LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124831.D
Acq On : 28 Jul 2021 17:08
Operator : JU/CG
Sample : M3165-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124831.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	9	rVB	8587	7066	3.58%	0.664%
2	5.087	507	510	513	rBB	2699	2784	1.41%	0.262%
3	5.481	573	577	580	rBV	110672	105217	53.33%	9.883%
4	6.492	745	749	752	rBV	117166	111310	56.41%	10.455%
5	6.869	810	813	816	rBB	39357	27368	13.87%	2.571%
6	7.433	905	909	912	rBB	88761	74798	37.91%	7.026%
7	8.051	1011	1014	1021	rBB	19229	15278	7.74%	1.435%
8	8.151	1028	1031	1034	rBB	50475	38225	19.37%	3.590%
9	9.227	1210	1214	1217	rBV	200986	153741	77.92%	14.441%
10	9.910	1326	1330	1333	rBB	54397	46362	23.50%	4.355%
11	10.698	1460	1464	1467	rBB	124263	99378	50.37%	9.335%
12	11.392	1579	1582	1585	rBV	59010	51598	26.15%	4.847%
13	11.910	1668	1670	1673	rBB	5061	3871	1.96%	0.364%
14	12.980	1848	1852	1855	rBV	211281	197307	100.00%	18.533%
15	13.545	1946	1948	1950	rBB	3411	2171	1.10%	0.204%
16	13.874	2002	2004	2006	rBV2	6074	5345	2.71%	0.502%
17	13.892	2006	2007	2015	rVB4	3978	6611	3.35%	0.621%
18	14.033	2027	2031	2034	rBV	53500	43047	21.82%	4.043%
19	14.192	2055	2058	2060	rBB	6390	4924	2.50%	0.463%
20	14.498	2107	2110	2112	rBB	5367	4427	2.24%	0.416%
21	14.786	2156	2159	2165	rBB2	19691	21479	10.89%	2.018%
22	15.145	2217	2220	2223	rBB	4347	4090	2.07%	0.384%
23	15.509	2277	2282	2288	rBB	29292	35555	18.02%	3.340%
24	15.968	2356	2360	2364	rBB2	2096	2668	1.35%	0.251%

