LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124878.D
Acq On : 30 Jul 2021 16:12
Operator : JU/CG
Sample : M3210-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(1.0-1.5)

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: BF124878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	7	11	14	rBB	4034	4181	1.38%	0.236%
2	5.104	510	513	519	rBB	5610	7794	2.57%	0.440%
3	5.493	574	579	582	rBV	192468	205321	67.74%	11.579%
4	6.504	745	751	754	rBV	195885	215699	71.17%	12.165%
5	6.869	810	813	816	rBB	49052	35905	11.85%	2.025%
6	7.440	905	910	912	rBV	146576	148138	48.88%	8.354%
7	8.051	1011	1014	1020	rBB	23249	18150	5.99%	1.024%
8	8.151	1028	1031	1034	rBV	64452	50526	16.67%	2.850%
9	9.234	1210	1215	1218	rBV	326696	300642	99.19%	16.955%
10	9.910	1326	1330	1333	rBV	80019	62489	20.62%	3.524%
11	10.704	1460	1465	1468	rBV	221786	197420	65.14%	11.134%
12	11.398	1579	1583	1585	rBV	83675	66005	21.78%	3.722%
13	11.416	1585	1586	1589	rVB	8473	6306	2.08%	0.356%
14	11.916	1669	1671	1674	rBB	5672	4284	1.41%	0.242%
15	12.610	1786	1789	1792	rBB	16507	13477	4.45%	0.760%
16	12.839	1823	1828	1831	rBB	13731	12843	4.24%	0.724%
17	12.986	1848	1853	1856	rBV	316087	303092	100.00%	17.093%
18	13.874	2002	2004	2012	rBB3	8717	11241	3.71%	0.634%
19	14.039	2027	2032	2034	rBV2	42261	42060	13.88%	2.372%
20	14.063	2034	2036	2038	rVB	5391	3618	1.19%	0.204%
21	14.498	2107	2110	2111	rBV	4296	3357	1.11%	0.189%
22	14.951	2184	2187	2191	rBB	5765	4197	1.38%	0.237%
23	15.080	2205	2209	2212	rBV2	4238	5867	1.94%	0.331%
24	15.145	2217	2220	2223	rBB	3642	3449	1.14%	0.195%
25	15.186	2224	2227	2233	rBV3	4231	7455	2.46%	0.420%
26	15.445	2268	2271	2274	rBB	3099	3424	1.13%	0.193%
27	15.515	2278	2283	2287	rBV	29723	32837	10.83%	1.852%
28	15.733	2316	2320	2323	rBB2	3695	3376	1.11%	0.190%

