LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087813.D
Acq On : 8 Jun 2016 16:51
Operator : UM/SJ
Sample : H3378-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-21

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-BF060716.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	1.655	3	6	8	rVB	3157569	5260842	100.00%	23.235%
2	1.758	13	15	24	rVB	214690	392056	7.45%	1.732%
3	1.884	24	26	39	rVB	1957423	3005668	57.13%	13.275%
4	2.044	39	40	89	rVB2	88682	542071	10.30%	2.394%
5	4.993	296	298	302	rBB	81503	96871	1.84%	0.428%
6	5.416	332	335	337	rBV	1314056	1197633	22.77%	5.289%
7	6.456	423	426	428	rBV	1346809	1308959	24.88%	5.781%
8	6.593	435	438	440	rBV	1229725	1293450	24.59%	5.713%
9	6.822	456	458	461	rBV	676670	574789	10.93%	2.539%
10	6.982	469	472	474	rBB	1076277	906654	17.23%	4.004%
11	7.382	505	507	509	rBV	652631	690129	13.12%	3.048%
12	8.113	568	571	573	rBV	860810	825925	15.70%	3.648%
13	9.188	663	665	668	rBV	1127351	1131624	21.51%	4.998%
14	9.588	698	700	702	rBV	297105	236222	4.49%	1.043%
15	9.873	722	725	727	rBV	848493	865802	16.46%	3.824%
16	10.651	791	793	796	rBV2	578107	730363	13.88%	3.226%
17	11.348	852	854	857	rBV2	605438	788383	14.99%	3.482%
18	12.559	958	960	963	rBV	86830	78279	1.49%	0.346%
19	12.776	976	979	983	rBV2	97794	149698	2.85%	0.661%
20	12.936	991	993	996	rVB	718001	886329	16.85%	3.915%
21	13.851	1071	1073	1077	rBV	40641	60907	1.16%	0.269%
22	13.988	1082	1085	1091	rVB	706281	719563	13.68%	3.178%
23	15.005	1172	1174	1180	rBV	44286	86486	1.64%	0.382%
24	15.417	1207	1210	1213	rBV	488650	609954	11.59%	2.694%
25	17.394	1379	1383	1393	rBV5	22940	95788	1.82%	0.423%
26	17.920	1426	1429	1435	rVB4	19372	54659	1.04%	0.241%
27	19.349	1549	1554	1561	rVB4	14276	52968	1.01%	0.234%

