LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125007.D
Acq On : 9 Aug 2021 18:16
Operator : JU/CG
Sample : M3299-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210562-COM-35

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125007.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	499	502	506	rBB	4461	4807	2.54%	0.415%
2	5.440	566	570	573	rBV	145988	142480	75.36%	12.301%
3	6.451	737	742	745	rBV	157007	145618	77.02%	12.572%
4	6.816	801	804	807	rBB	43852	32460	17.17%	2.802%
5	7.381	896	900	903	rBB	105932	96170	50.86%	8.303%
6	8.004	1004	1006	1012	rBB	8053	6795	3.59%	0.587%
7	8.098	1019	1022	1026	rBB	56942	45293	23.96%	3.910%
8	9.175	1201	1205	1208	rBV	215644	179611	95.00%	15.507%
9	9.851	1317	1320	1324	rBB	57688	51042	27.00%	4.407%
10	10.645	1451	1455	1458	rBB	121344	102427	54.17%	8.843%
11	11.339	1570	1573	1576	rBV	69794	53319	28.20%	4.603%
12	11.863	1659	1662	1664	rBB	3259	2957	1.56%	0.255%
13	12.645	1792	1795	1799	rBB2	4804	5695	3.01%	0.492%
14	12.927	1839	1843	1846	rBB	215090	189073	100.00%	16.323%
15	13.810	1990	1993	1995	rBV	1657	2311	1.22%	0.200%
16	13.839	1995	1998	2002	rVB	7925	8785	4.65%	0.758%
17	13.974	2018	2021	2025	rBB	45845	38333	20.27%	3.309%
18	14.439	2095	2100	2103	rBV	3420	3881	2.05%	0.335%
19	14.739	2148	2151	2153	rBB	3151	2686	1.42%	0.232%
20	15.068	2204	2207	2211	rBB	4594	4986	2.64%	0.430%
21	15.433	2264	2269	2274	rBV2	24314	30905	16.35%	2.668%
22	15.863	2339	2342	2347	rBB2	3489	5153	2.73%	0.445%
23	16.362	2423	2427	2432	rBB	2571	3505	1.85%	0.303%

Sum of corrected areas: 1158292

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
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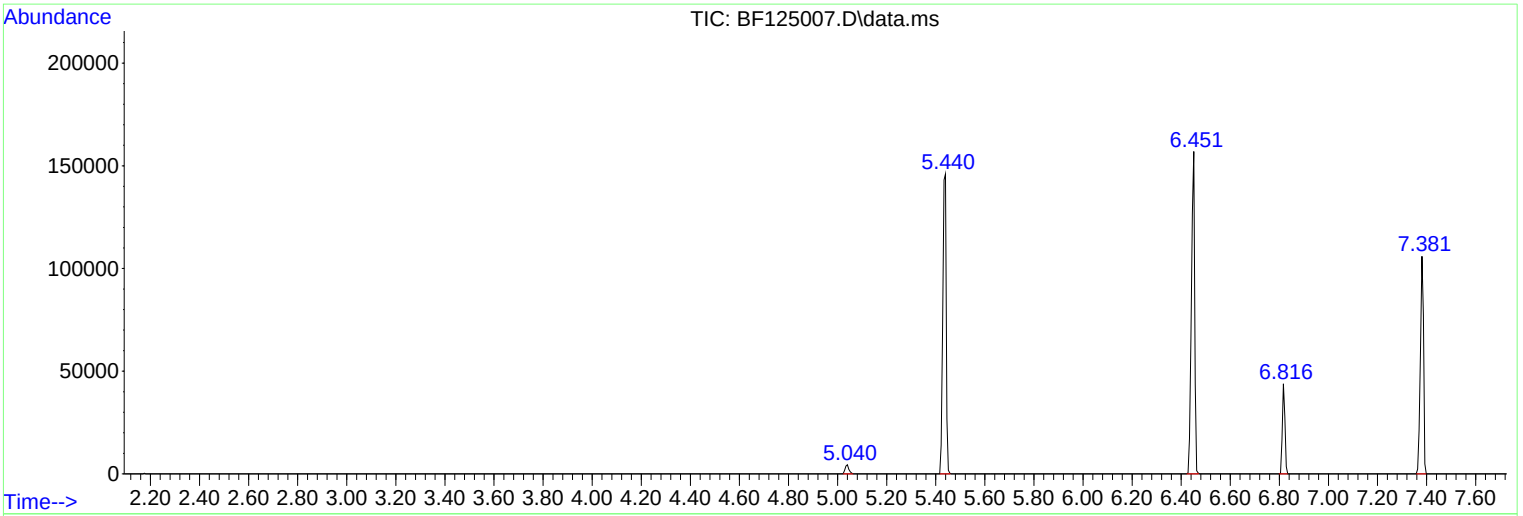
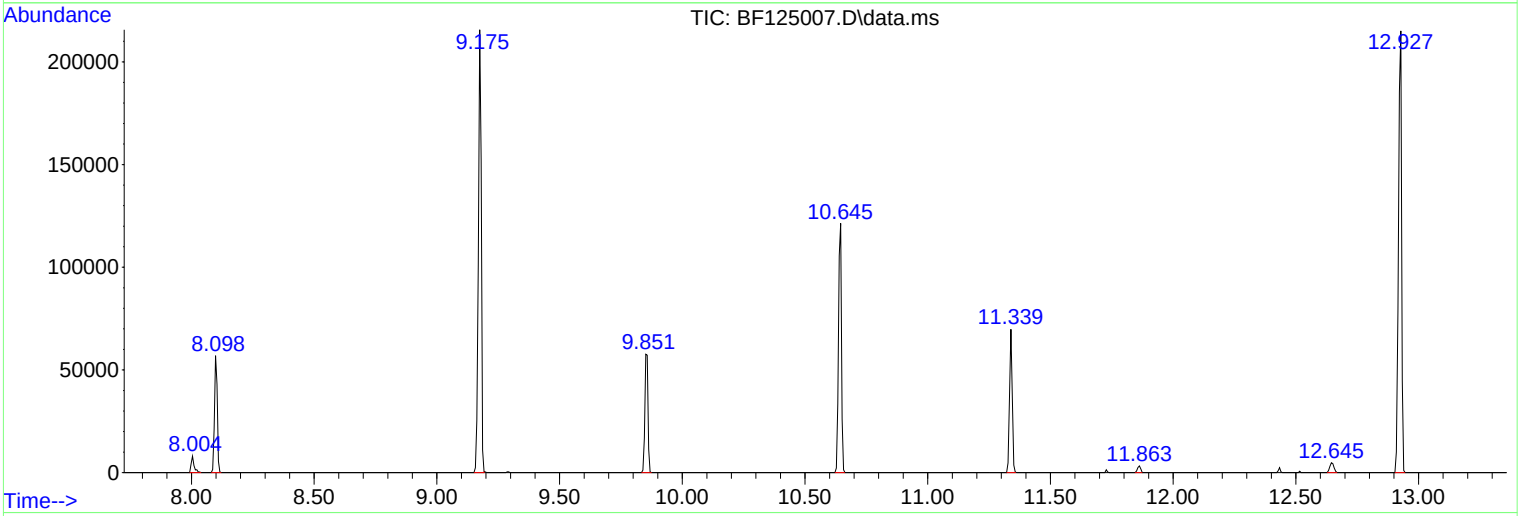
Misc :
ALS Vial : 4 Sample Multiplier: 1

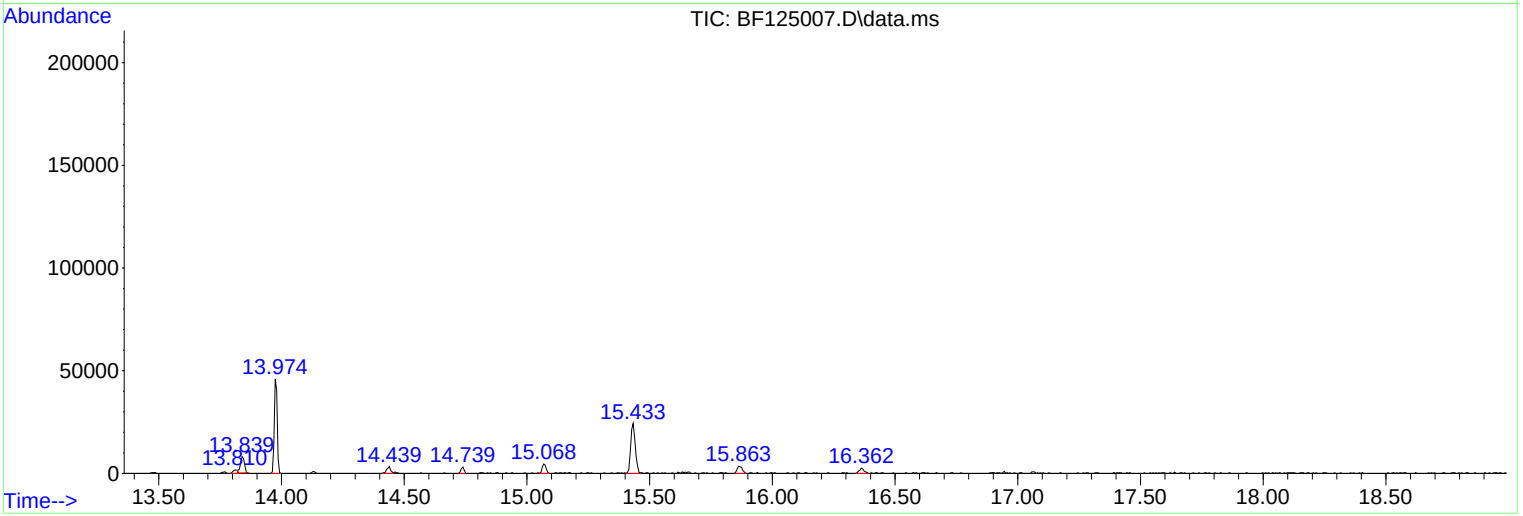
Instrument :
BNA_F
ClientSampleId :
20210562-COM-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Data File : BF125007.D