Sum of corrected areas: 1773153

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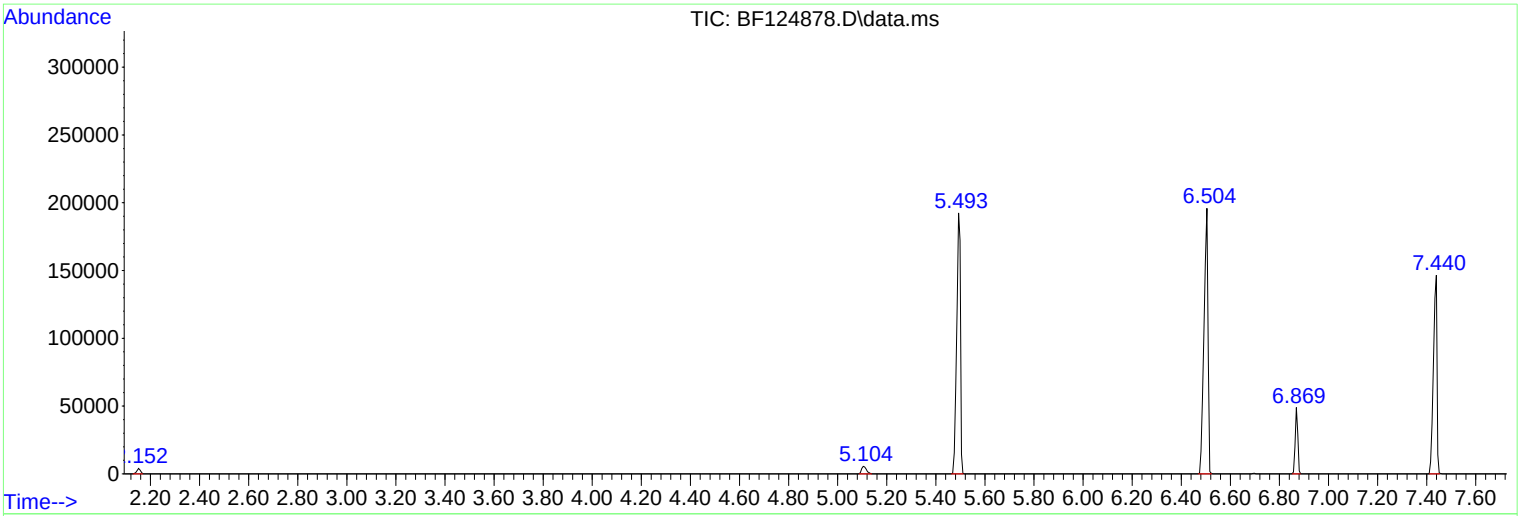
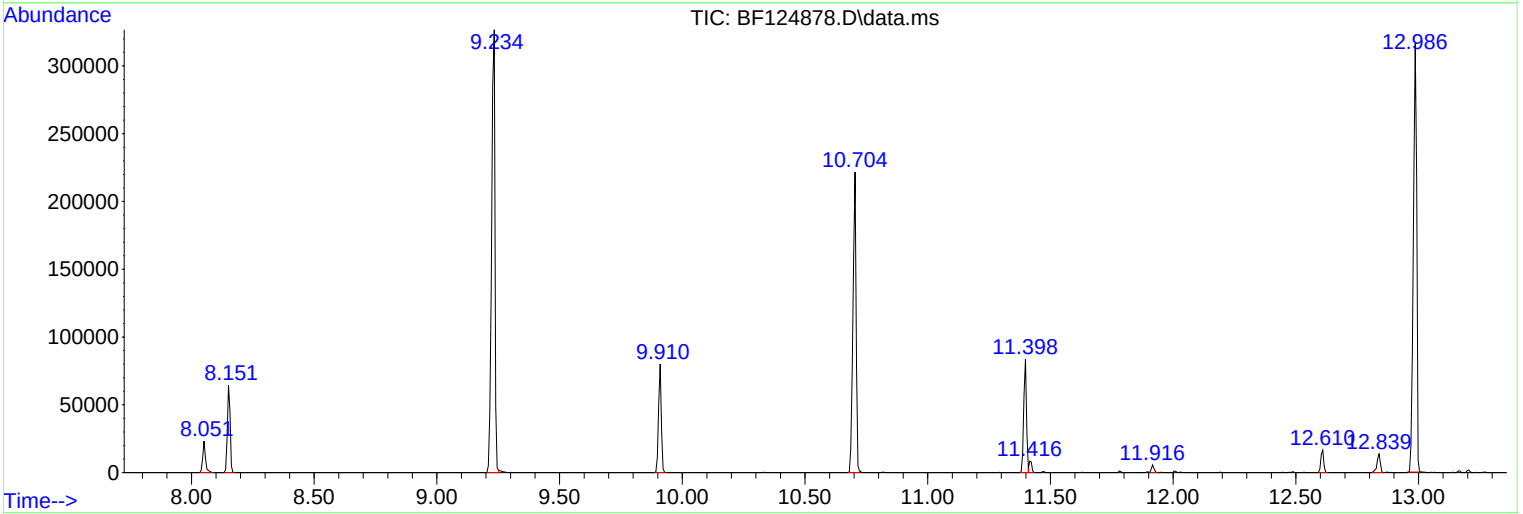
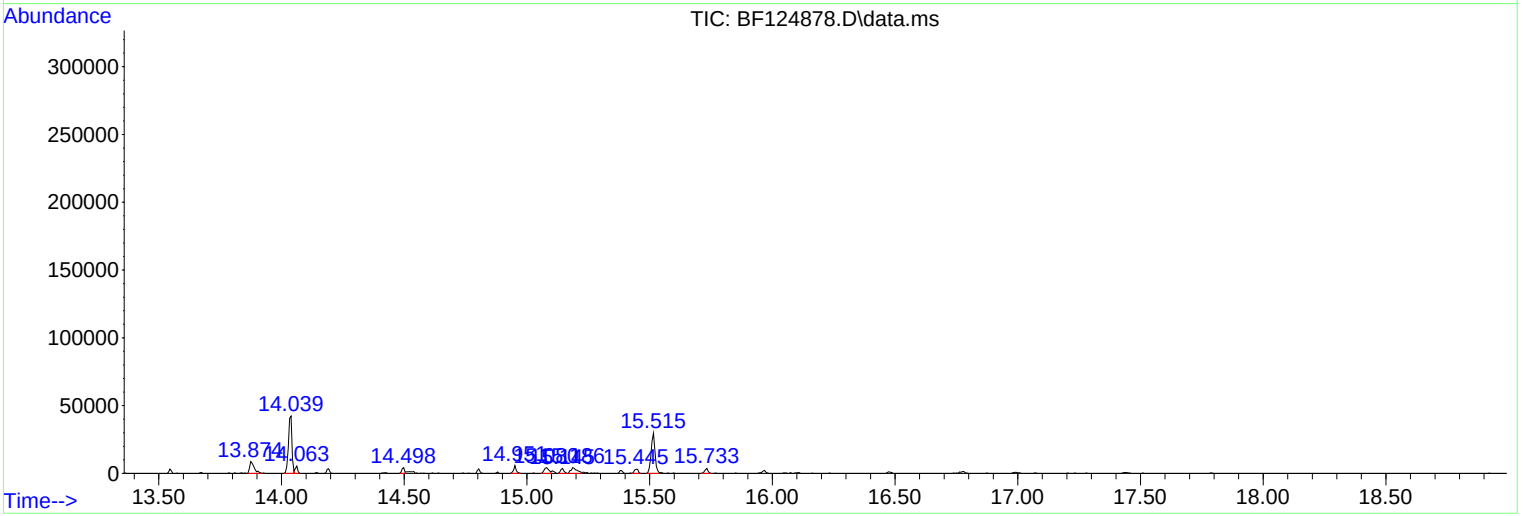
Instrument :
BNA_F
ClientSampleId :
SB-2(1.0-1.5)