Sum of corrected areas: 22642072

LSC Report - Integrated Chromatogram

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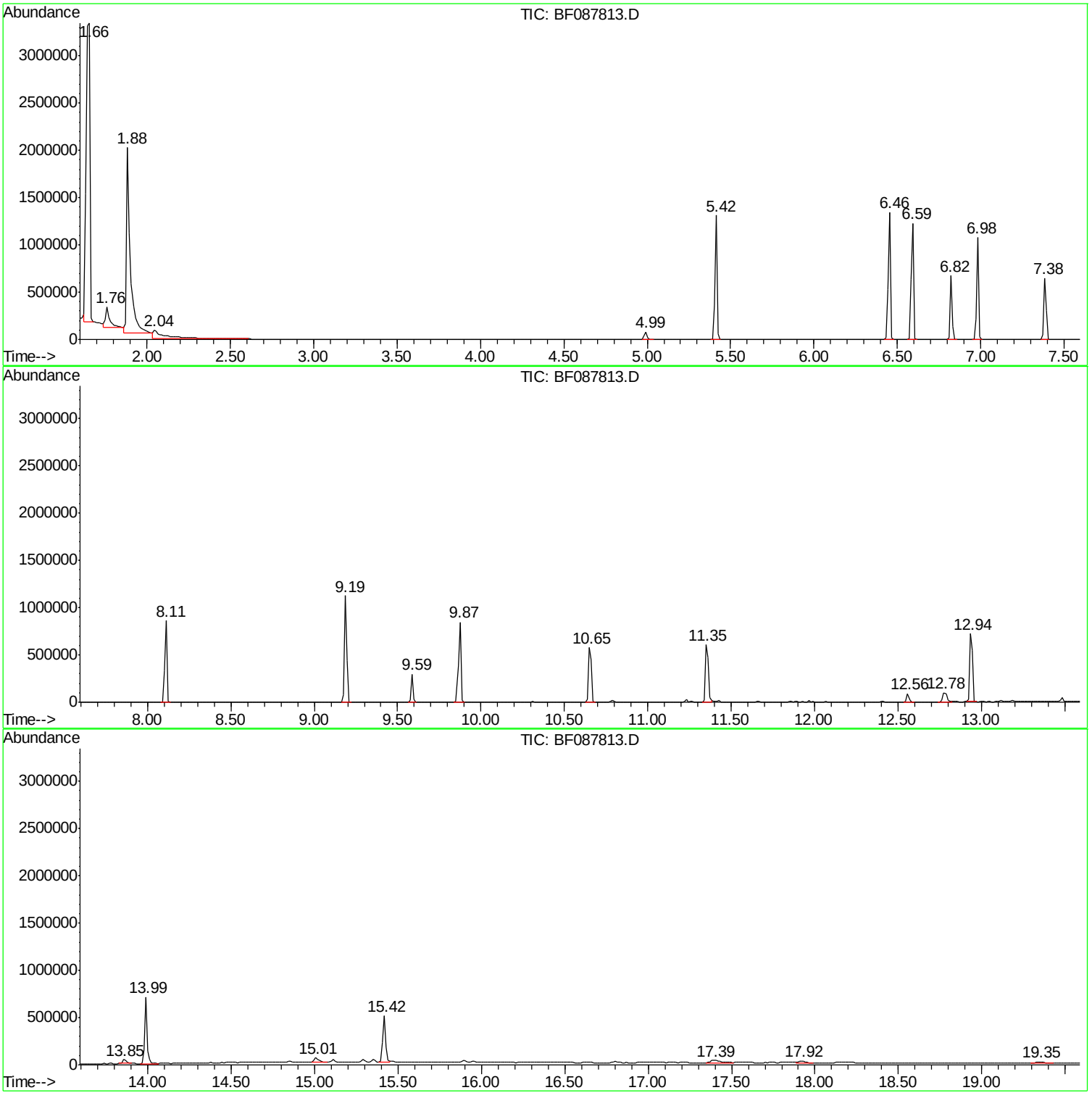
Instrument : BNA_F
ClientSampleId : SS-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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Sample : H3378-11
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ClientSampleId : SS-21

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

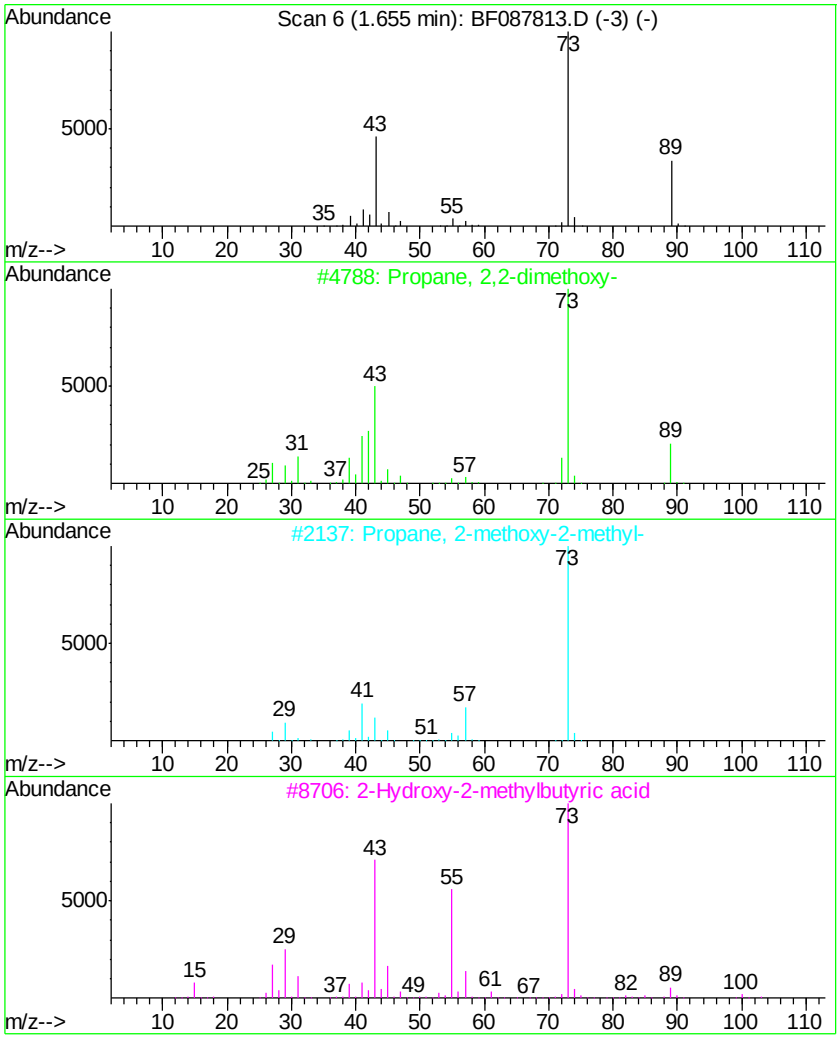
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