Sum of corrected areas: 1064620

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BNA_F
ClientSampleId :
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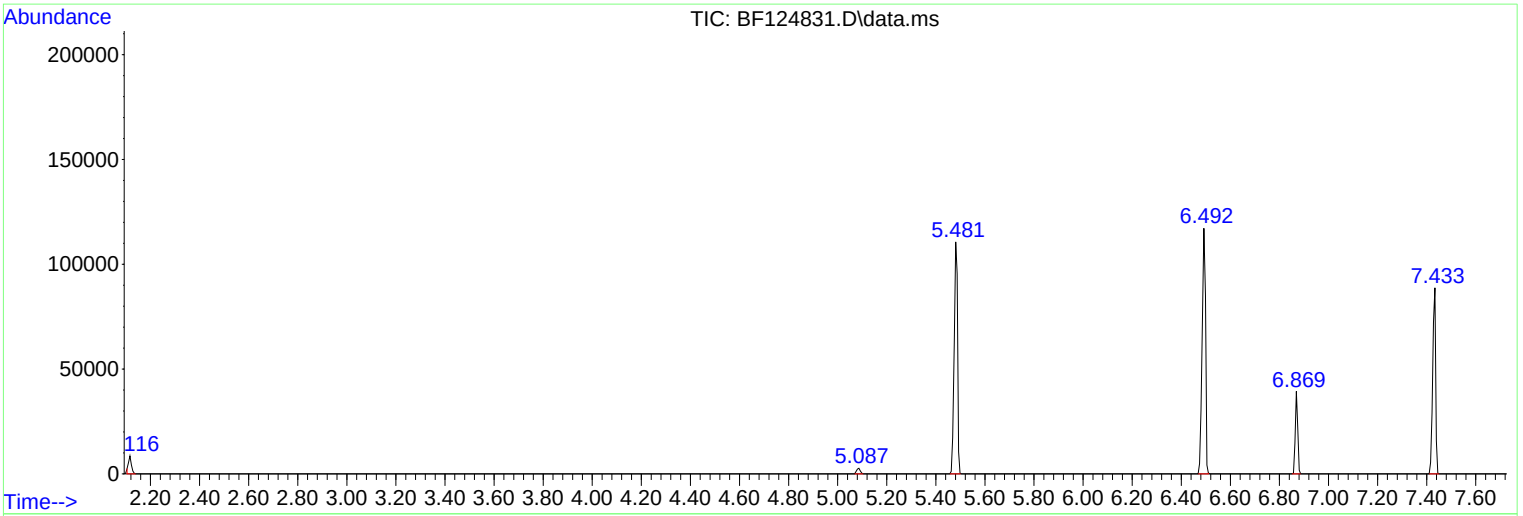
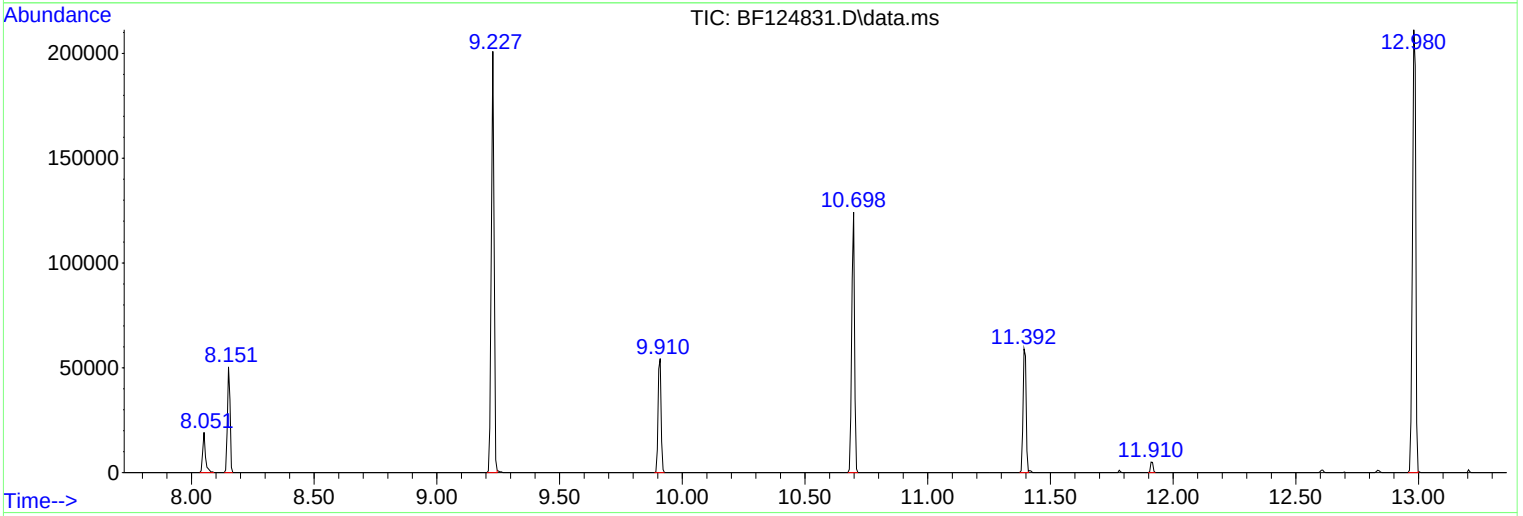
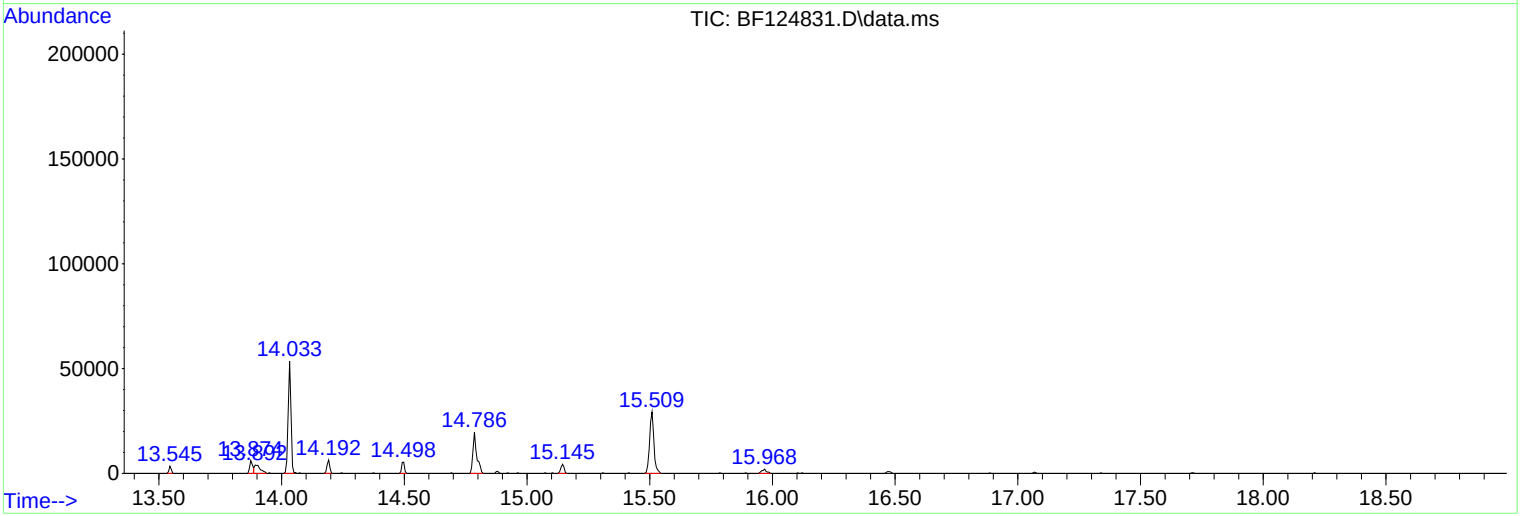
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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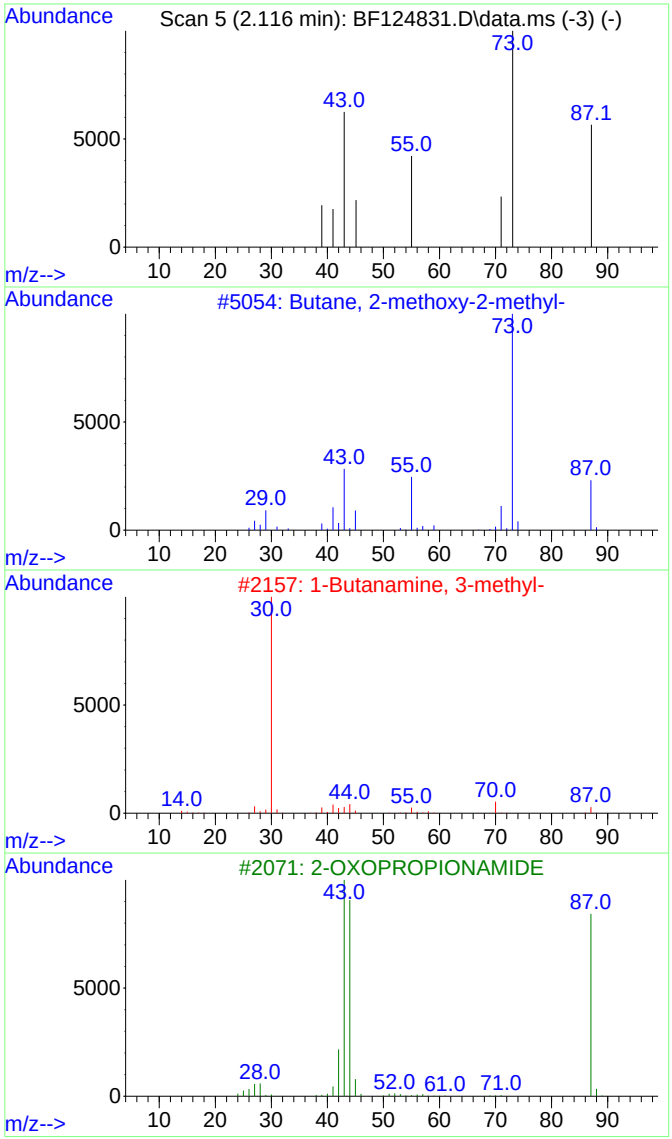
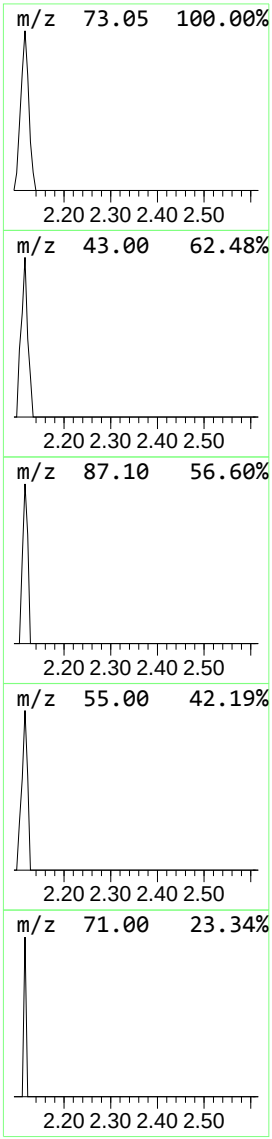
Peak Number 1 unknown2.116 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	5.16 ng	7066	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
2	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5
3	2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	4
4	Isobutylamine	73	C4H11N	000078-81-9	4
5	1-Pentanamine	87	C5H13N	000110-58-7	4