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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Data File : BF124878.D
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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TIC Library : C:\Database\NIST20.L
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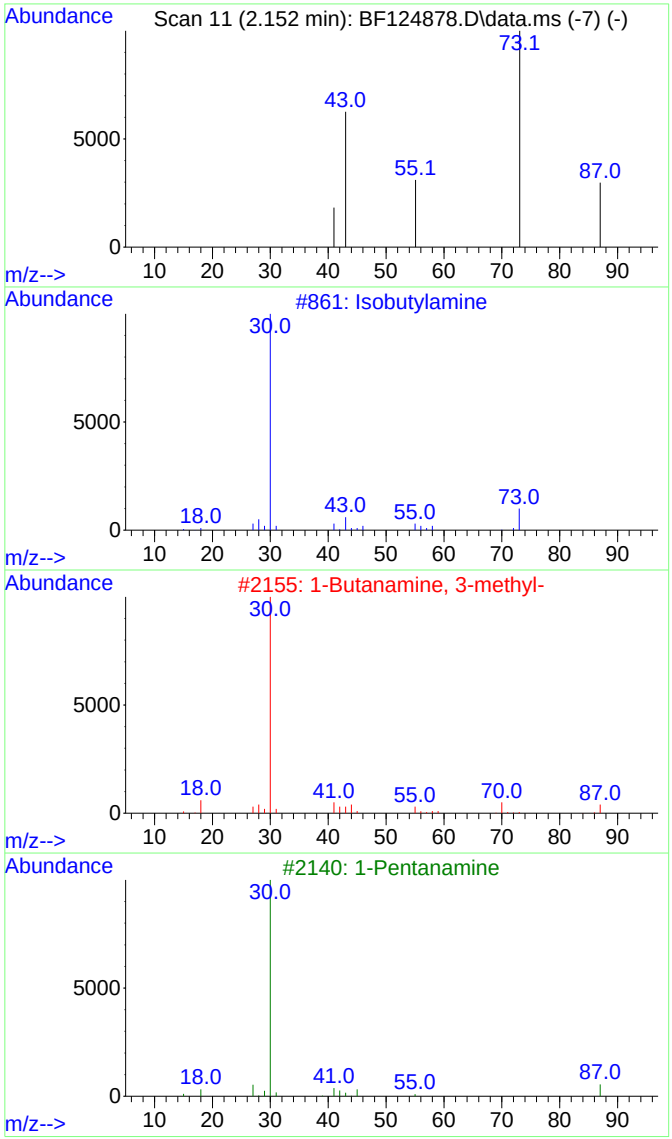
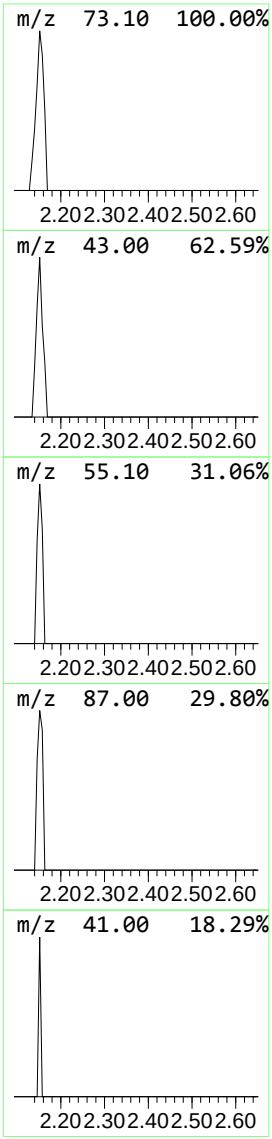
Peak Number 1 unknown2.152 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	2.33 ng	4181	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutylamine	73	C4H11N	000078-81-9	4
2	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	3
3	1-Pentanamine	87	C5H13N	000110-58-7	3
4	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	2
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	2





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Data File : BF124878.D
Acq On : 30 Jul 2021 16:12
Operator : JU/CG
Sample : M3210-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(1.0-1.5)