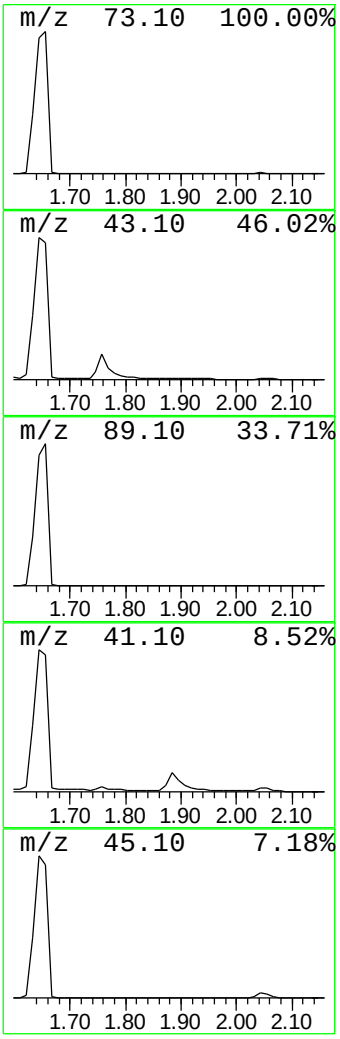
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.66	183.05 ng	5260840	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087813.D
Acq On : 8 Jun 2016 16:51
Operator : UM/SJ
Sample : H3378-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

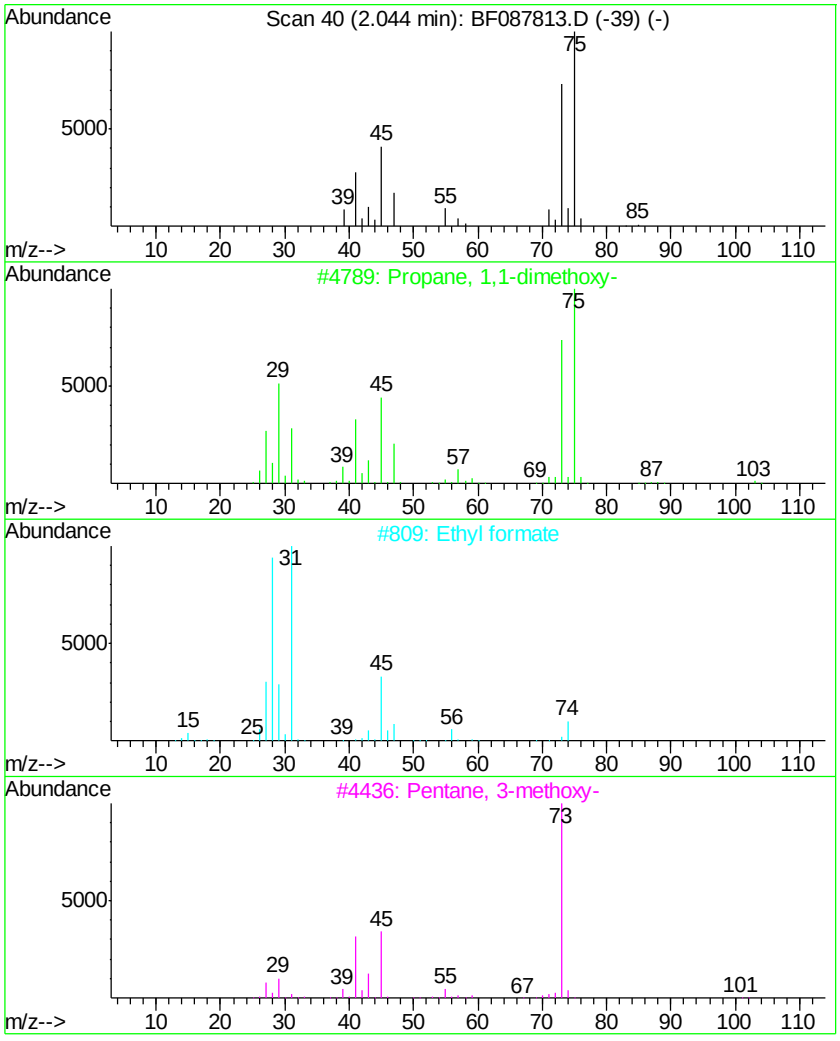
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

