LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087554.D
Acq On : 30 May 2016 17:03
Operator : UM/SJ
Sample : H3317-08
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24

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-BF052316.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	4.730	273	275	288	rBV	30800	123429	3.10%	0.469%
2	5.393	331	333	365	rBV	520114	1546424	38.83%	5.876%
3	7.050	476	478	483	rBV	314911	759636	19.08%	2.886%
4	7.130	483	485	502	rVB	1959201	3321920	83.42%	12.623%
5	7.473	513	515	526	rBV	496594	719088	18.06%	2.732%
6	7.702	532	535	551	rVB	2192745	2843296	71.40%	10.804%
7	8.387	593	595	623	rBV	1591159	2493589	62.62%	9.475%
8	9.508	691	693	712	rBV	546907	925641	23.24%	3.517%
9	11.279	845	848	851	rBV	3272788	3982333	100.00%	15.132%
10	12.331	937	940	952	rBV	684657	1030143	25.87%	3.914%
11	13.154	1009	1012	1015	rVB2	26069	41032	1.03%	0.156%
12	13.622	1051	1053	1068	rBV	1277000	2460812	61.79%	9.351%
13	13.931	1077	1080	1085	rVB	26341	42628	1.07%	0.162%
14	14.742	1149	1151	1167	rVB	533691	935659	23.50%	3.555%
15	15.154	1183	1187	1193	rBV	36451	75347	1.89%	0.286%
16	16.823	1330	1333	1340	rBV	56611	118355	2.97%	0.450%
17	16.925	1340	1342	1345	rVB	177773	191049	4.80%	0.726%
18	17.085	1354	1356	1359	rBV	2488453	3142674	78.92%	11.941%
19	17.851	1421	1423	1426	rBV	103318	120811	3.03%	0.459%
20	18.160	1447	1450	1456	rVB	24369	52306	1.31%	0.199%
21	18.331	1463	1465	1471	rBV2	30239	71282	1.79%	0.271%
22	18.468	1474	1477	1489	rBV	274721	668234	16.78%	2.539%
23	20.149	1622	1624	1640	rBV2	224418	651706	16.36%	2.476%

Sum of corrected areas: 26317394

LSC Report - Integrated Chromatogram

