LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095482.D
Acq On : 27 May 2017 3:54
Operator : SJ/MA
Sample : I3316-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-3

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-BF050217.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	5.095	534	537	552	rBV2	22424	71555	2.25%	0.405%
2	5.737	642	646	680	rBV	171957	677367	21.34%	3.831%
3	7.254	901	904	913	rBV	26423	50804	1.60%	0.287%
4	7.331	913	917	927	rVV	93479	279913	8.82%	1.583%
5	7.413	927	931	960	rVB	769388	1687058	53.16%	9.543%
6	7.742	983	987	1002	rVB	358556	474605	14.95%	2.685%
7	7.978	1022	1027	1051	rBV	1638348	2175167	68.53%	12.304%
8	8.648	1136	1141	1179	rBV	738711	1584635	49.93%	8.963%
9	9.766	1327	1331	1358	rBV2	300571	733541	23.11%	4.149%
10	10.936	1526	1530	1544	rBV	59625	111887	3.53%	0.633%
11	11.089	1551	1556	1569	rVB	37974	64275	2.03%	0.364%
12	11.530	1626	1631	1656	rBV	2021406	3173817	100.00%	17.953%
13	11.707	1656	1661	1666	rBV	18911	35249	1.11%	0.199%
14	11.977	1699	1707	1719	rVB5	15861	41729	1.31%	0.236%
15	12.077	1719	1724	1728	rBV2	25466	44357	1.40%	0.251%
16	12.242	1747	1752	1771	rBV	78142	175755	5.54%	0.994%
17	12.595	1807	1812	1817	rBV2	436219	633446	19.96%	3.583%
18	12.648	1817	1821	1832	rVB	338838	537906	16.95%	3.043%
19	12.954	1868	1873	1883	rBV	87177	175541	5.53%	0.993%
20	13.495	1960	1965	1977	rBV2	148720	243898	7.68%	1.380%
21	13.901	2030	2034	2051	rBV	319117	617078	19.44%	3.490%
22	15.001	2216	2221	2224	rBV	312819	404856	12.76%	2.290%
23	15.042	2224	2228	2240	rVV	353097	649128	20.45%	3.672%
24	15.142	2241	2245	2255	rVB2	23482	49167	1.55%	0.278%
25	15.942	2375	2381	2397	rVB4	31779	81438	2.57%	0.461%