Acq On : 9 Aug 2021 18:16
Operator : JU/CG
Sample : M3299-02
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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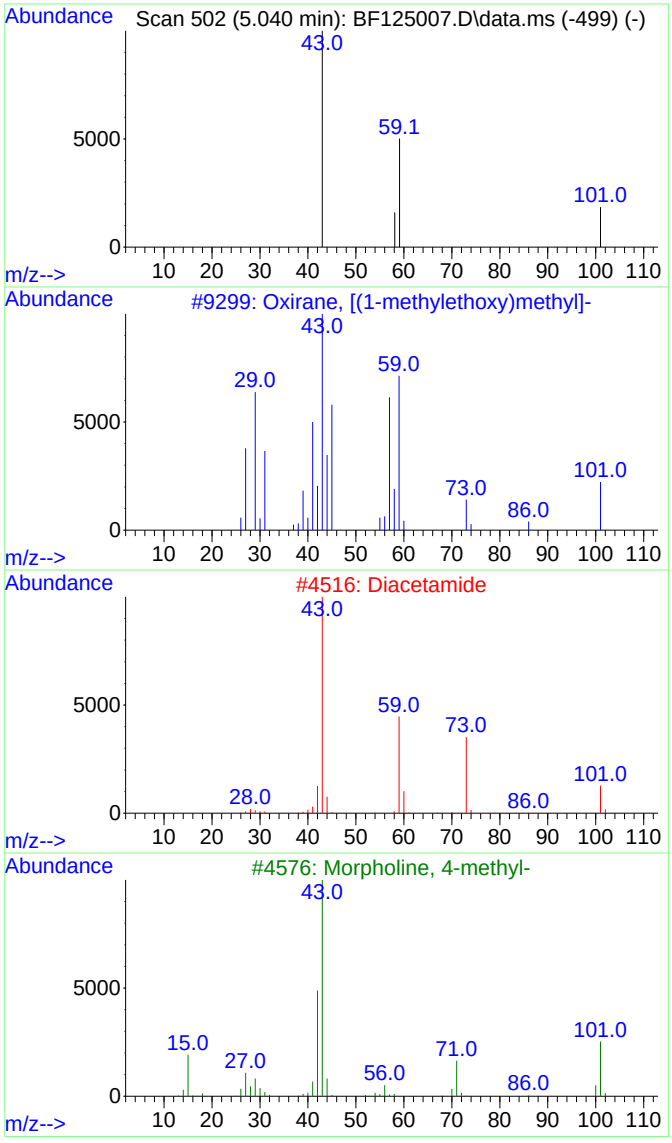
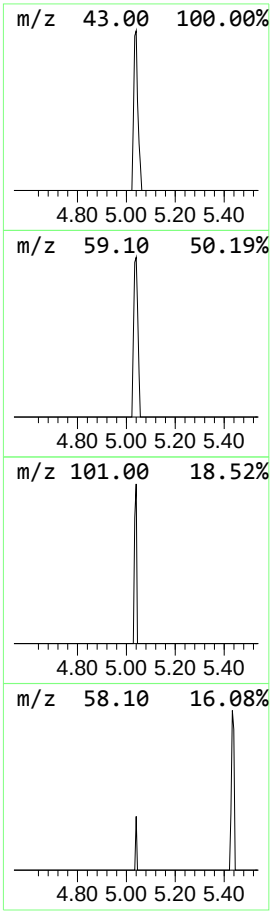
Peak Number 1 unknown5.040 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.96 ng	4807	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	9
2	Diacetamide	101	C4H7NO2	000625-77-4	7
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	4
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	3
5	Propylamine	59	C3H9N	000107-10-8	3





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Data File : BF125007.D
Acq On : 9 Aug 2021 18:16
Operator : JU/CG
Sample : M3299-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210562-COM-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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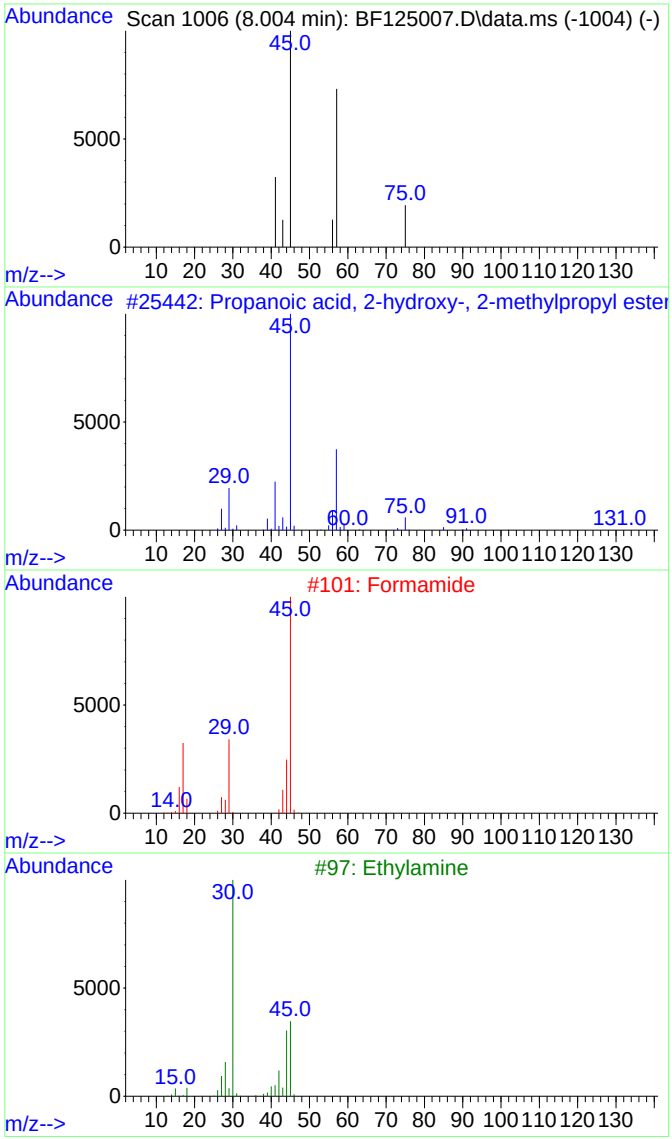
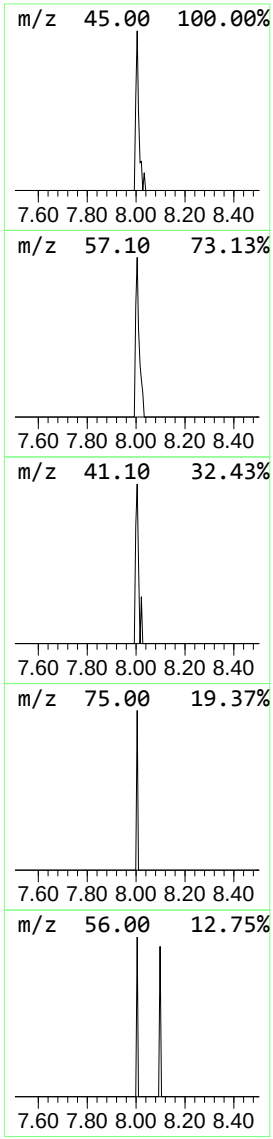