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Operator : UM/SJ
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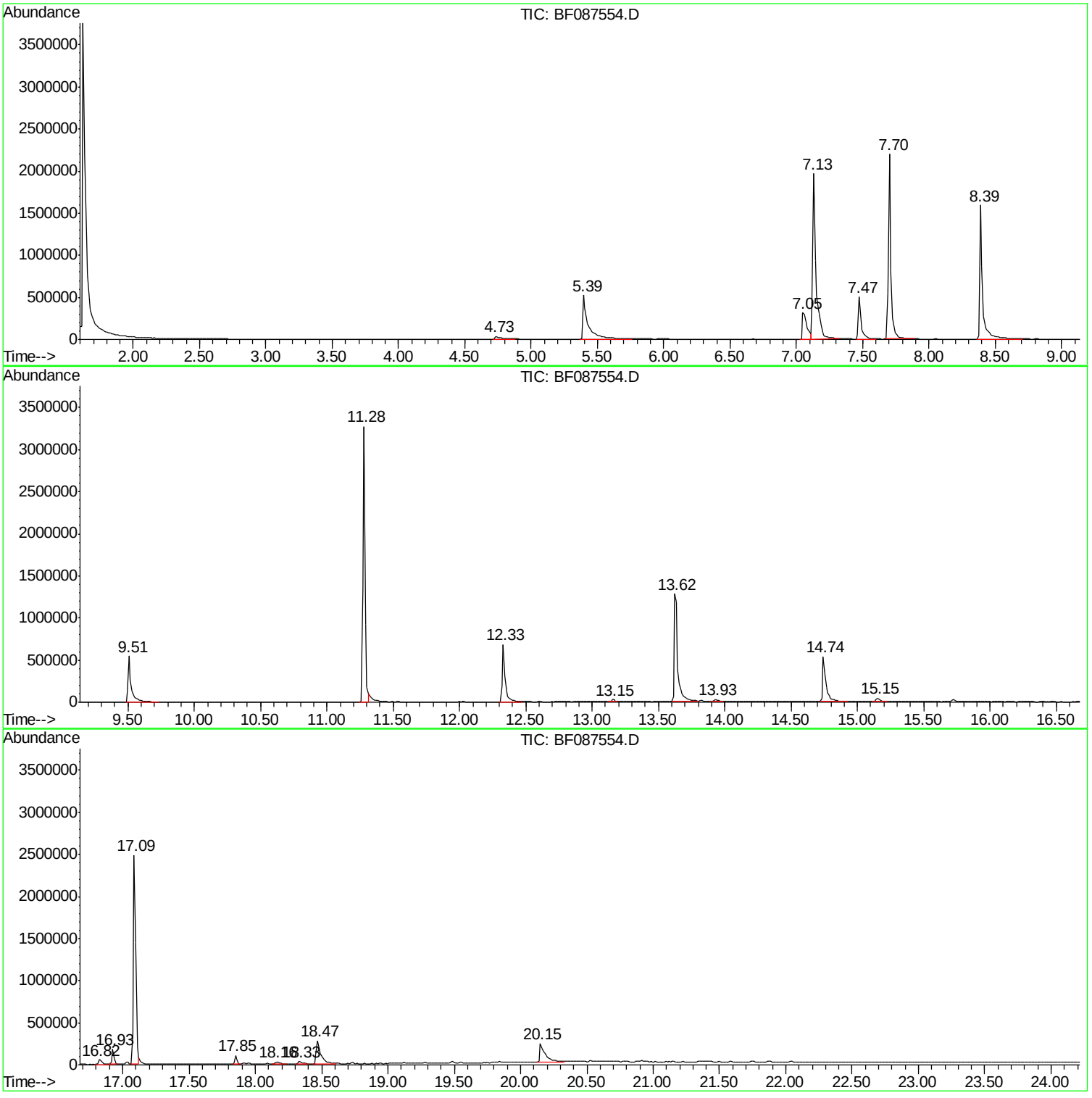
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087554.D
Acq On : 30 May 2016 17:03
Operator : UM/SJ
Sample : H3317-08
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

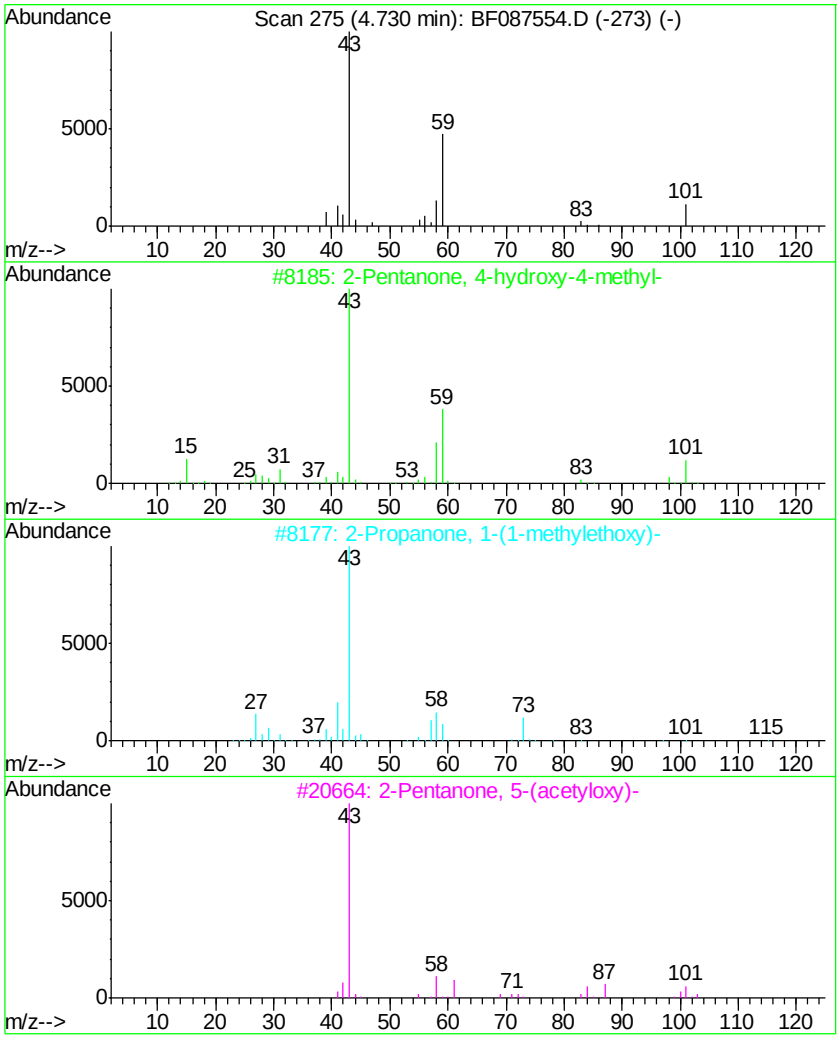
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

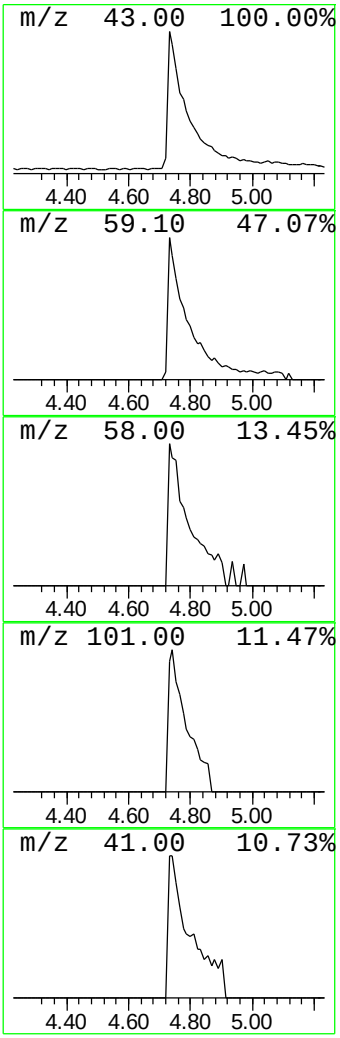
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	3.43 ng	123429	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
3	2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
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Operator : UM/SJ
Sample : H3317-08