26	16.795	2521	2526	2540	rBV	123342	188976	5.95%	1.069%
27	17.095	2569	2577	2587	rBV	84668	129108	4.07%	0.730%
28	17.318	2610	2615	2629	rBV	1473433	1842081	58.04%	10.420%
29	18.683	2842	2847	2863	rBV	259640	447691	14.11%	2.532%
30	20.365	3128	3133	3141	rBV	159282	296890	9.35%	1.679%

Sum of corrected areas: 17678918

LSC Report - Integrated Chromatogram

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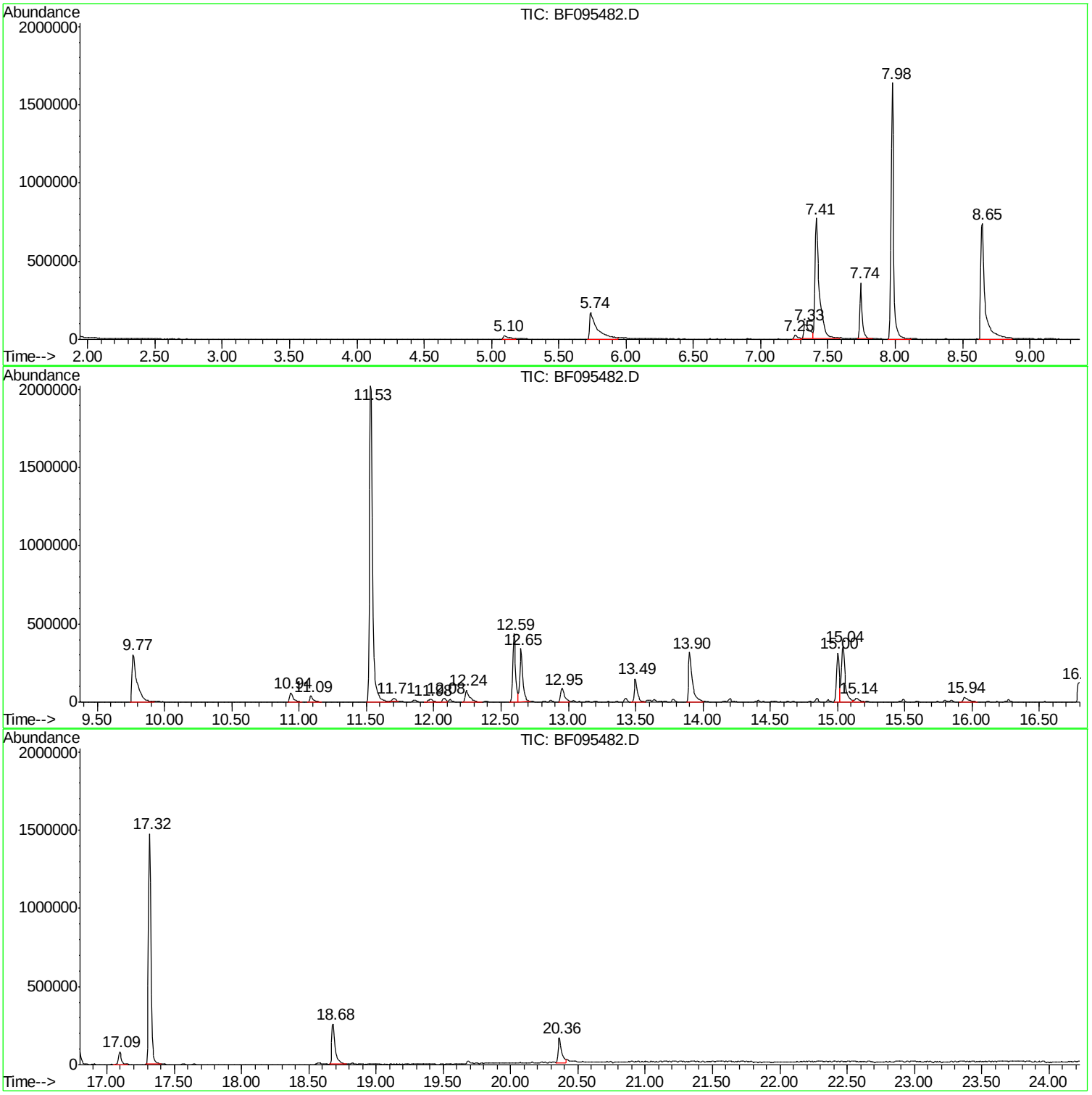
Operator : SJ/MA
Sample : I3316-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095482.D
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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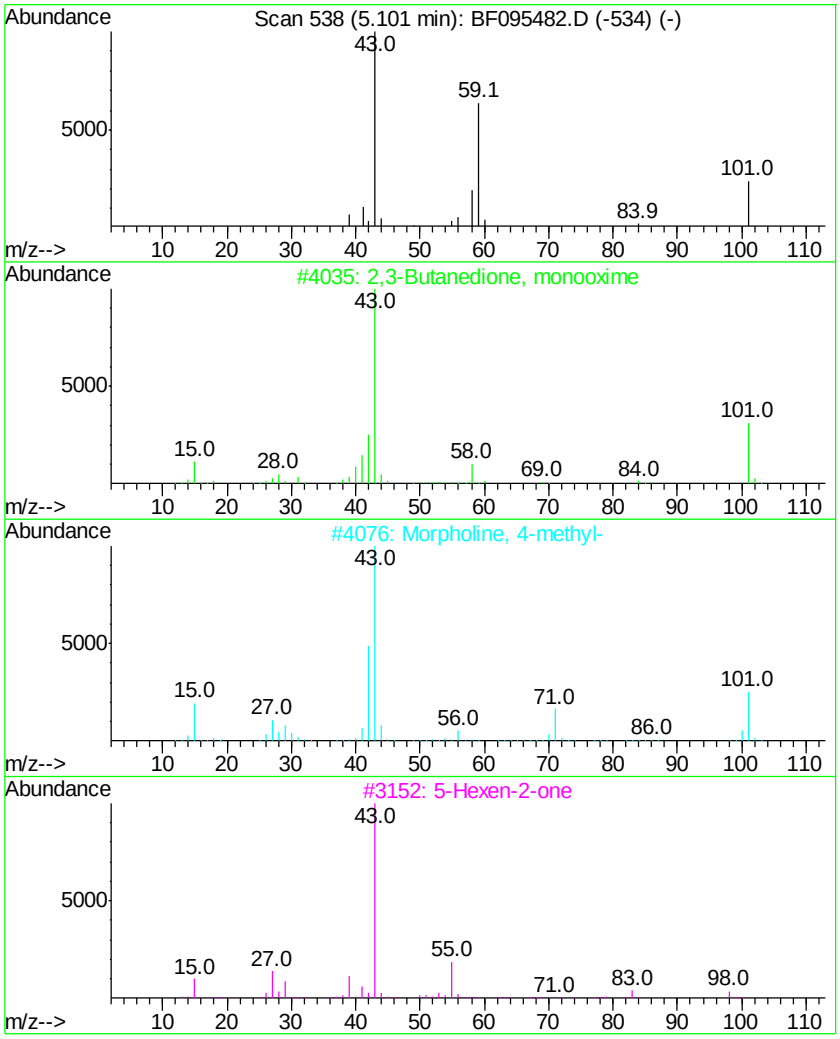
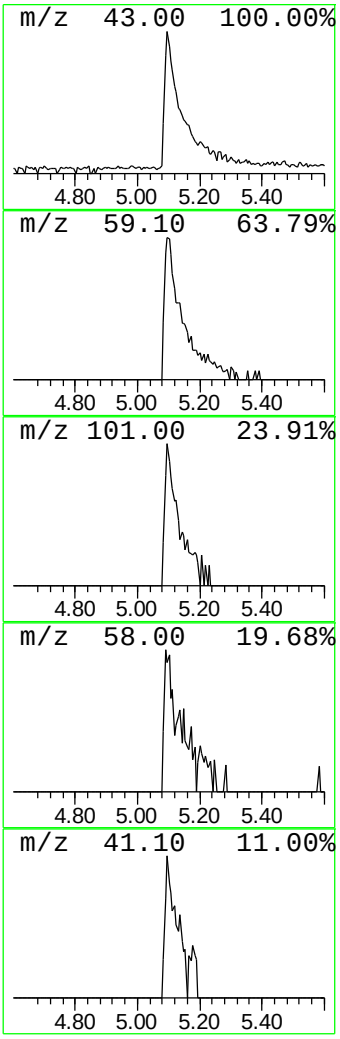
Peak Number 1 unknown5.10 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	3.02 ng	71555	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	5