Peak Number 2 unknown8.004 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	3.00 ng	6795	Naphthalene-d8	8.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	4
2	Formamide	45	CH3NO	000075-12-7	3
3	Ethylamine	45	C2H7N	000075-04-7	3
4	Methane, nitroso-	45	CH3NO	000865-40-7	3
5	Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	3





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Acq On : 9 Aug 2021 18:16
Operator : JU/CG
Sample : M3299-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210562-COM-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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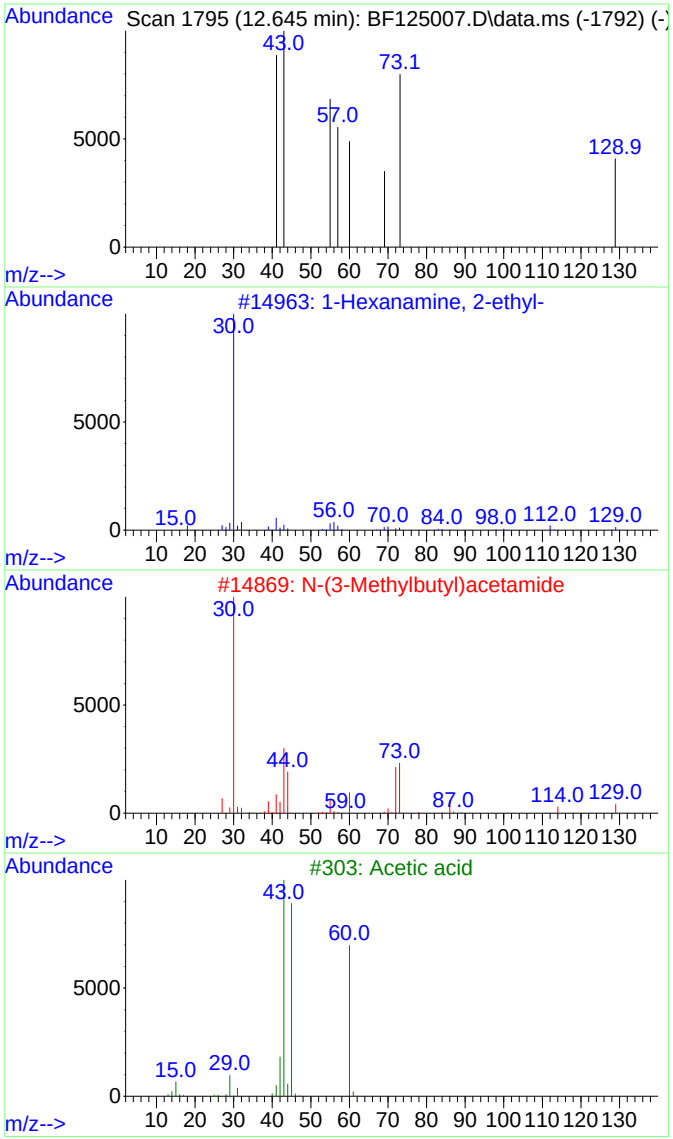
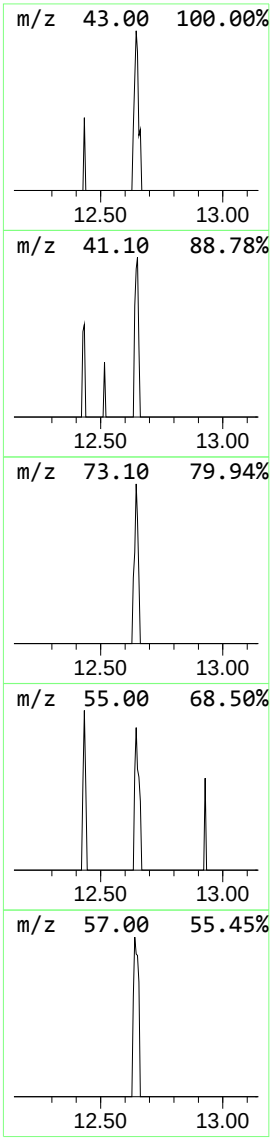
Peak Number 3 unknown12.645 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.14 ng	5695	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanamine, 2-ethyl-	129	C8H19N	000104-75-6	5
2	N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	4