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Sample : M3165-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-3

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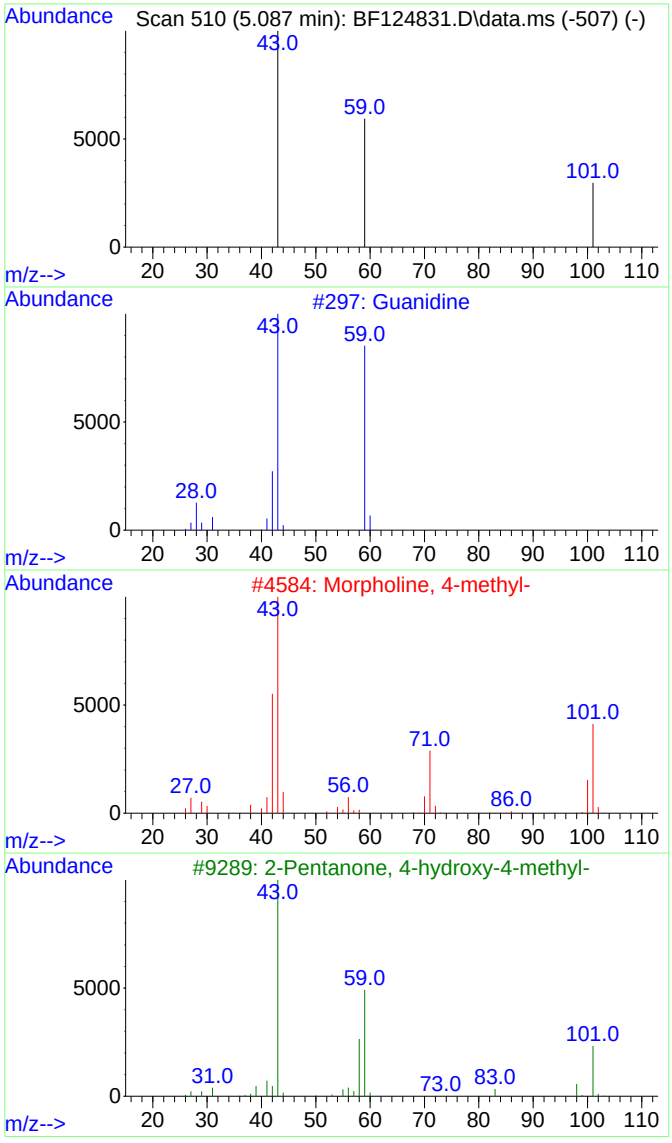
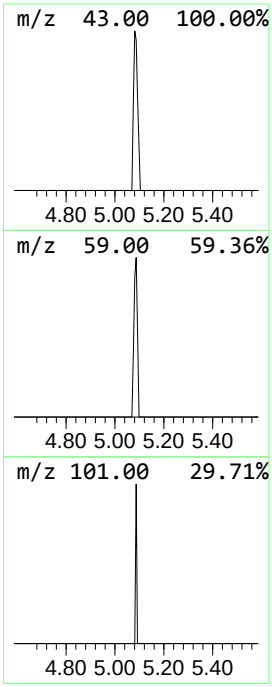
Peak Number 2 unknown5.087 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	2.03 ng	2784	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanidine	59	CH5N3	000113-00-8	4
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	4
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	4
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	4
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	4