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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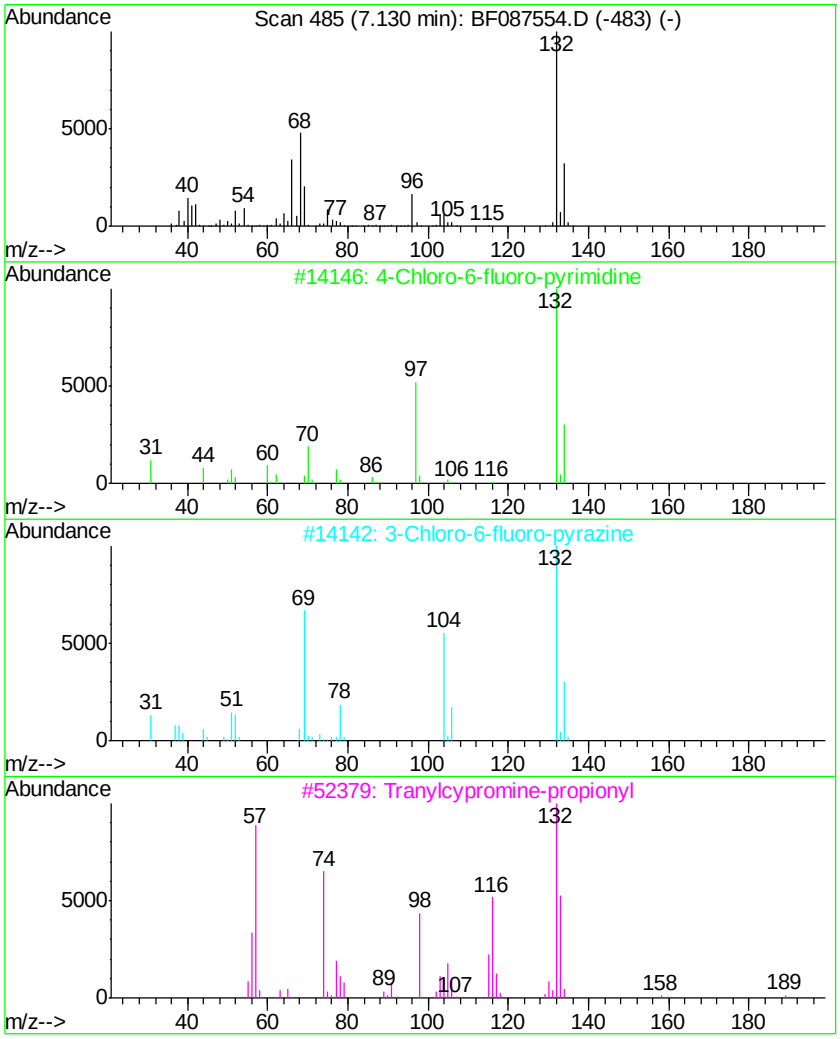
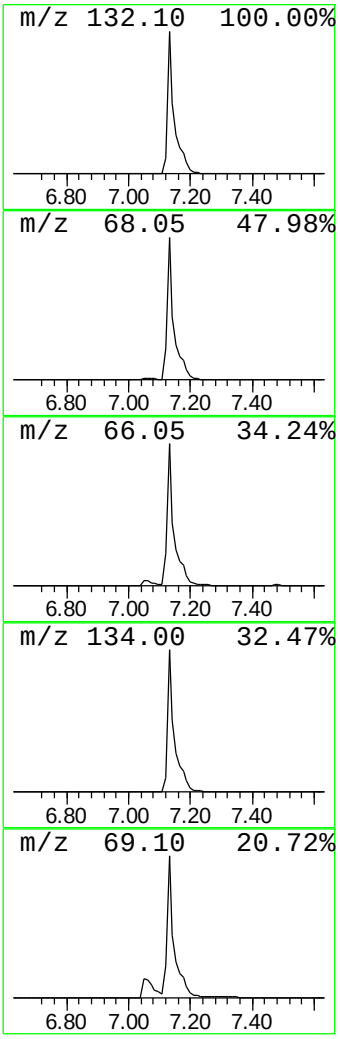
Peak Number 2 unknown7.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	92.39 ng	3321920	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087554.D
Acq On : 30 May 2016 17:03
Operator : UM/SJ
Sample : H3317-08
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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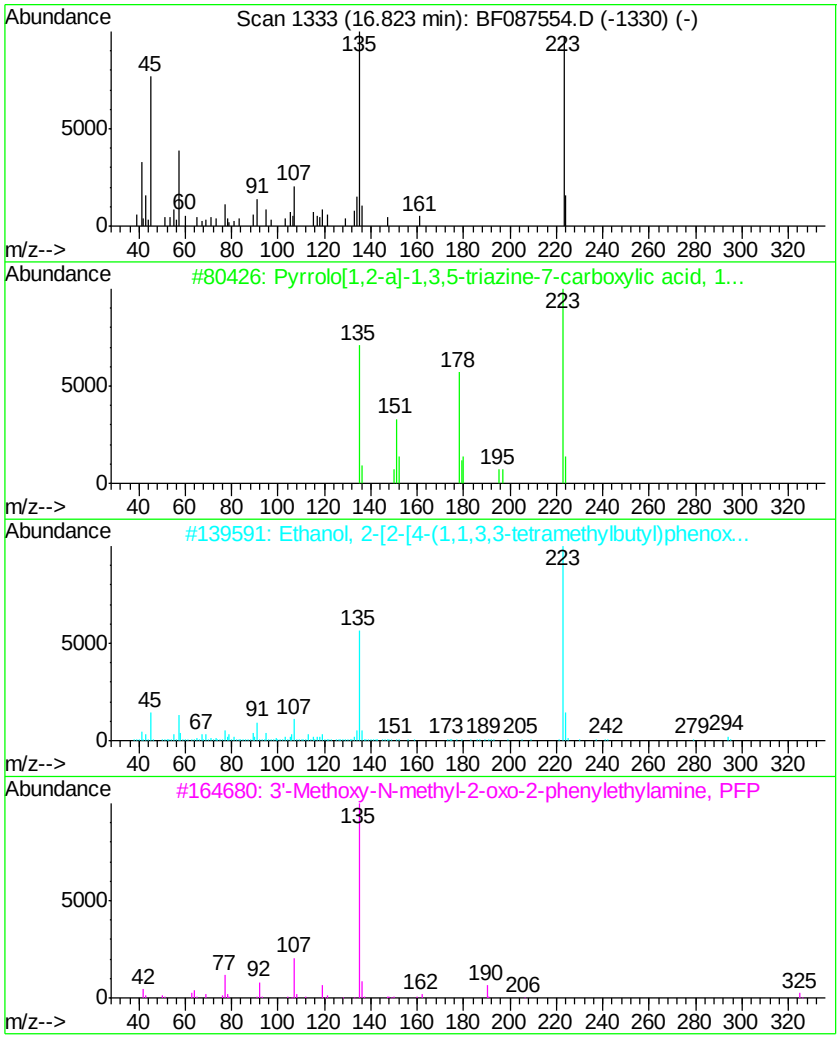
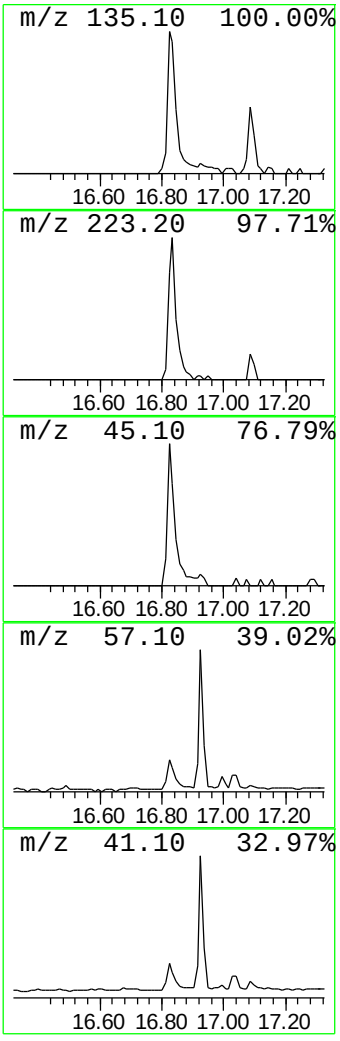
Peak Number 4 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.82	3.54 ng	118355	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
2	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	43
3	3'-Methoxy-N-methyl-2-oxo-2-phen...	325	C13H12F5NO3	1000099-92-9	22