3	Acetic acid	60	C2H4O2	000064-19-7	4
4	3-Pentane isothiocyanate	129	C6H11NS	201224-89-7	4
5	N-Pentylacetamide	129	C7H15NO	002524-60-9	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125007.D
Acq On : 9 Aug 2021 18:16
Operator : JU/CG
Sample : M3299-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210562-COM-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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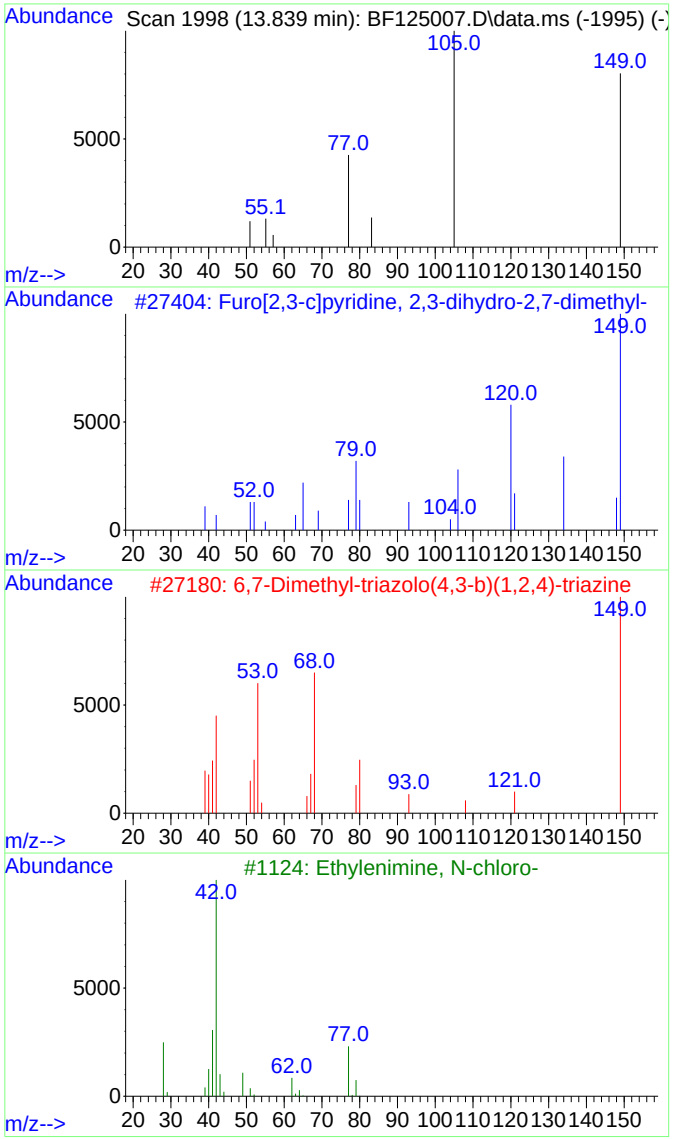
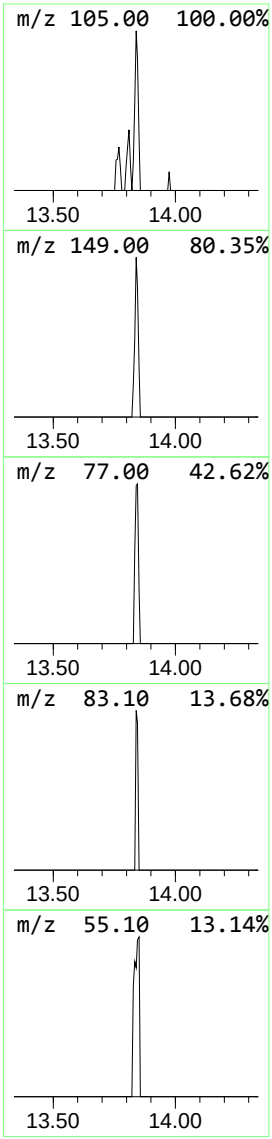
Peak Number 4 unknown13.839 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	4.58 ng	8785	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furo[2,3-c]pyridine, 2,3-dihydro...	149	C9H11NO	069022-82-8	4
2	6,7-Dimethyl-triazolo(4,3-b)(1,2...	149	C6H7N5	061139-73-9	4
3	Ethylenimine, N-chloro-	77	C2H4ClN	010165-13-6	3
4	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	2
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125007.D