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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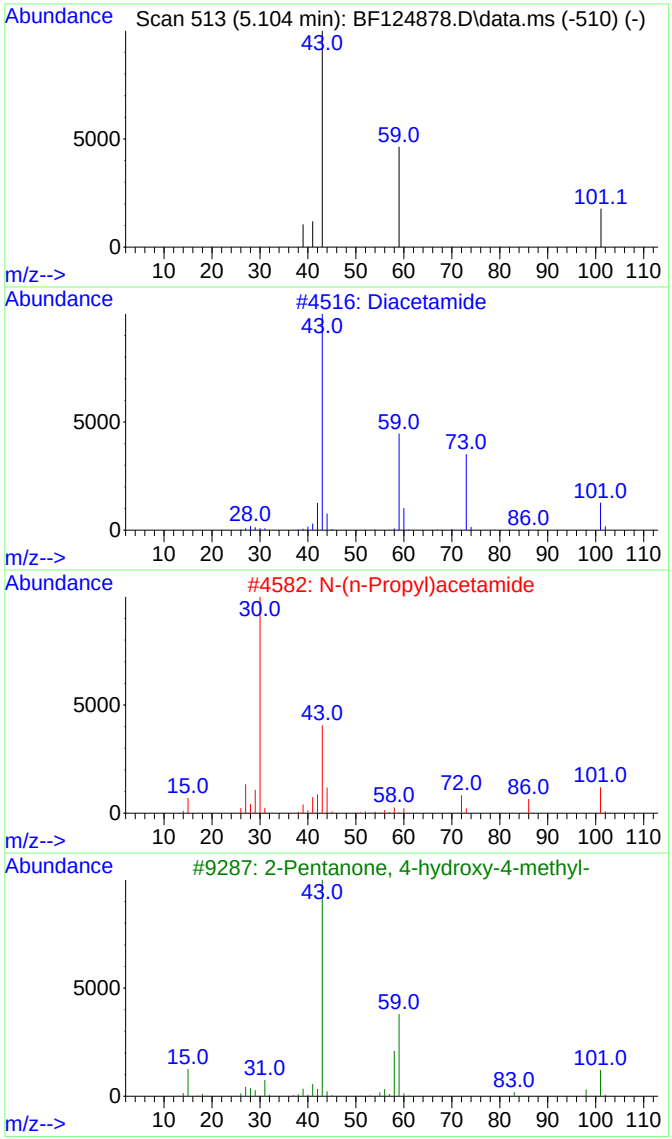
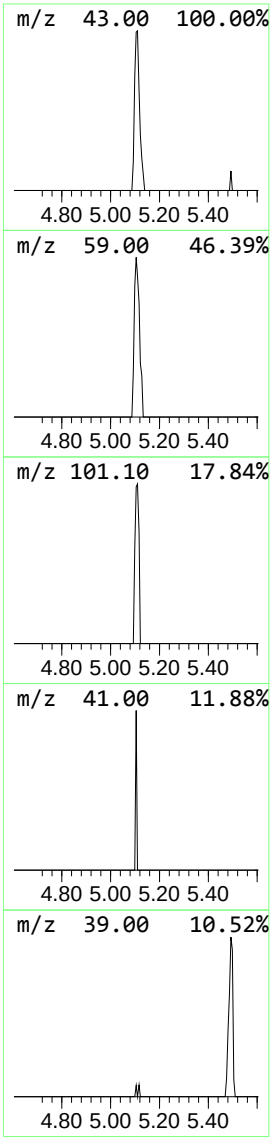
Peak Number 2 unknown5.104 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	4.34 ng	7794	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diacetamide	101	C4H7NO2	000625-77-4	7
2	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	4
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	4
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	4
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	3





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Data File : BF124878.D
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Operator : JU/CG
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(1.0-1.5)

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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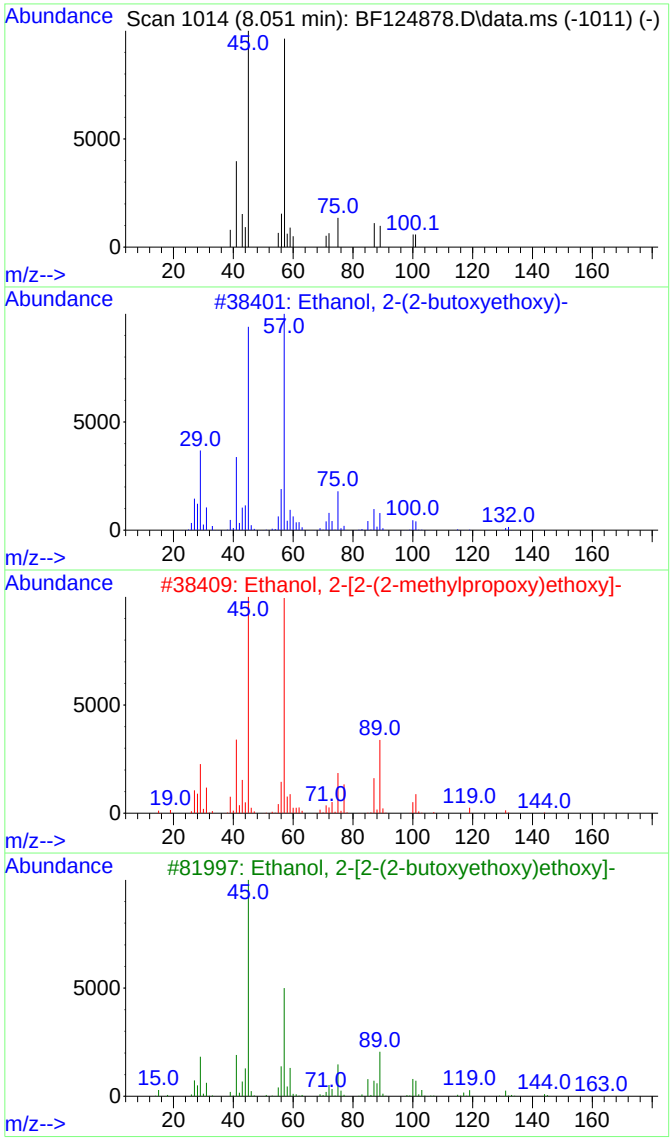
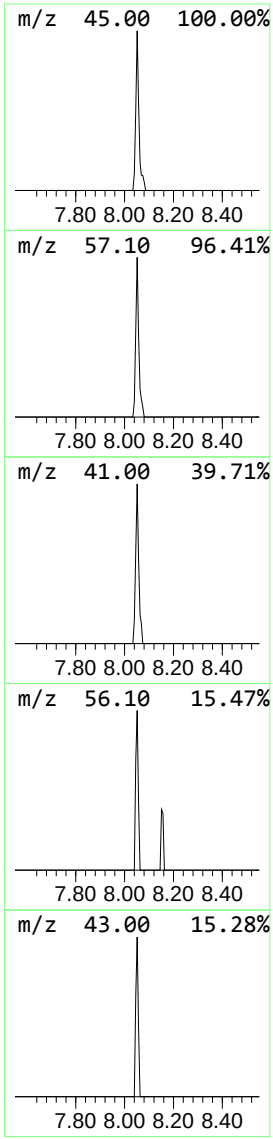
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	7.18 ng	18150	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
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	45
4	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40
5	Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	39