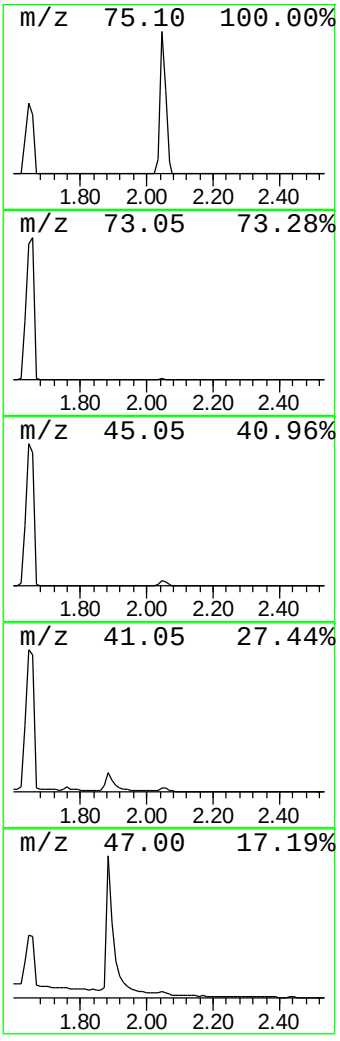
****

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.04	18.86 ng	542071	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2	Ethyl formate	74	C3H6O2	000109-94-4	9
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4	Formamide, N-methylthio	75	C2H5NS	018952-41-5	7
5	Methane, nitroso-	45	CH3NO	000865-40-7	5