Acq On : 9 Aug 2021 18:16
Operator : JU/CG
Sample : M3299-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210562-COM-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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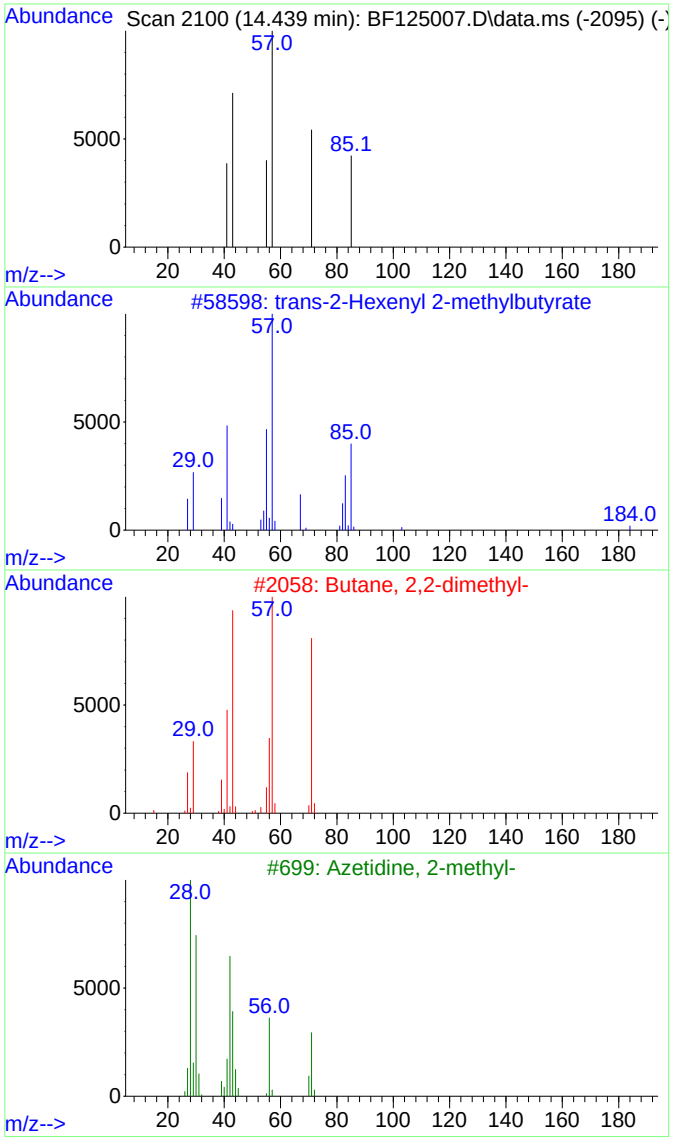
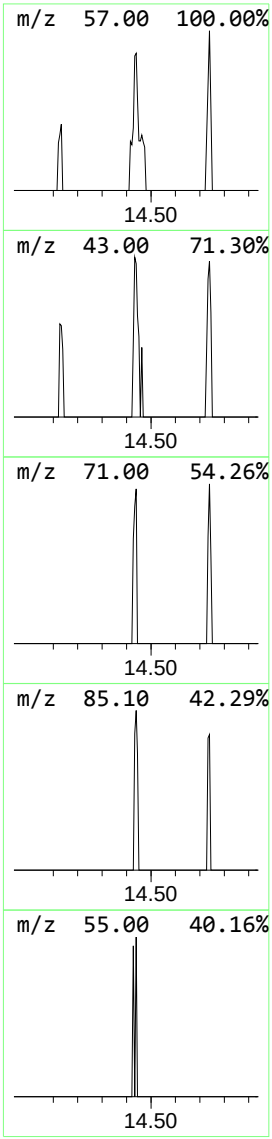
Peak Number 5 unknown14.439 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.439	2.02 ng	3881	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
2	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
3	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
4	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
5	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4





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Sample : M3299-02
Misc :
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Instrument :
BNA_F
ClientSampleId :
20210562-COM-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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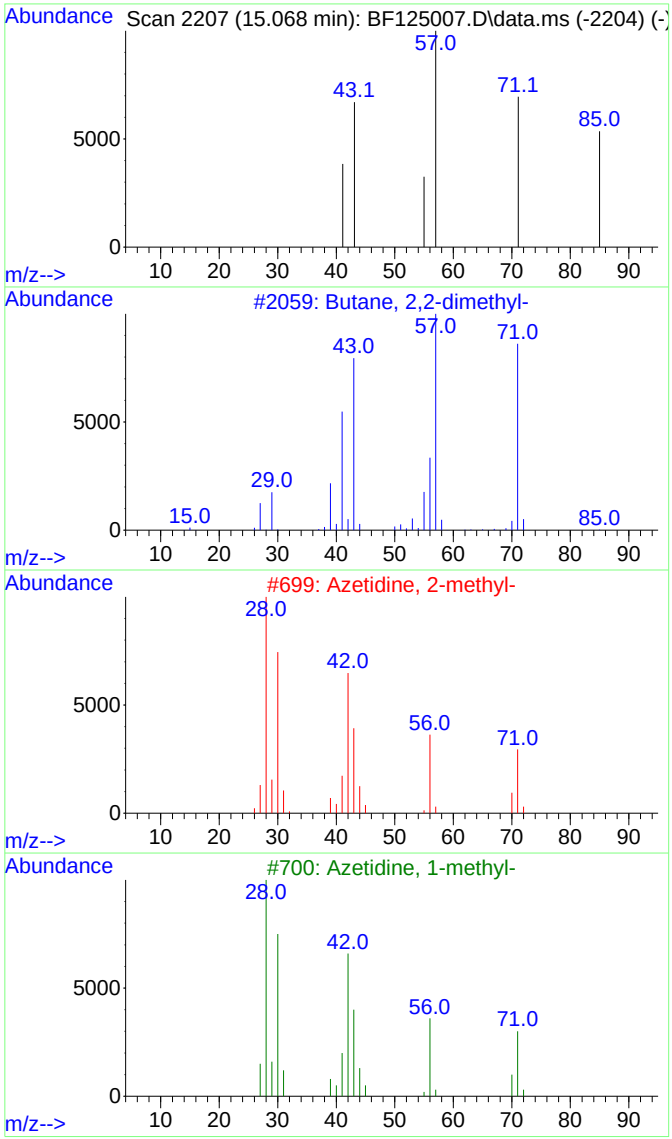