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Instrument : BNA_F
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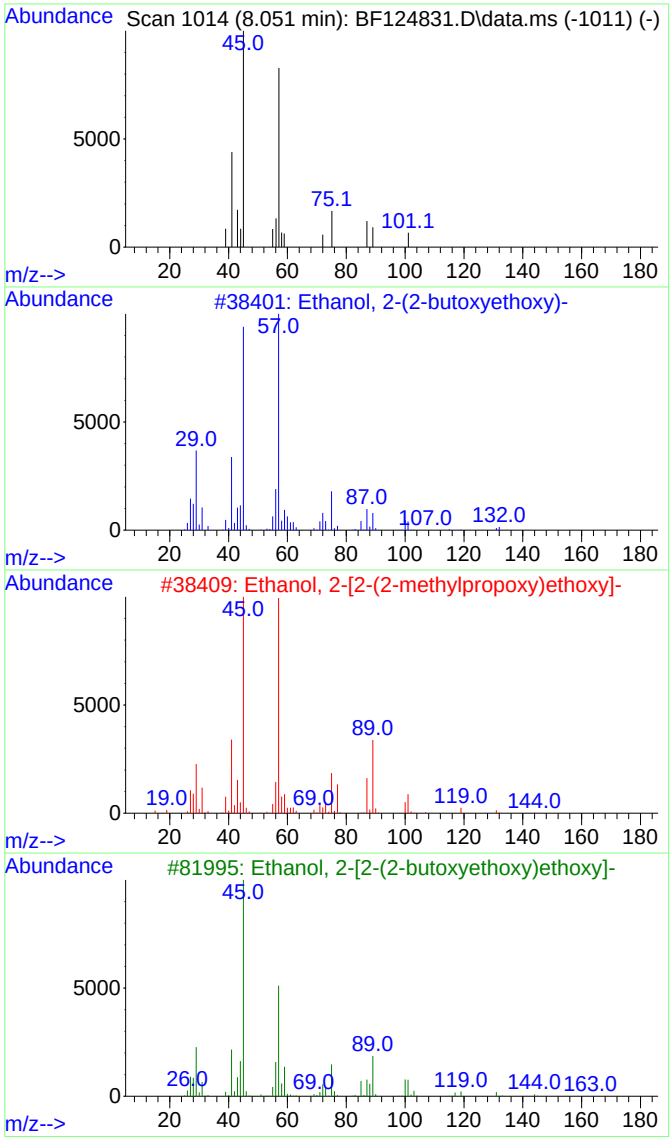
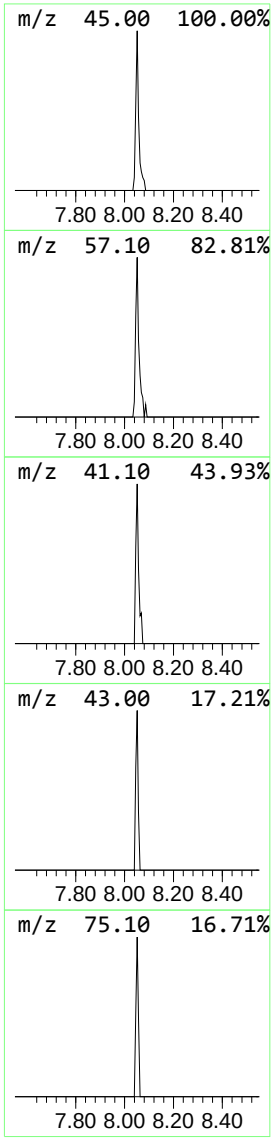
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	7.99 ng	15278	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	39
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	36





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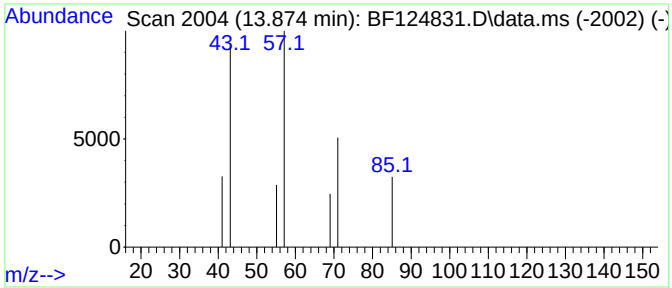
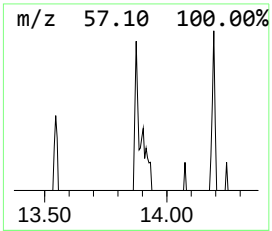
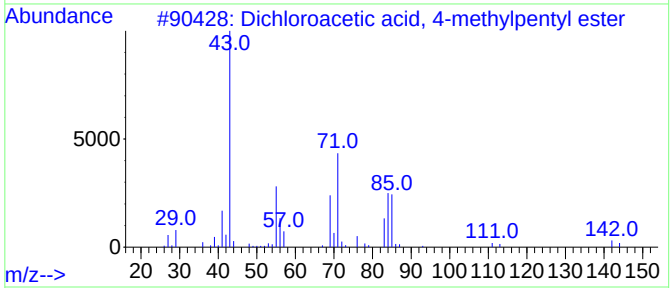
Peak Number 4 unknown13.874 Concentration Rank 5