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Data File : BF087813.D
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Operator : UM/SJ
Sample : H3378-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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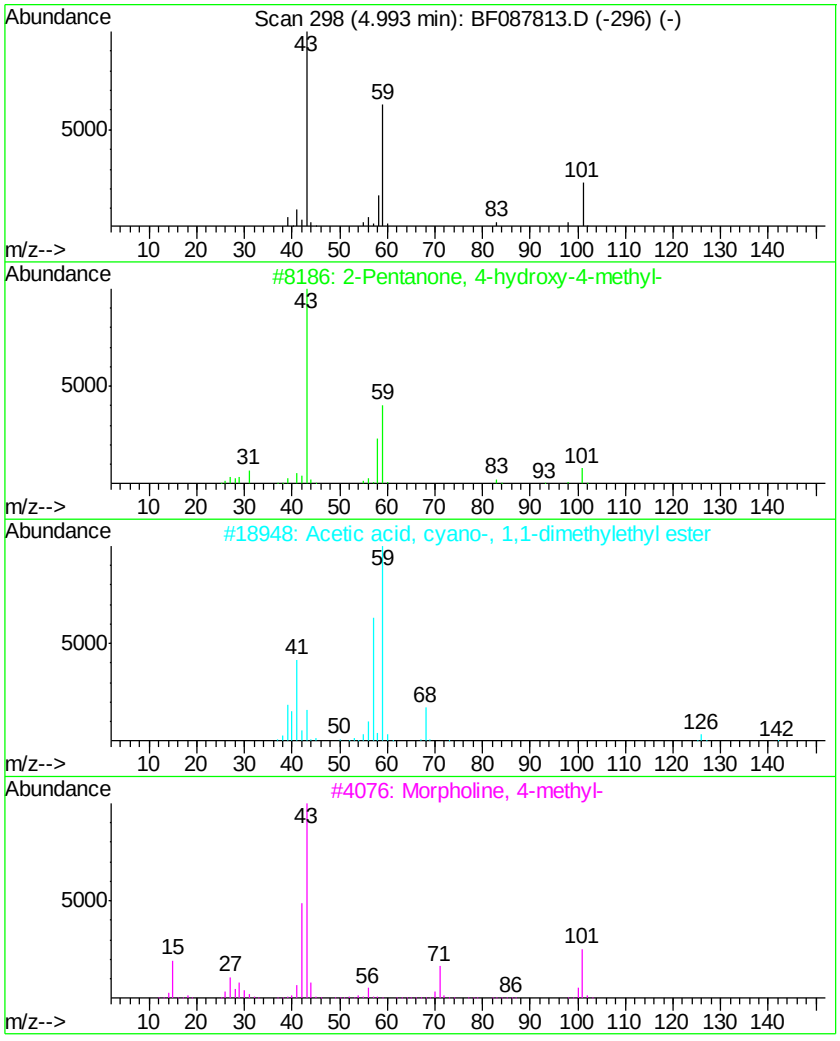
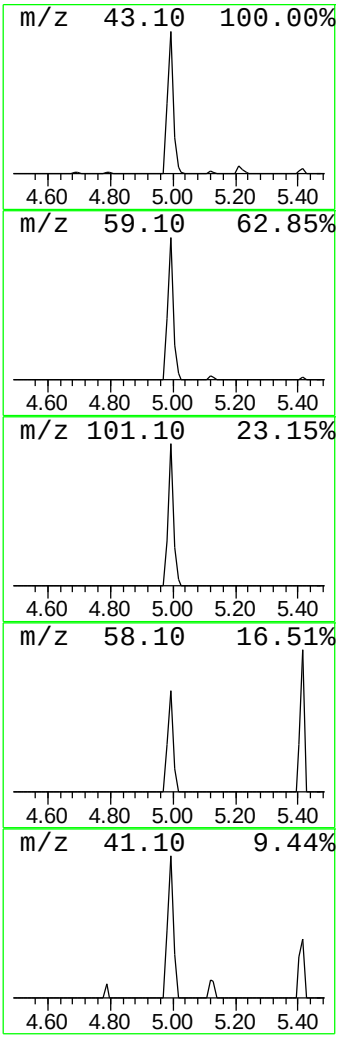
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	3.37 ng	96871	1,4-Dichlorobenzene-d4	6.82