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	5
3	5-Hexen-2-one	98	C6H10O	000109-49-9	5
4	Diacetamide	101	C4H7NO2	000625-77-4	4
5	Guanidine	59	CH5N3	000113-00-8	4





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095482.D
Acq On : 27 May 2017 3:54
Operator : SJ/MA
Sample : I3316-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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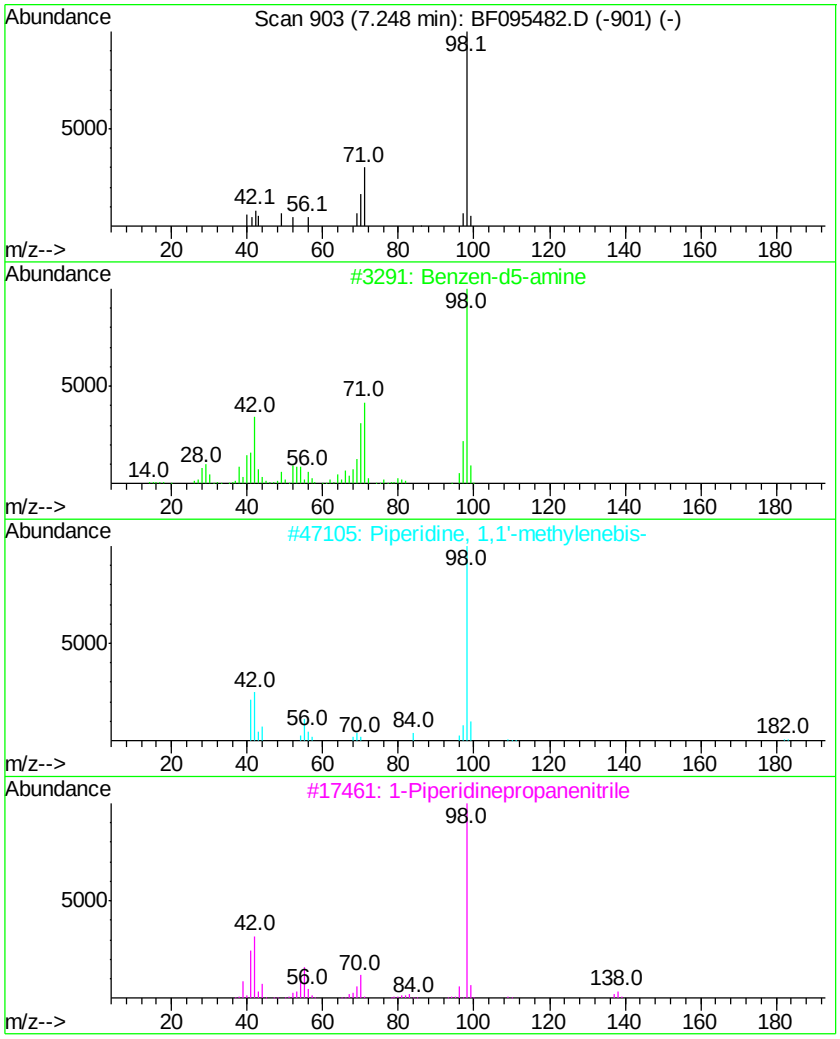
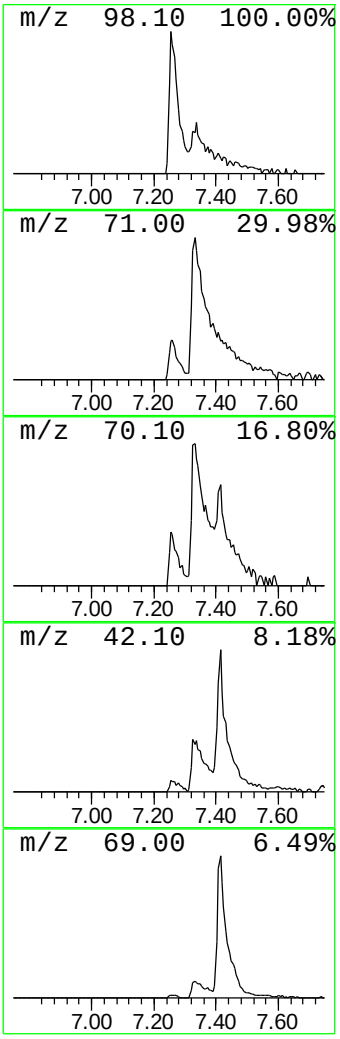
Peak Number 2 Benzen-d5-amine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.25	2.14 ng	50804	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzen-d5-amine	98	C6H2D5N	004165-61-1	86
2	Piperidine, 1,1'-methylenebis-	182	C11H22N2	000880-09-1	59
3	1-Piperidinepropanenitrile	138	C8H14N2	003088-41-3	59
4	3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	50