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Acq On : 30 Jul 2021 16:12
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(1.0-1.5)

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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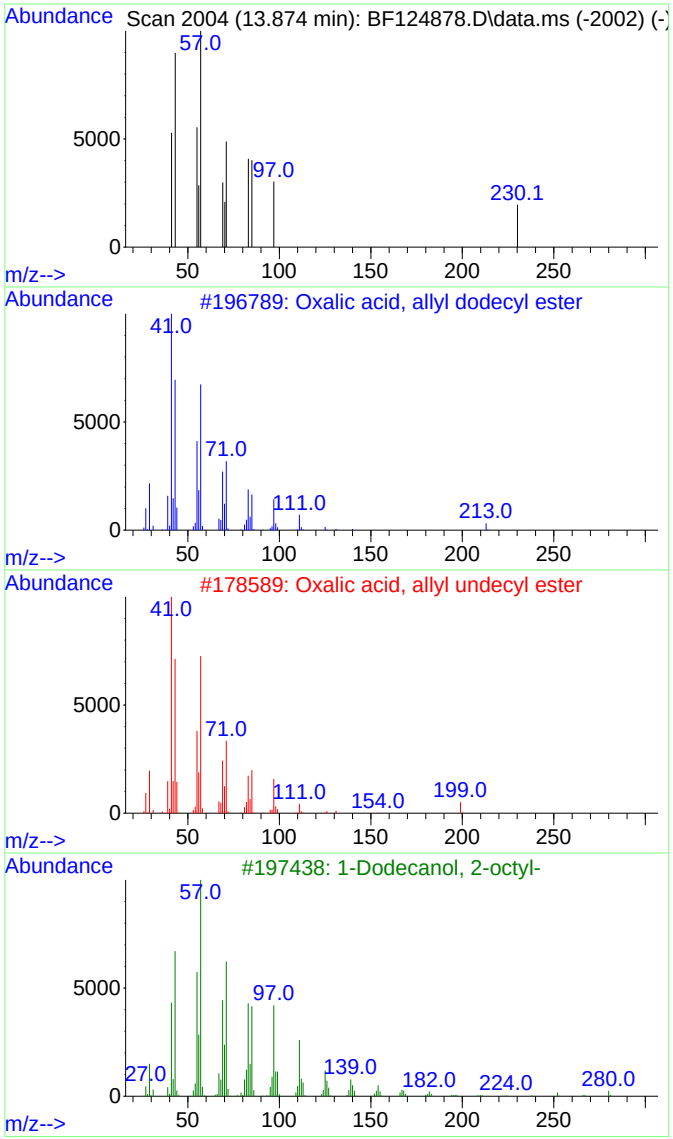
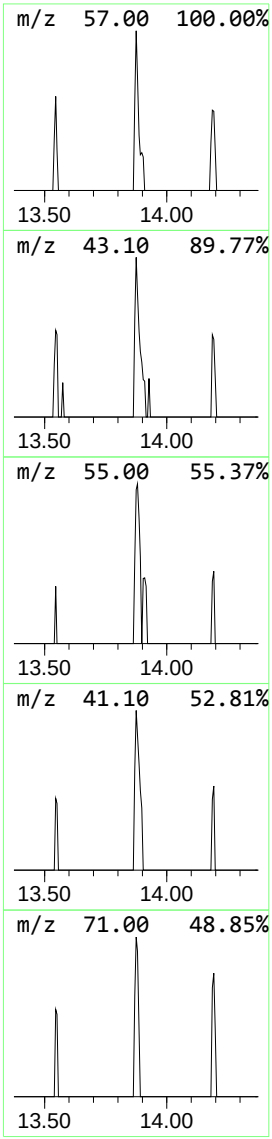
Peak Number 4 Oxalic acid, allyl dodecyl ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.35 ng	11241	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	78
2	Oxalic acid, allyl undecyl ester	284	C16H28O4	1000309-23-9	78
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	78
4	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	78
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	78





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Instrument :
BNA_F
ClientSampleId :
SB-2(1.0-1.5)