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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : BNA_F
ClientSampleId : SS-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
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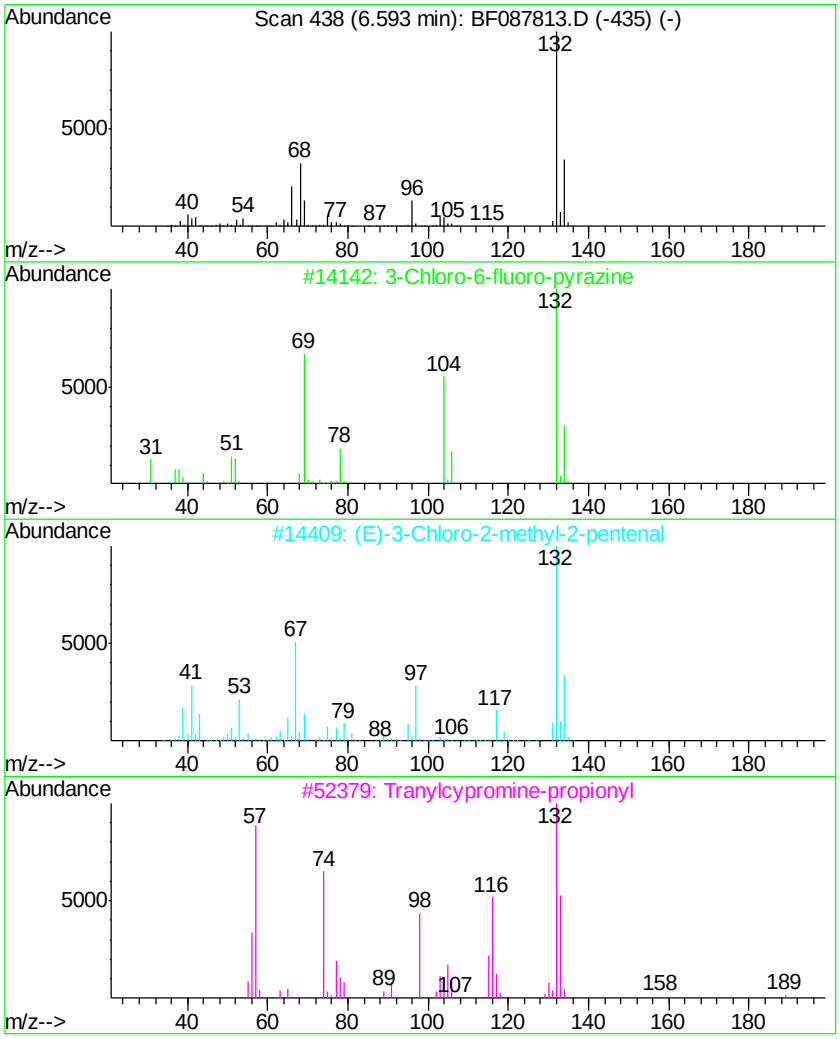
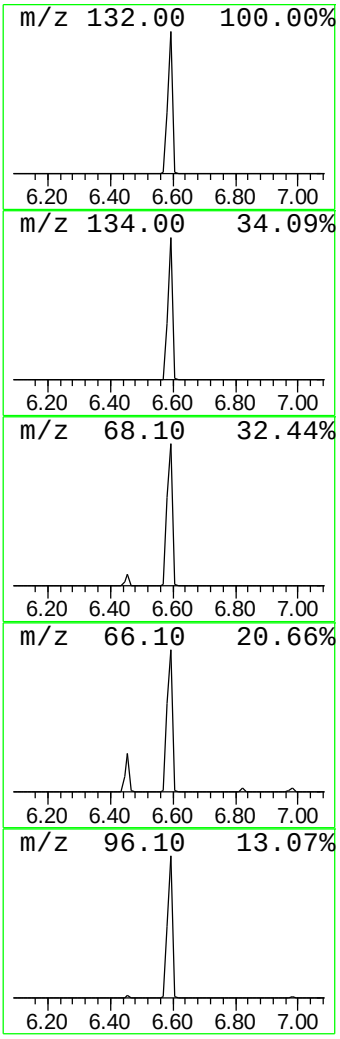
Peak Number 6 unknown6.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	45.01 ng	1293450	1,4-Dichlorobenzene-d4	6.82