5	1-Methyl-2-piperidinemethanol	129	C7H15NO	020845-34-5	45





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
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Acq On : 27 May 2017 3:54
Operator : SJ/MA
Sample : I3316-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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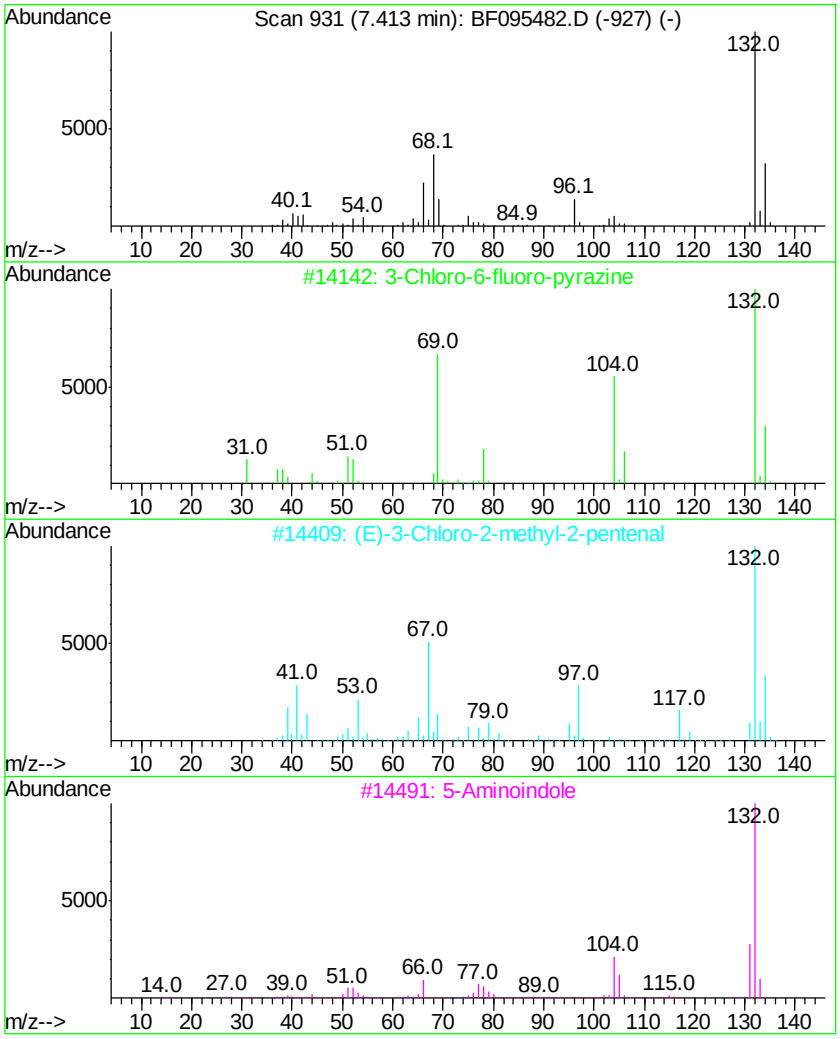
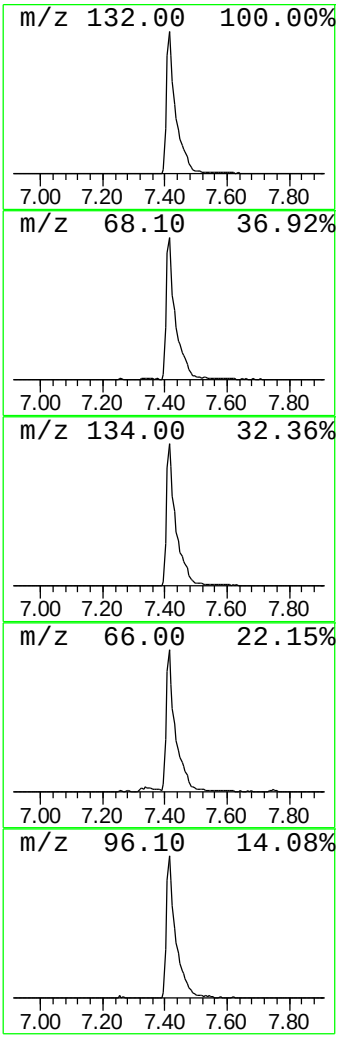
Peak Number 3 unknown7.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	71.09 ng	1687060	1,4-Dichlorobenzene-d4	7.74

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	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10





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ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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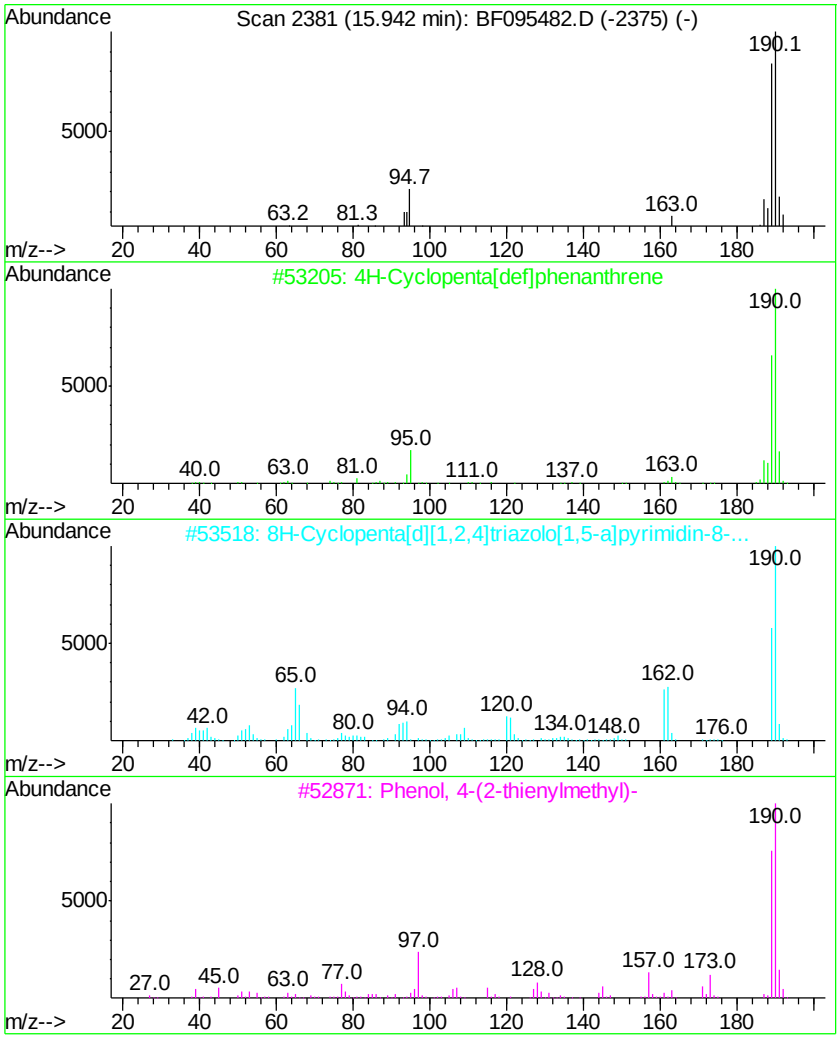