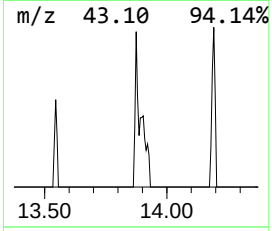
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.48 ng	5345	Chrysene-d12	14.033

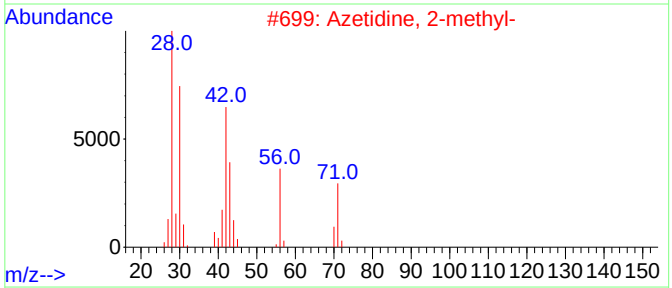
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	9
2	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
3	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
4	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
5	2-Propenamide	71	C3H5NO	000079-06-1	4

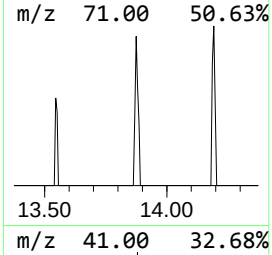


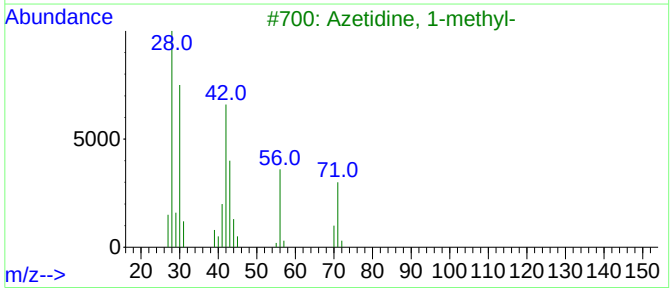


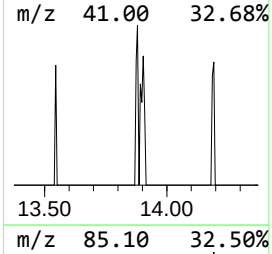


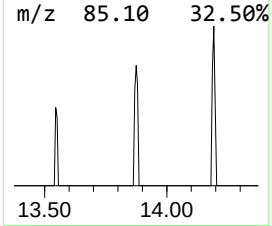












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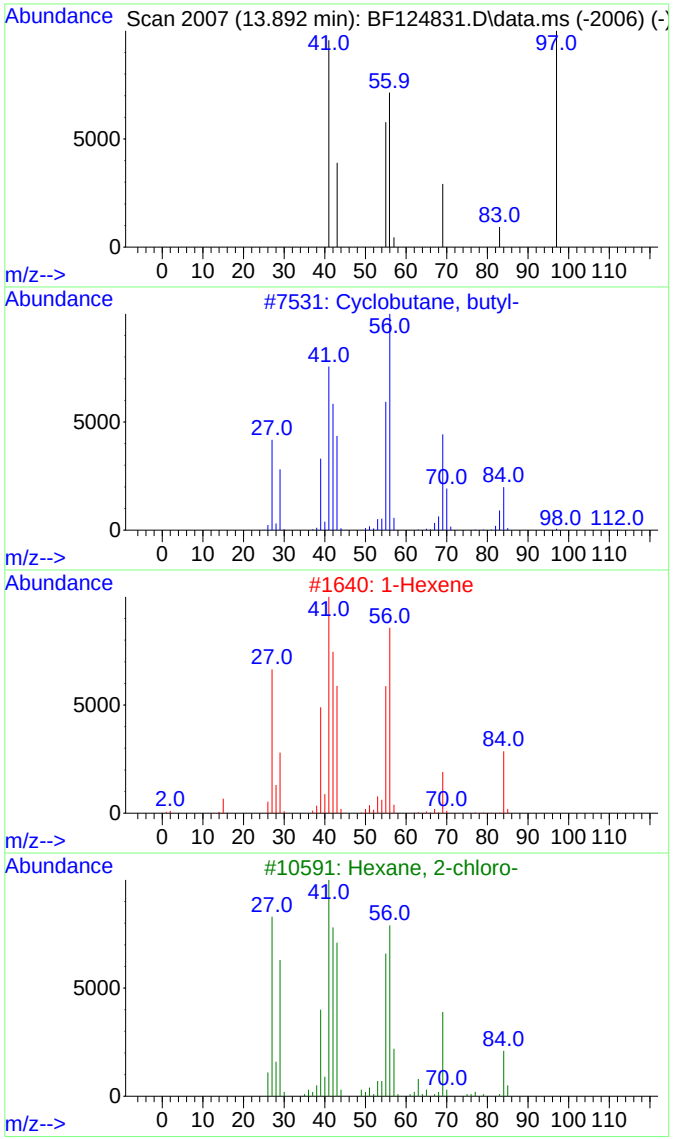
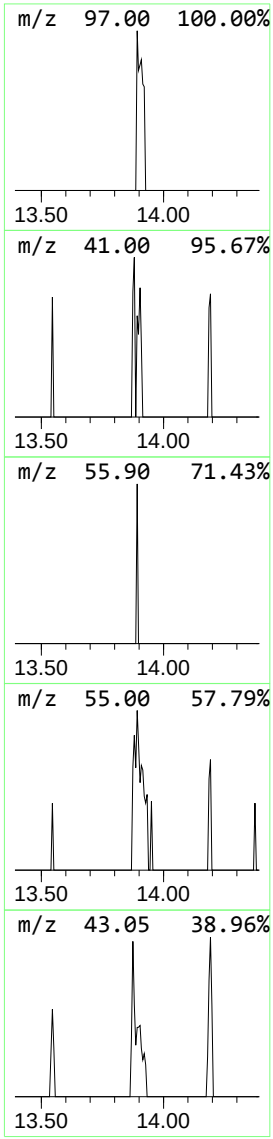
****