4	2H-1,4-Benzoxazine, 3,4-dihydro-	135	C8H9NO	005735-53-5	18
5	1-Dodecanone, 2-(imidazol-1-yl)-...	356	C22H32N2O2	1000137-95-7	14





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Data File : BF087554.D
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Operator : UM/SJ
Sample : H3317-08
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
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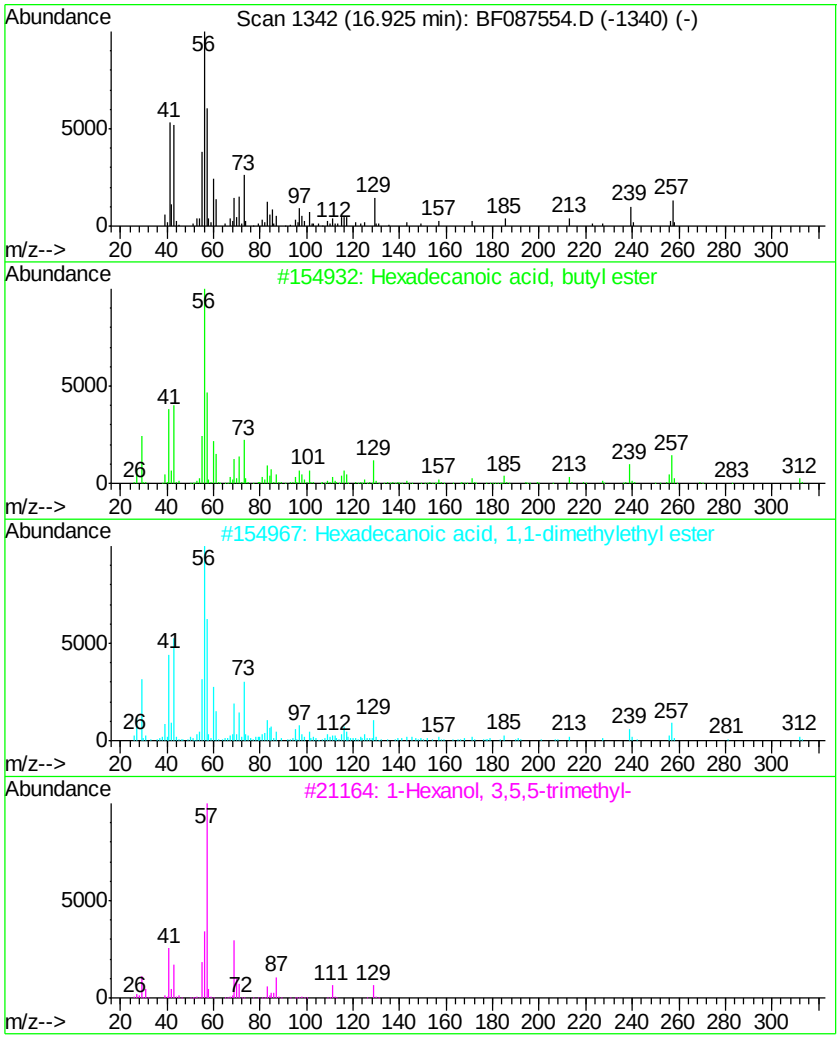
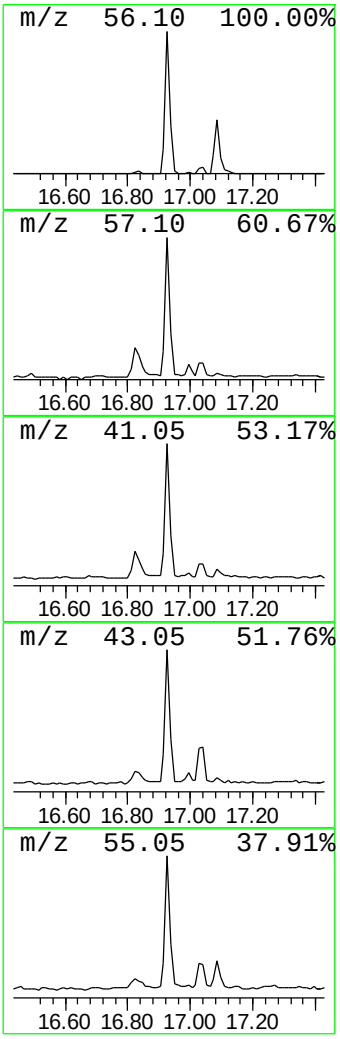
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	5.72 ng	191049	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3	1-Hexanol, 3,5,5-trimethyl-	144	C9H20O	003452-97-9	38
4	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35





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Data File : BF087554.D
