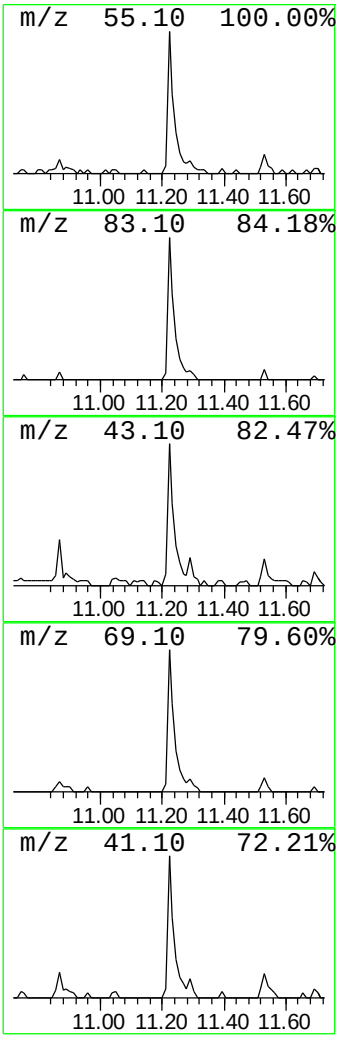
Peak Number 6 1-Hexadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.22	13.14 ng	172885	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	95
2	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	91





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Instrument : BNA_F
ClientSampleId : SB-56-17.0-18.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
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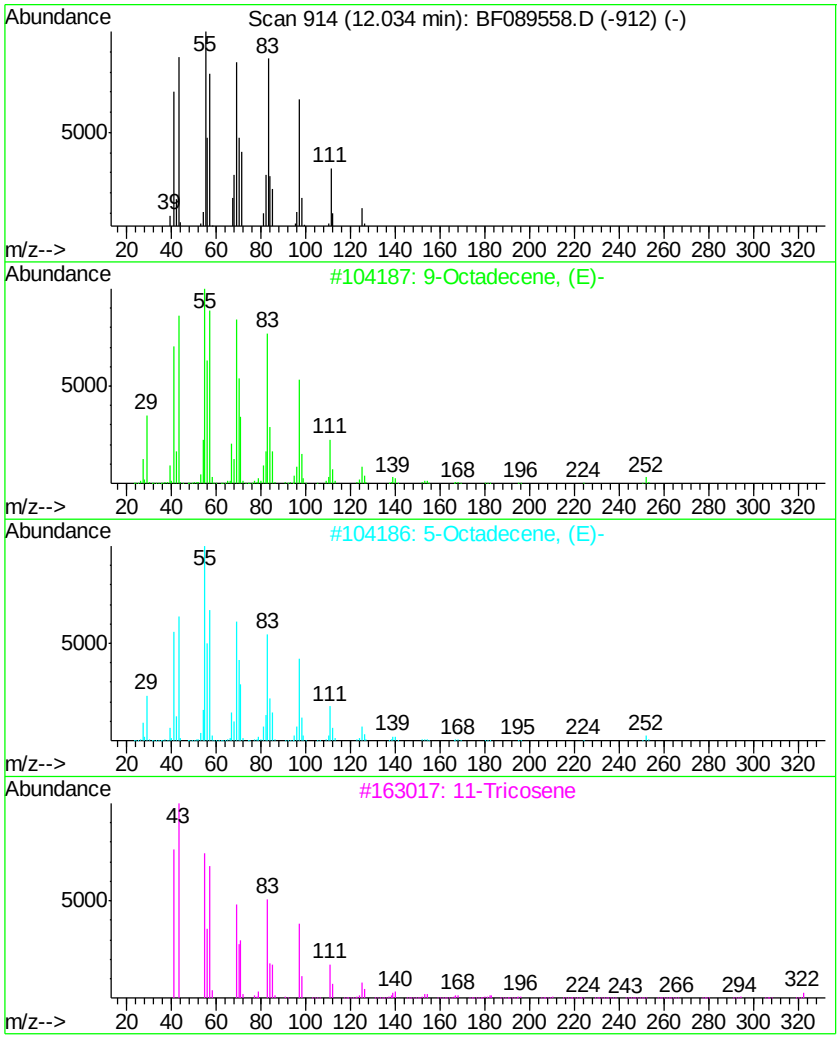
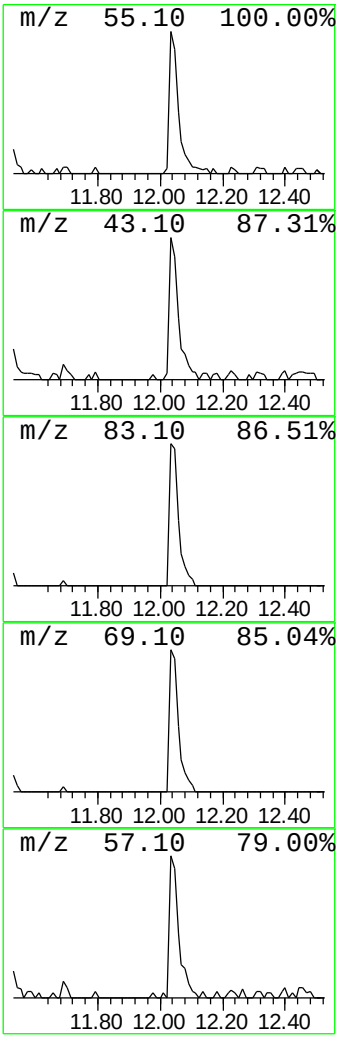
****