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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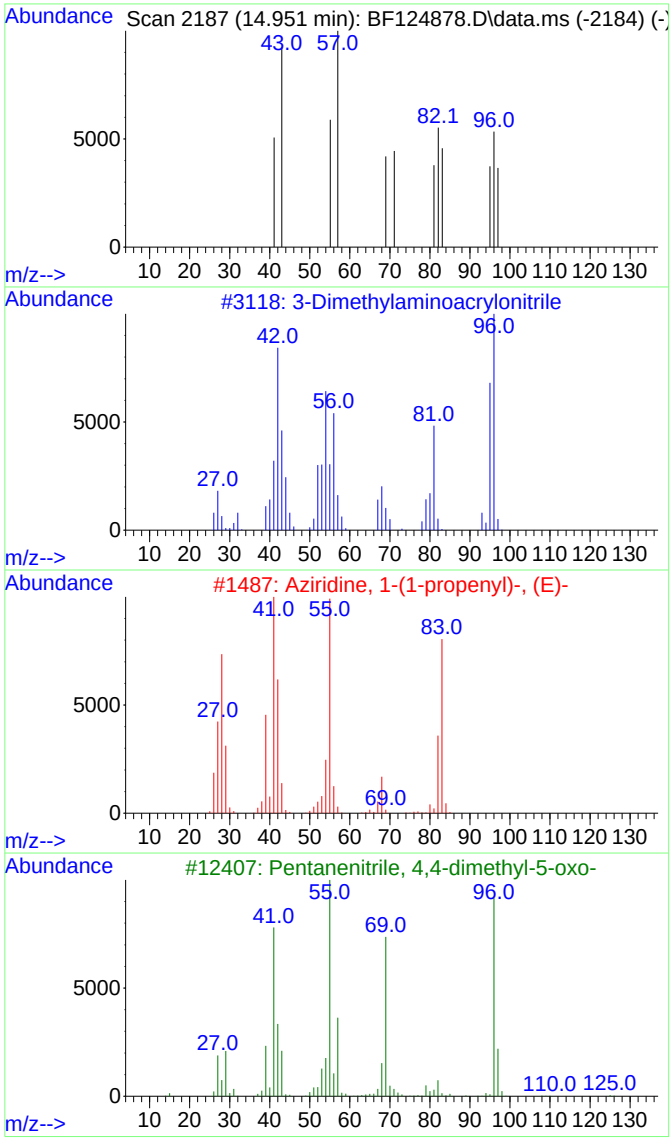
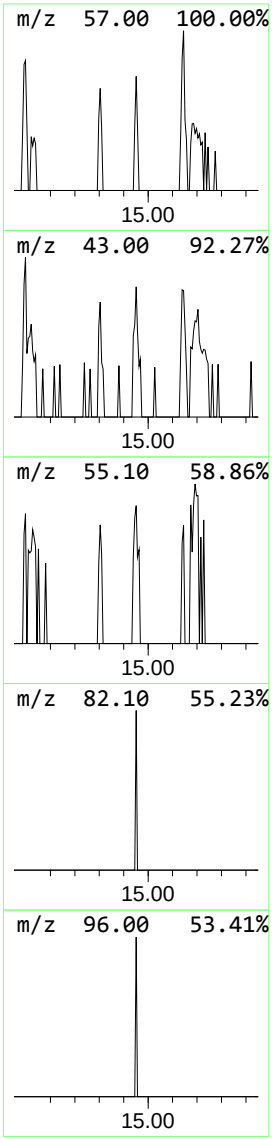
Peak Number 5 unknown14.951 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.951	2.56 ng	4197	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Dimethylaminoacrylonitrile	96	C5H8N2	002407-68-3	9
2	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7
3	Pentanenitrile, 4,4-dimethyl-5-oxo-	125	C7H11NO	006140-61-0	7
4	1H-Imidazole, 1,5-dimethyl-	96	C5H8N2	010447-93-5	5
5	2,4-Dimethylfuran	96	C6H8O	003710-43-8	5





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Instrument : BNA_F
ClientSampleId : SB-2(1.0-1.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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TIC Library : C:\Database\NIST20.L
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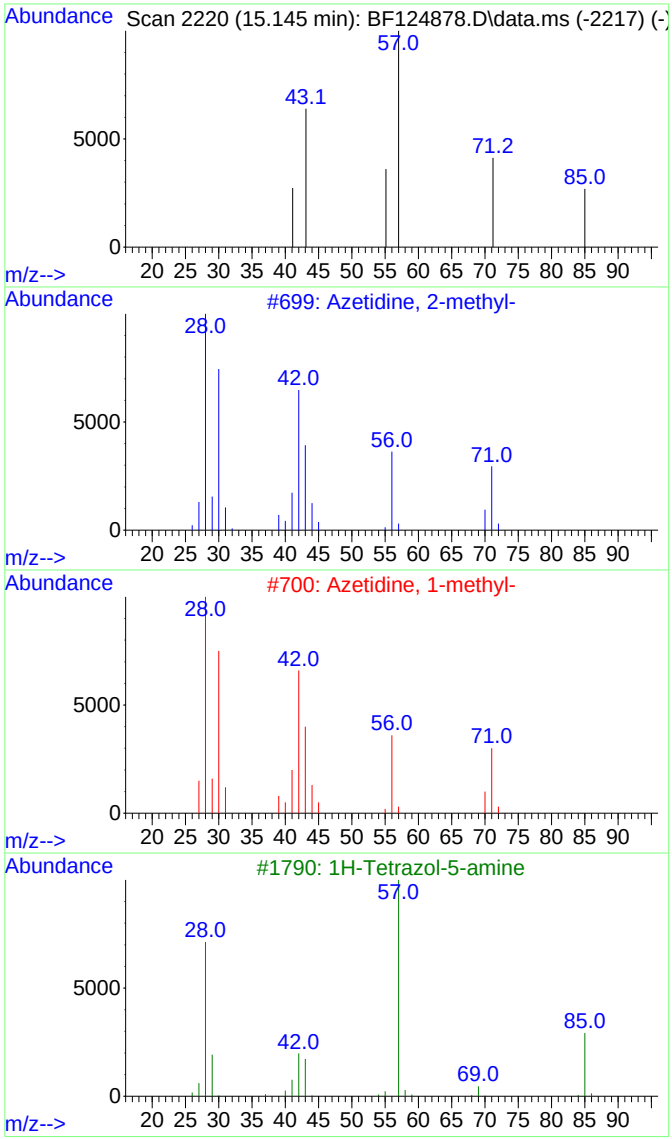
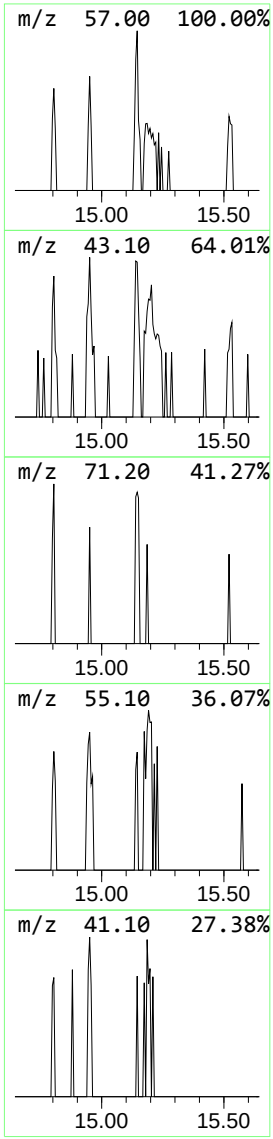
Peak Number 6 unknown15.145 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	2.10 ng	3449	Perylene-d12	15.515