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : H3378-11
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Instrument : BNA_F
ClientSampleId : SS-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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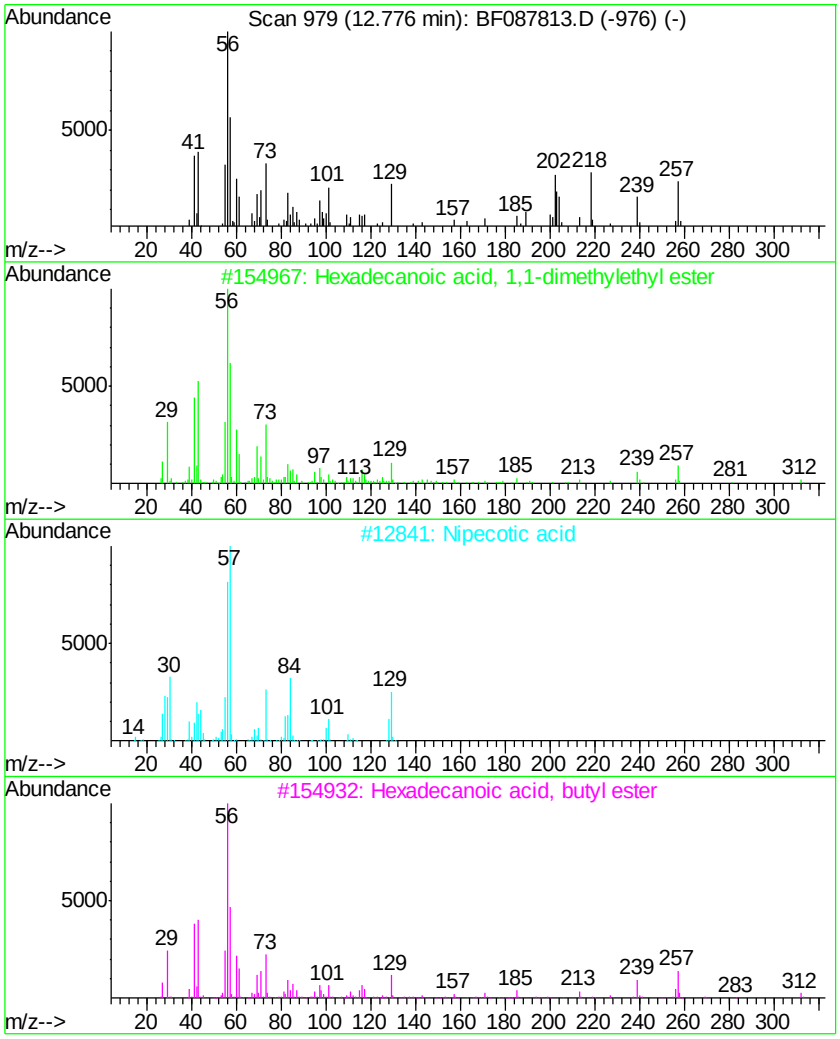
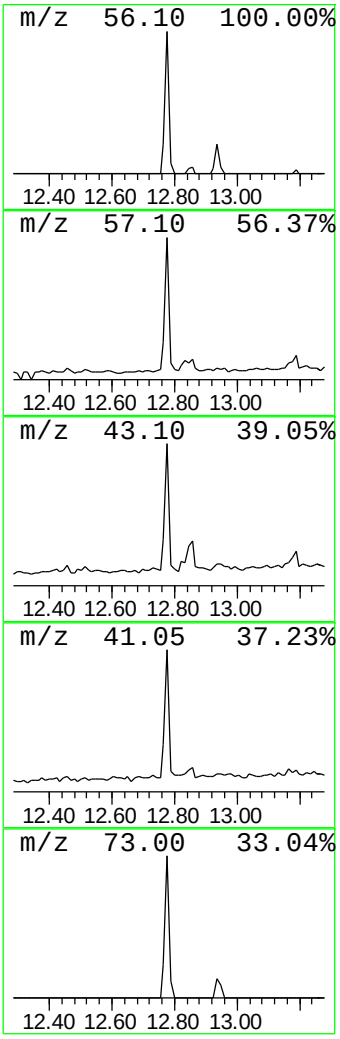
Peak Number 8 unknown12.78 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	4.16 ng	149698	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
2	Nipecotic acid	129	C6H11NO2	000498-95-3	37
3	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	30
4	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	22
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	22