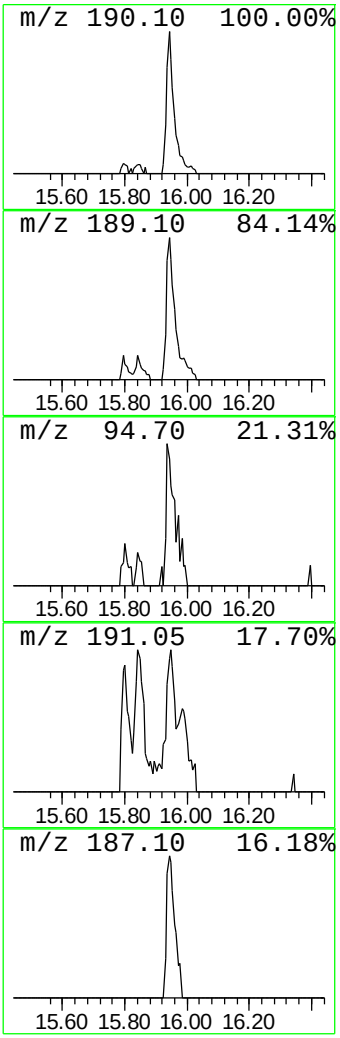
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	4.02 ng	81438	Phenanthrene-d10	15.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2	8H-Cyclopenta[d][1,2,4]triazolo[...	190	C9H10N4O	1000337-56-4	72
3	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	64
4	Cyclohepta[cd][2]benzothiophene,...	190	C12H14S	199807-57-3	64
5	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052617\
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ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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
unknown5.10	5.10	3.0	ng	71555	1	7.74	474605	20.0
Benzen-d5-amine	7.25	2.1	ng	50804	1	7.74	474605	20.0
unknown7.41	7.41	71.1	ng	1687060	1	7.74	474605	20.0
4H-Cyclopenta[def...	15.94	4.0	ng	81438	4	15.00	404856	20.0