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	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	4
5	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3





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Data File : BF124878.D
Acq On : 30 Jul 2021 16:12
Operator : JU/CG
Sample : M3210-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(1.0-1.5)

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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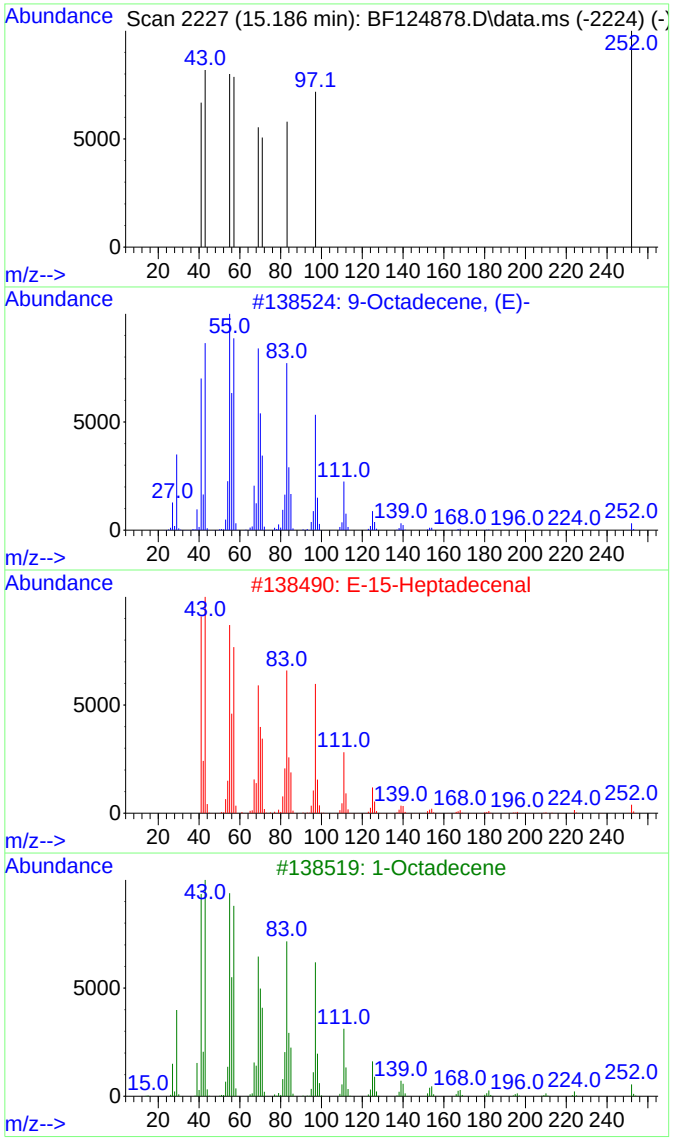
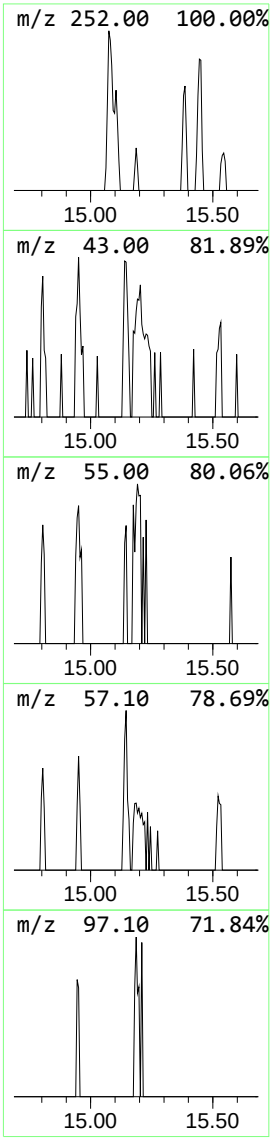
Peak Number 7 9-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	4.54 ng	7455	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecene, (E)-	252	C18H36	007206-25-9	72
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	64
3	1-Octadecene	252	C18H36	000112-88-9	64
4	1-Hexacosene	364	C26H52	018835-33-1	50
5	1-Tetracosene	336	C24H48	010192-32-2	50