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Instrument : BNA_F
ClientSampleId : SS-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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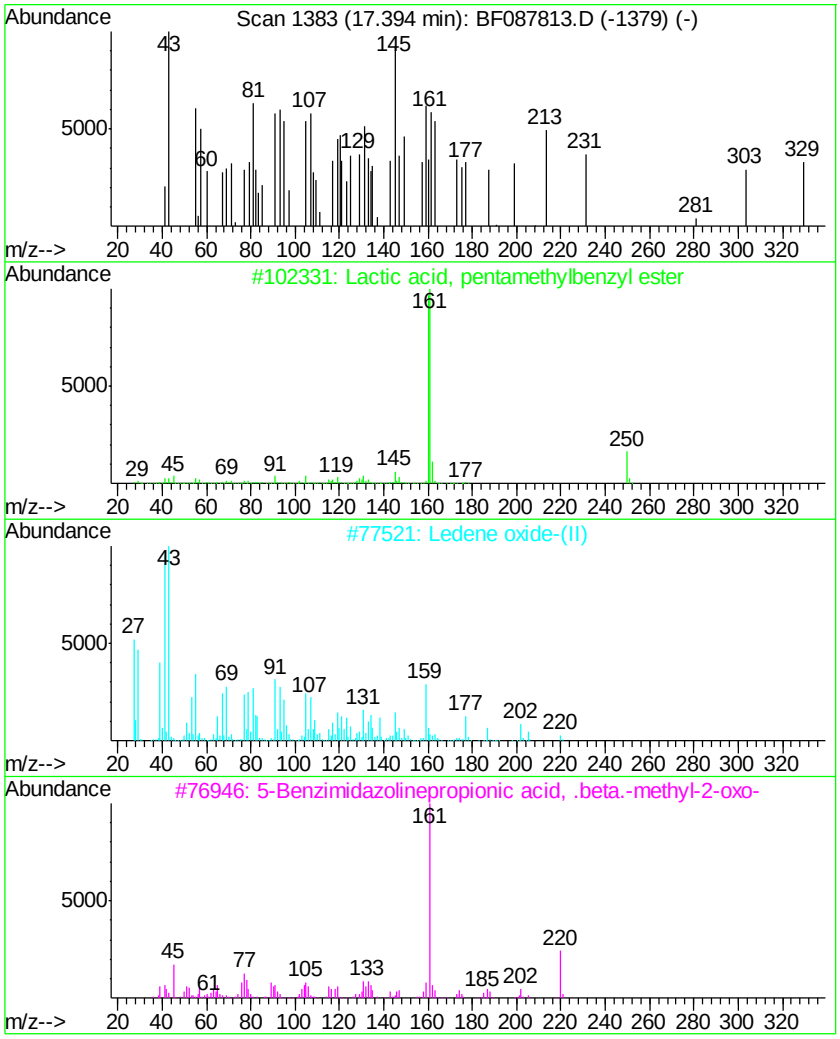
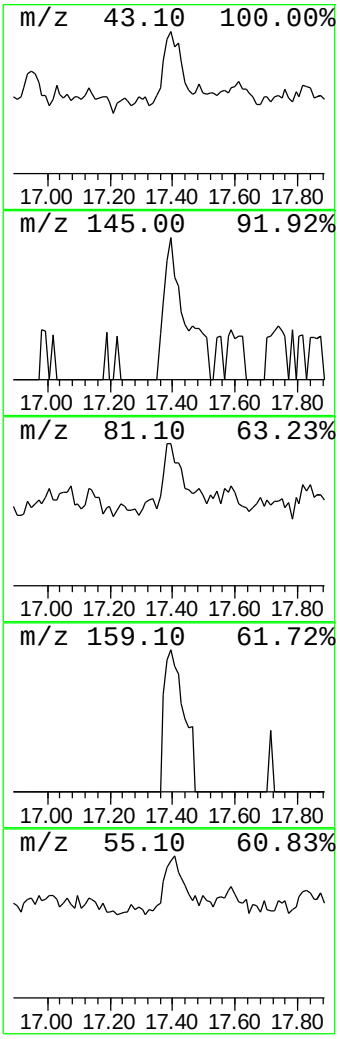
Peak Number 10 unknown17.39 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	3.14 ng	95788	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lactic acid, pentamethylbenzyl e...	250	C15H22O3	019405-32-4	12
2	Ledene oxide-(II)	220	C15H24O	1000159-36-7	11
3	5-Benzimidazolinepropionic acid,...	220	C11H12N2O3	021190-17-0	10
4	Benzeneethanol, .alpha.-methyl-3...	178	C12H18O	054518-11-5	10
5	N-(6-Chloro-5-hydroxy-4-pyridazi...	187	C6H6ClN3O2	098142-22-4	10





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
Propane, 2,2-dime...	1.66	183.1	ng	5260840	1	6.82	574789	20.0
Propane, 1,1-dime...	2.04	18.9	ng	542071	1	6.82	574789	20.0
2-Pentanone, 4-hy...	4.99	3.4	ng	96871	1	6.82	574789	20.0
unknown6.59	6.59	45.0	ng	1293450	1	6.82	574789	20.0
unknown12.78	12.78	4.2	ng	149698	5	13.99	719563	20.0
unknown17.39	17.39	3.1	ng	95788	6	15.42	609954	20.0