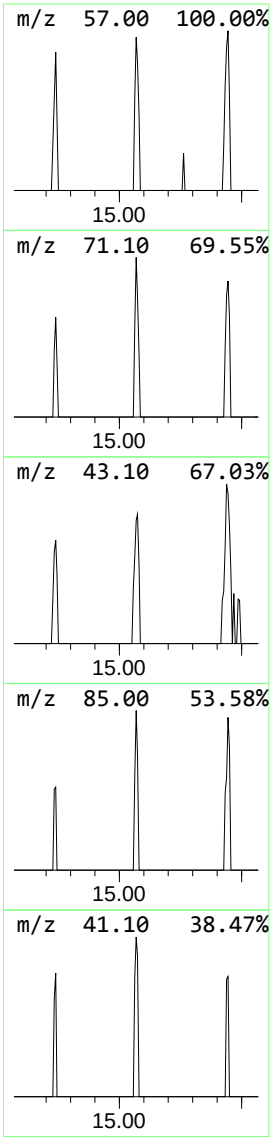
Peak Number 6 unknown15.069 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.069	3.23 ng	4986	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
2	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
3	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
4	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
5	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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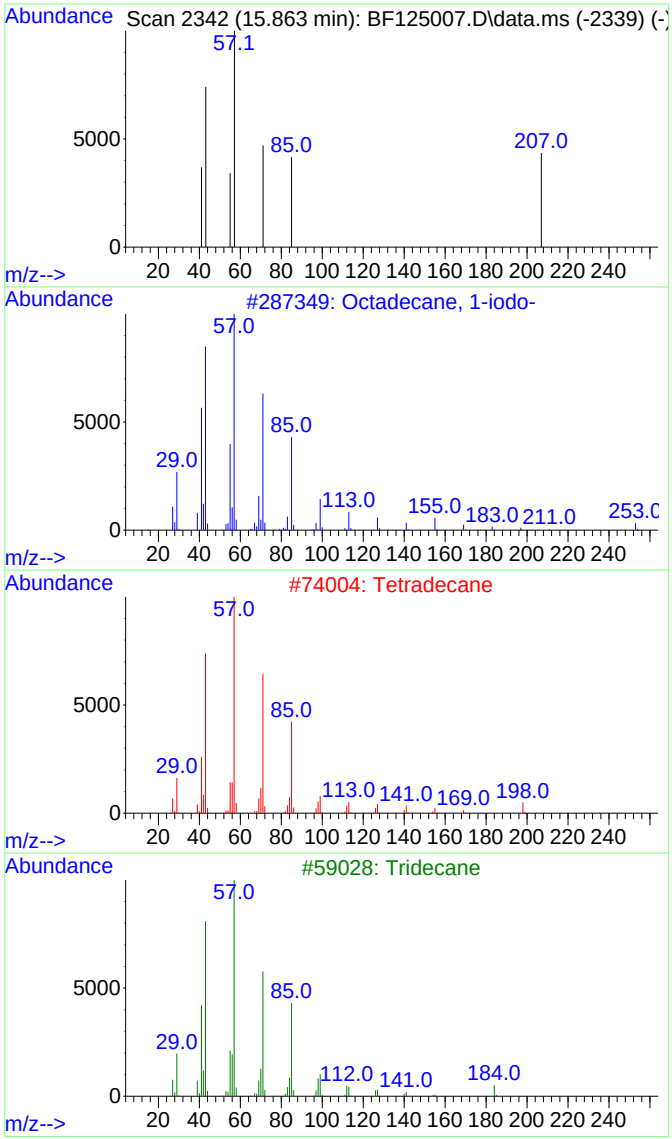
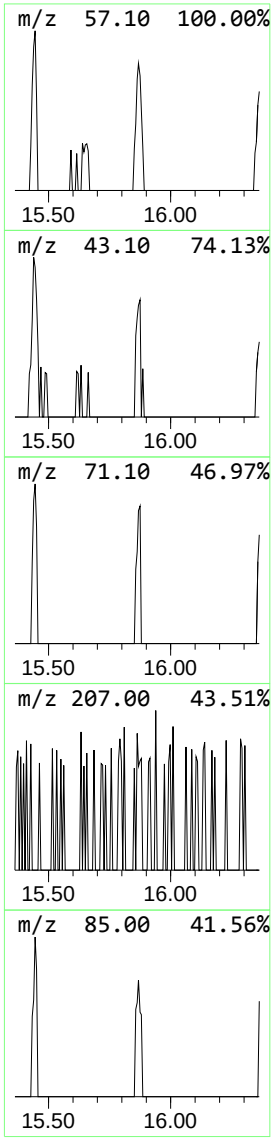
Peak Number 7 unknown15.863 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.863	3.33 ng	5153	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	42
2	Tetradecane	198	C14H30	000629-59-4	9
3	Tridecane	184	C13H28	000629-50-5	9
4	Nonadecane	268	C19H40	000629-92-5	9
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	9