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SB-2(1.0-1.5)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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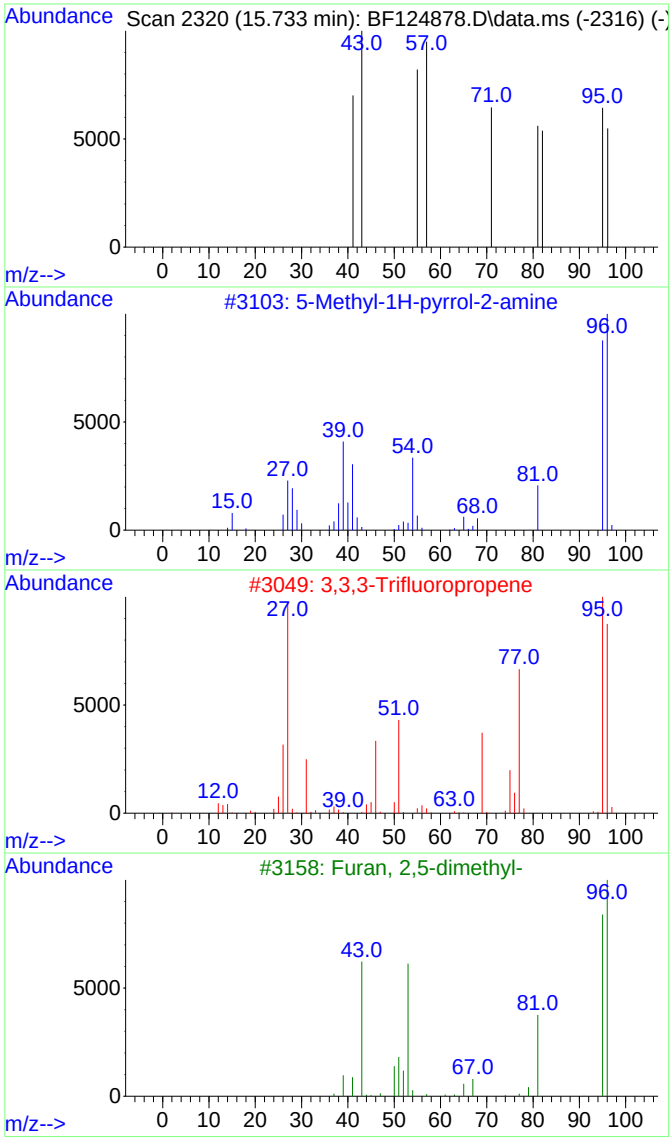
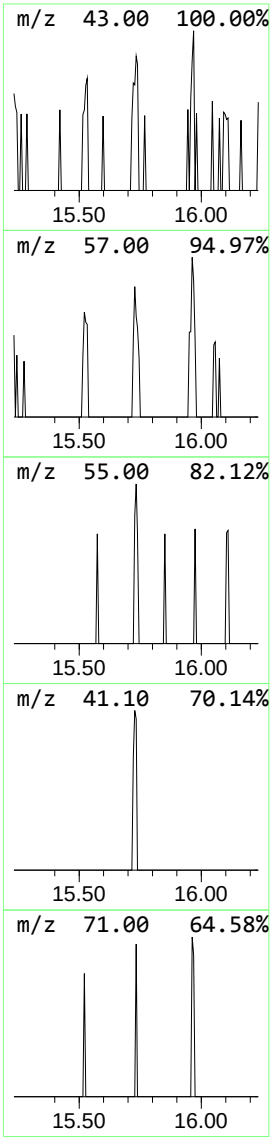
Peak Number 8 unknown15.733 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	2.06 ng	3376	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-1H-pyrrol-2-amine	96	C5H8N2	1000436-81-3	5
2	3,3,3-Trifluoropropene	96	C3H3F3	000677-21-4	5
3	Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	5
4	Pyrazole, 1,4-dimethyl-	96	C5H8N2	001072-68-0	5
5	3-Heptyne	96	C7H12	002586-89-2	5





Tentatively Identified Compound (LSC) summary

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Data File : BF124878.D
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Instrument : BNA_F
ClientSampleId : SB-2(1.0-1.5)

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
unknown2.152	2.152	2.3	ng	4181	1	6.869	35905	20.0
unknown5.104	5.104	4.3	ng	7794	1	6.869	35905	20.0
Ethanol, 2-(2-b...	8.051	7.2	ng	18150	2	8.151	50526	20.0
Oxalic acid, al...	13.874	5.3	ng	11241	5	14.039	42060	20.0
unknown14.951	14.951	2.6	ng	4197	6	15.515	32837	20.0
unknown15.145	15.145	2.1	ng	3449	6	15.515	32837	20.0
9-Octadecene, (E)-	15.186	4.5	ng	7455	6	15.515	32837	20.0
unknown15.733	15.733	2.1	ng	3376	6	15.515	32837	20.0