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Operator : UM/SJ
Sample : H3317-08
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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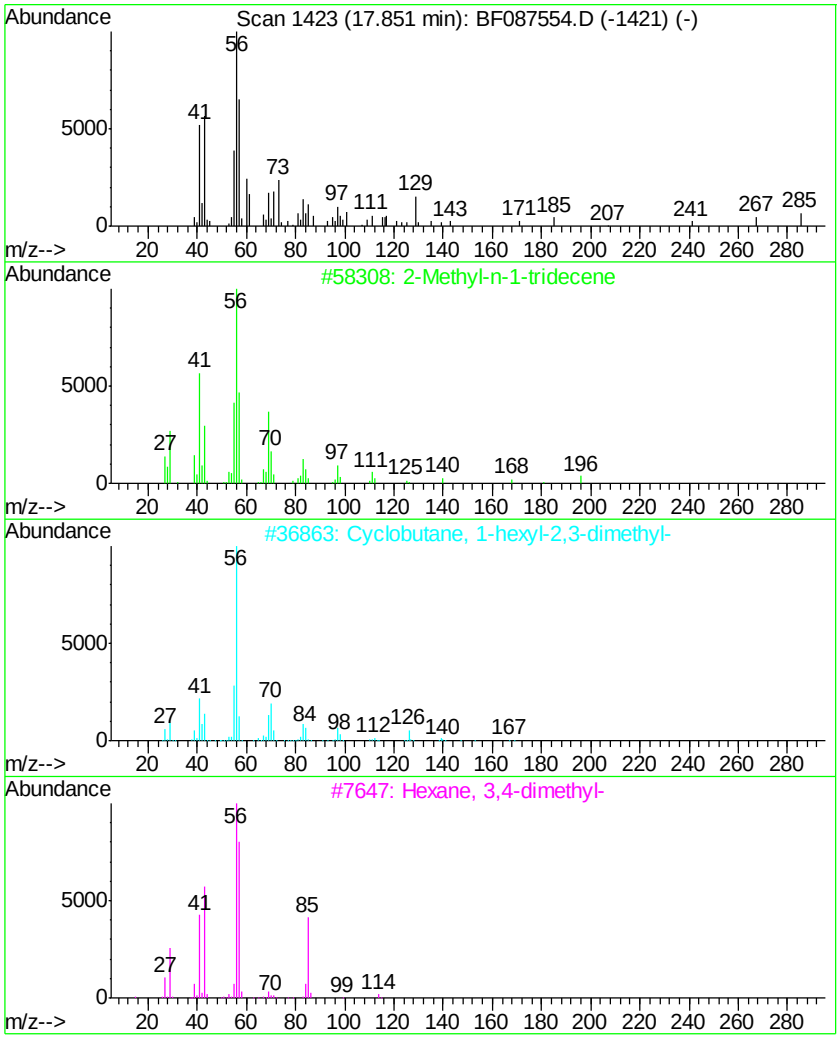
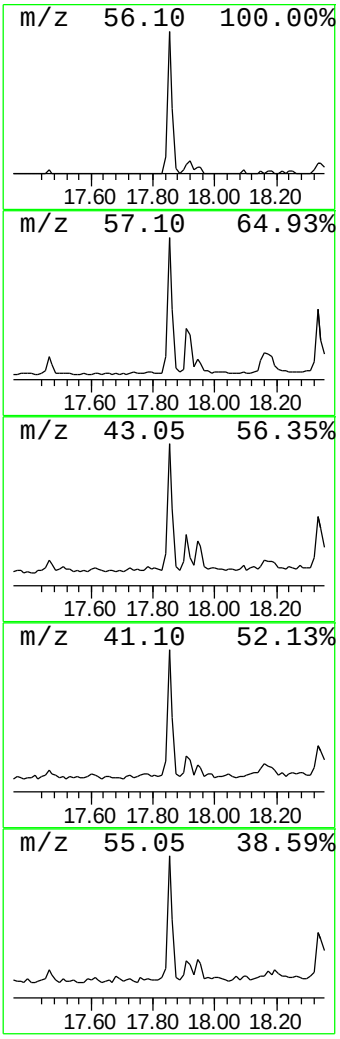
Peak Number 6 unknown17.85 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	3.62 ng	120811	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
2	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
3	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
4	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37
5	Cyclobutanone, 3,3-dimethyl-	98	C6H10O	001192-33-2	35





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Instrument : BNA_F
ClientSampleId : MW-24

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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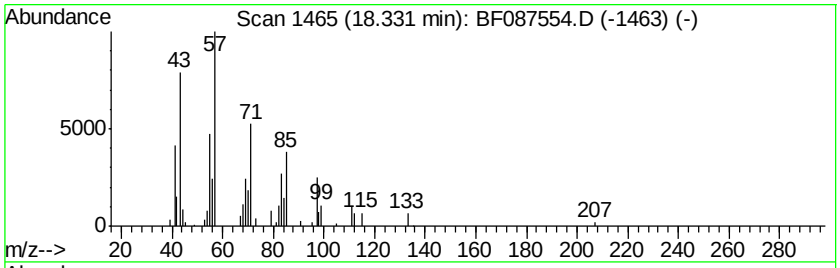
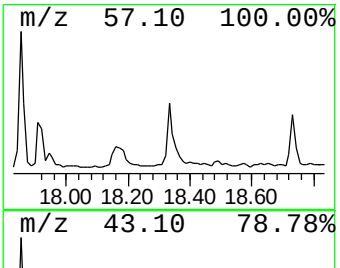
Peak Number 7 1-Octadecanesulphonyl chloride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	2.13 ng	71282	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	80
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	72
4	Dodecane	170	C12H26	000112-40-3	53
5	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	53





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	4.73	3.4	ng	123429	1	7.47	719088	20.0
unknown7.13	7.13	92.4	ng	3321920	1	7.47	719088	20.0
Pyrrolo[1,2-a]-1,...	16.82	3.5	ng	118355	5	18.47	668234	20.0
Hexadecanoic acid...	16.93	5.7	ng	191049	5	18.47	668234	20.0
unknown17.85	17.85	3.6	ng	120811	5	18.47	668234	20.0
1-Octadecanesulph...	18.33	2.1	ng	71282	5	18.47	668234	20.0