Peak Number 7 9-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	14.60 ng	192100	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
3	11-Tricosene	322	C23H46	052078-56-5	91
4	Cetene	224	C16H32	000629-73-2	58
5	1-Hexadecanol	242	C16H34O	036653-82-4	58





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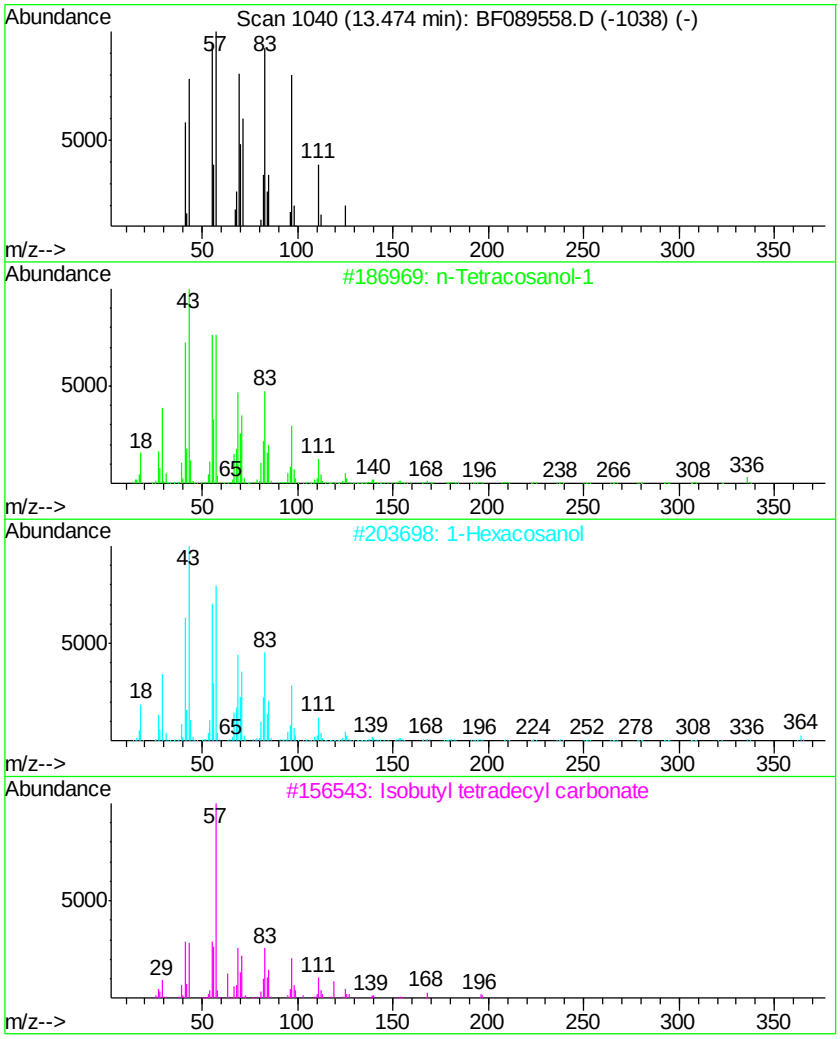
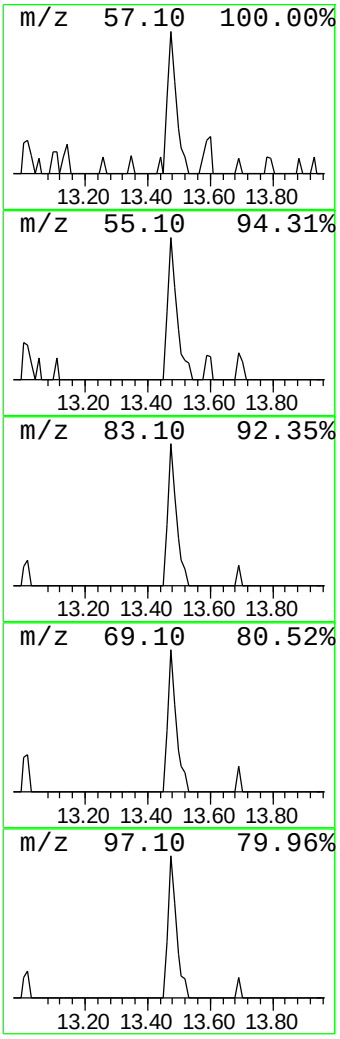
****

Peak Number 8 unknown13.47 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	4.47 ng	49768	Chrysene-d12	13.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	49
2	1-Hexacosanol	382	C26H54O	000506-52-5	49
3	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	47
4	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	43
5	Cyclotetradecane	196	C14H28	000295-17-0	43





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...	4.56	36.1	ng	433538	1	6.47	240280	20.0
unknown6.24	6.24	103.1	ng	1238690	1	6.47	240280	20.0
Octane, 2,4,6-tri...	10.42	2.7	ng	36121	4	10.97	263212	20.0
1-Hexadecanol	11.22	13.1	ng	172885	4	10.97	263212	20.0
9-Octadecene, (E)-	12.03	14.6	ng	192100	4	10.97	263212	20.0
unknown13.47	13.47	4.5	ng	49768	5	13.59	222591	20.0