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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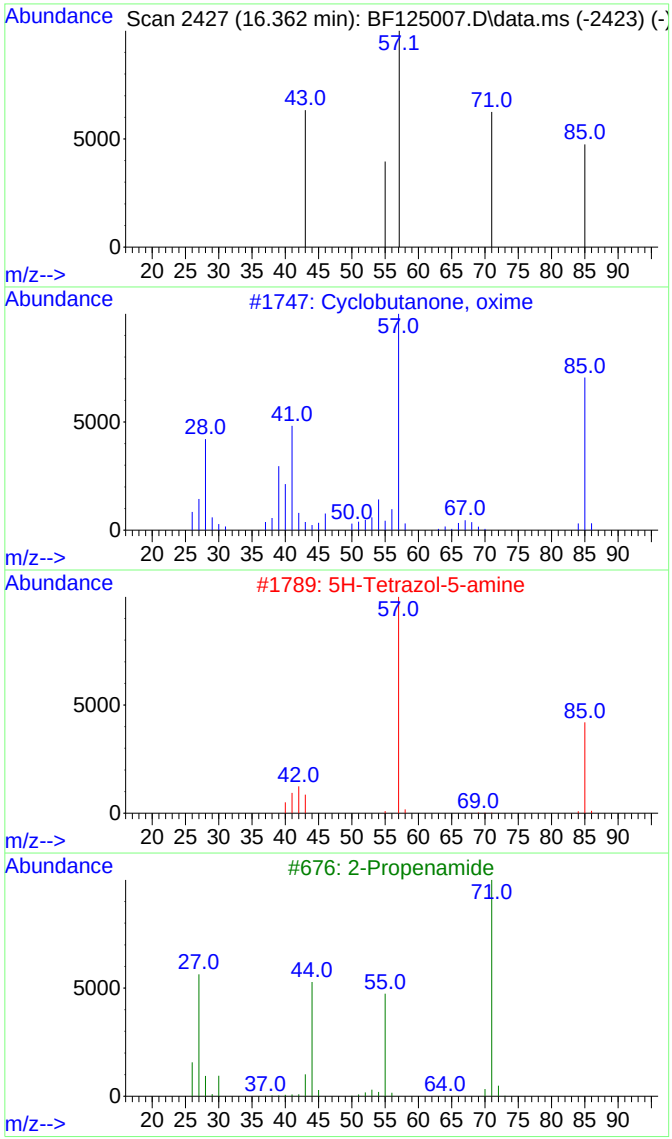
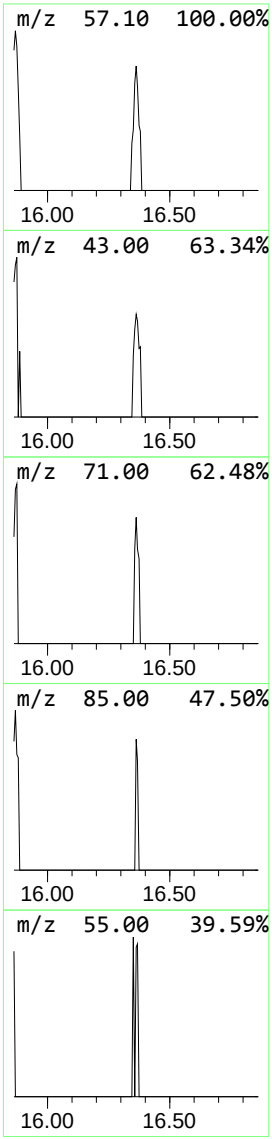
Peak Number 8 unknown16.363 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.363	2.27 ng	3505	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
2	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
3	2-Propenamide	71	C3H5NO	000079-06-1	4
4	Azetidine, 1,2-dimethyl-	85	C5H11N	051764-32-0	4
5	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125007.D
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.040	5.040	3.0	ng	4807	1	6.816	32460	20.0
unknown8.004	8.004	3.0	ng	6795	2	8.098	45293	20.0
unknown12.645	12.645	2.1	ng	5695	4	11.339	53319	20.0
unknown13.839	13.839	4.6	ng	8785	5	13.974	38333	20.0
unknown14.439	14.439	2.0	ng	3881	5	13.974	38333	20.0
unknown15.069	15.069	3.2	ng	4986	6	15.433	30905	20.0
unknown15.863	15.863	3.3	ng	5153	6	15.433	30905	20.0
unknown16.363	16.363	2.3	ng	3505	6	15.433	30905	20.0