Peak Number 5 unknown13.892 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.07 ng	6611	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, butyl-	112	C8H16	013152-44-8	16
2	1-Hexene	84	C6H12	000592-41-6	9
3	Hexane, 2-chloro-	120	C6H13Cl	000638-28-8	9
4	Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	9
5	2-Propenal	56	C3H4O	000107-02-8	7





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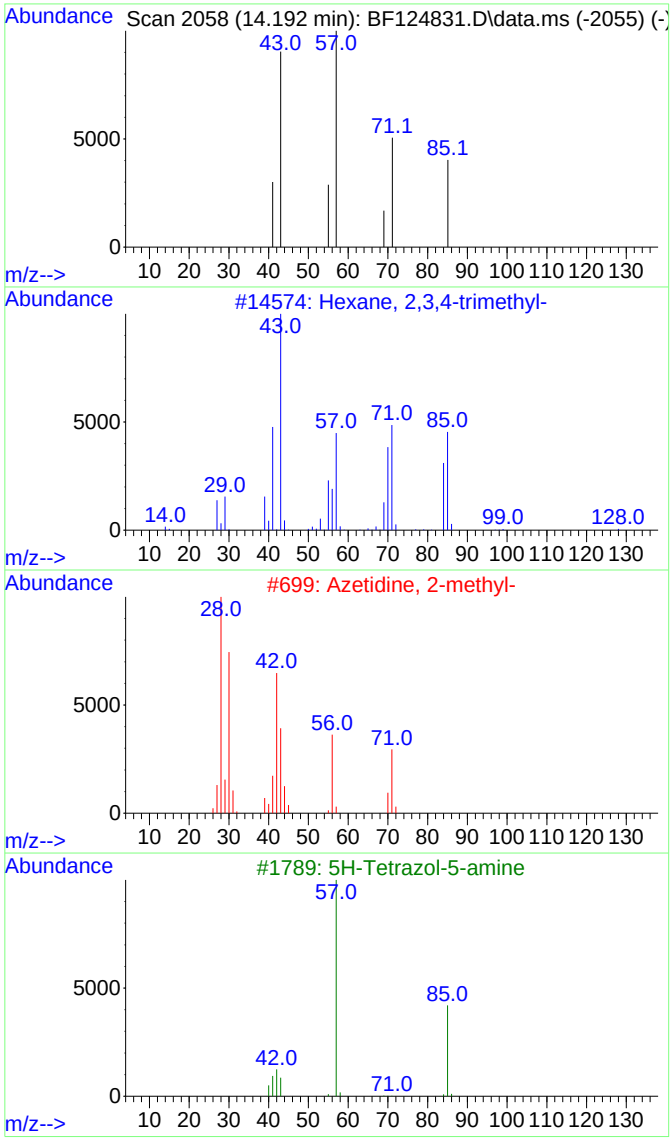
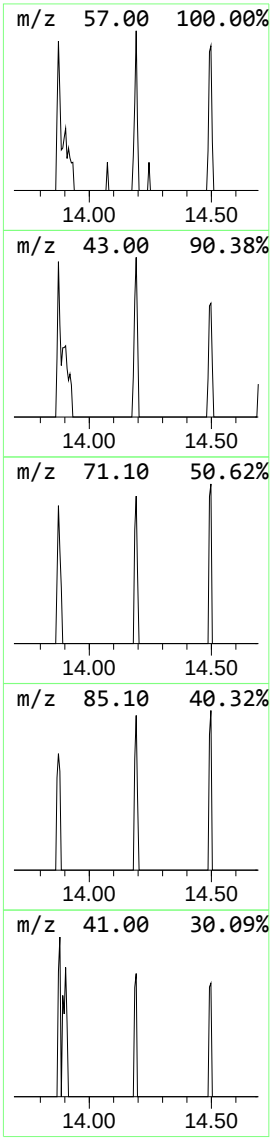
Peak Number 6 unknown14.192 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	2.29 ng	4924	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	43
2	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
3	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4	2-Propenamide	71	C3H5NO	000079-06-1	4
5	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4





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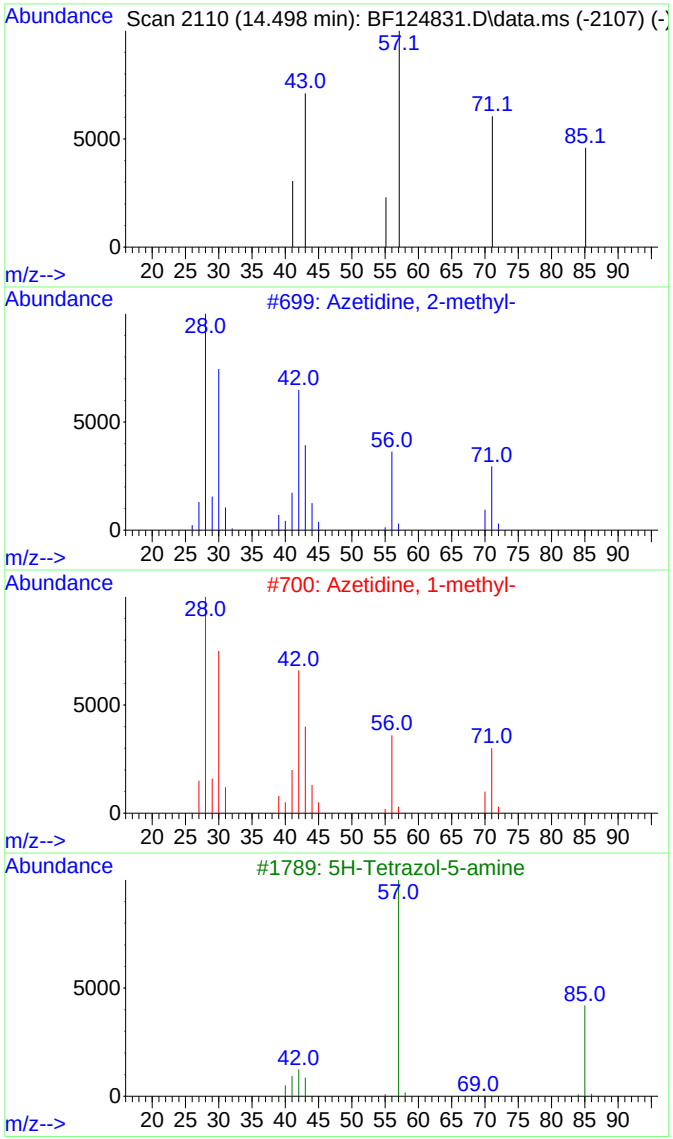
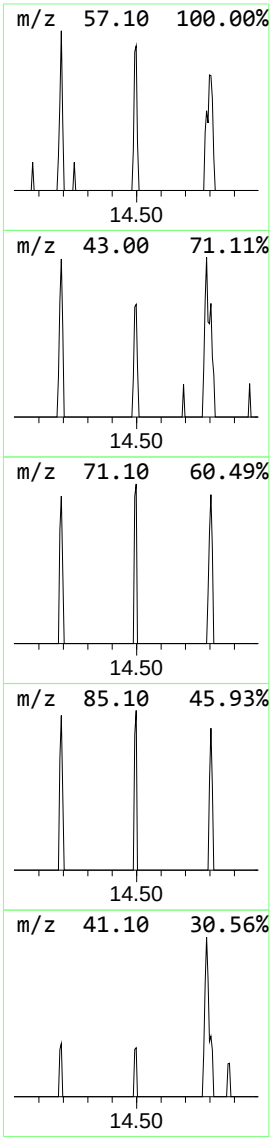
Peak Number 7 unknown14.498 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	2.06 ng	4427	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
2	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
3	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4	2-Propen-1-amine	57	C3H7N	000107-11-9	4
5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	4





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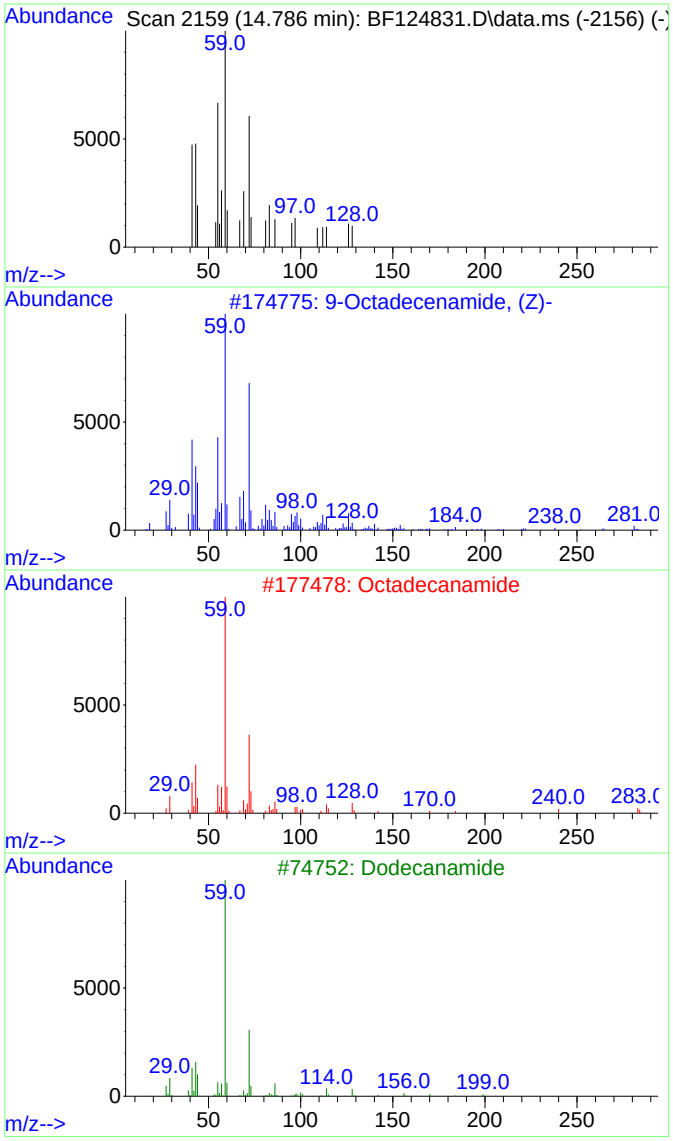
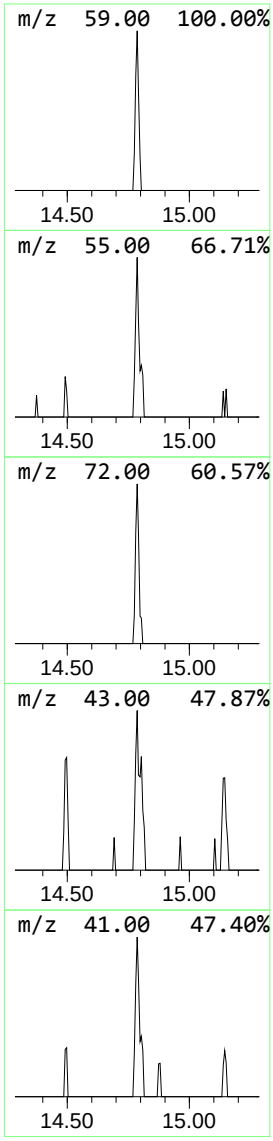
Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	12.08 ng	21479	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
2	Octadecanamide	283	C18H37NO	000124-26-5	42
3	Dodecanamide	199	C12H25NO	001120-16-7	42
4	Hexadecanamide	255	C16H33NO	000629-54-9	42
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124831.D
Acq On : 28 Jul 2021 17:08
Operator : JU/CG
Sample : M3165-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

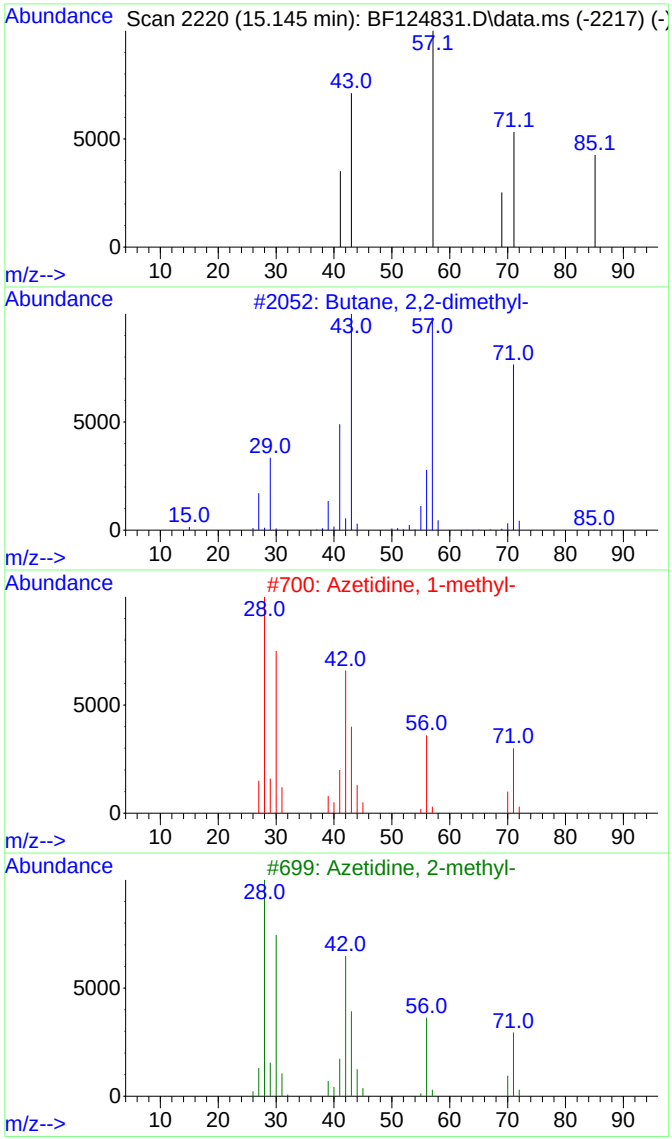
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

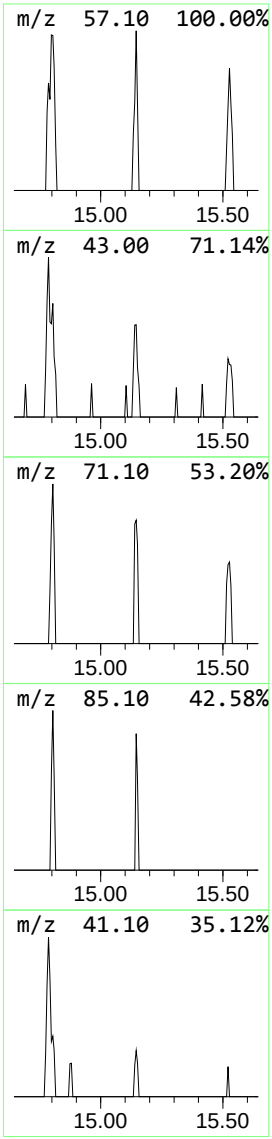
****

Peak Number 9 unknown15.145 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	2.30 ng	4090	Perylene-d12	15.509

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124831.D
Acq On : 28 Jul 2021 17:08
Operator : JU/CG
Sample : M3165-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.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
unknown2.116	2.116	5.2	ng	7066	1	6.869	27368	20.0
unknown5.087	5.087	2.0	ng	2784	1	6.869	27368	20.0
Ethanol, 2-(2-b...	8.051	8.0	ng	15278	2	8.151	38225	20.0
unknown13.874	13.874	2.5	ng	5345	5	14.033	43047	20.0
unknown13.892	13.892	3.1	ng	6611	5	14.033	43047	20.0
unknown14.192	14.192	2.3	ng	4924	5	14.033	43047	20.0
unknown14.498	14.498	2.1	ng	4427	5	14.033	43047	20.0
9-Octadecenamid...	14.786	12.1	ng	21479	6	15.509	35555	20.0
unknown15.145	15.145	2.3	ng	4090	6	15.509	35555	20.0