LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124642.D
Acq On : 20 Jul 2021 23:13
Operator : JU/CG
Sample : M3096-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-071921

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-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124642.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	20	24	28	rBB	10796	11877	7.32%	1.123%
2	5.122	513	516	520	rBB	9785	10914	6.73%	1.032%
3	5.516	579	583	586	rBB	127789	112917	69.60%	10.679%
4	6.516	748	753	756	rBB	116647	120317	74.16%	11.379%
5	6.898	816	818	821	rBB	43414	36947	22.77%	3.494%
6	7.463	909	914	916	rBB	89071	79975	49.30%	7.564%
7	8.080	1016	1019	1022	rBB	18674	13824	8.52%	1.307%
8	8.186	1033	1037	1040	rBB	66572	53921	33.24%	5.100%
9	9.263	1215	1220	1223	rBV	202538	162231	100.00%	15.343%
10	9.945	1332	1336	1339	rBB	79909	66081	40.73%	6.250%
11	10.727	1466	1469	1472	rBB	110445	93591	57.69%	8.851%
12	11.427	1585	1588	1591	rBV	74532	61576	37.96%	5.823%
13	11.951	1672	1677	1680	rBB	19882	16594	10.23%	1.569%
14	12.521	1772	1774	1776	rBV	3205	2239	1.38%	0.212%
15	12.733	1808	1810	1812	rBB	6610	4531	2.79%	0.429%
16	13.015	1854	1858	1861	rBB	149245	120603	74.34%	11.406%
17	13.904	2007	2009	2014	rBB	7437	7843	4.83%	0.742%
18	14.068	2033	2037	2040	rBB	31967	28131	17.34%	2.660%
19	14.539	2114	2117	2122	rBB2	5992	7004	4.32%	0.662%
20	15.192	2225	2228	2231	rBV2	4955	5722	3.53%	0.541%
21	15.221	2231	2233	2240	rVB2	5137	6104	3.76%	0.577%
22	15.556	2285	2290	2293	rBV	23850	26584	16.39%	2.514%
23	16.033	2368	2371	2375	rBB	4386	5527	3.41%	0.523%
24	17.662	2644	2648	2654	rBB	1436	2322	1.43%	0.220%

Sum of corrected areas: 1057375

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ClientSampleId :
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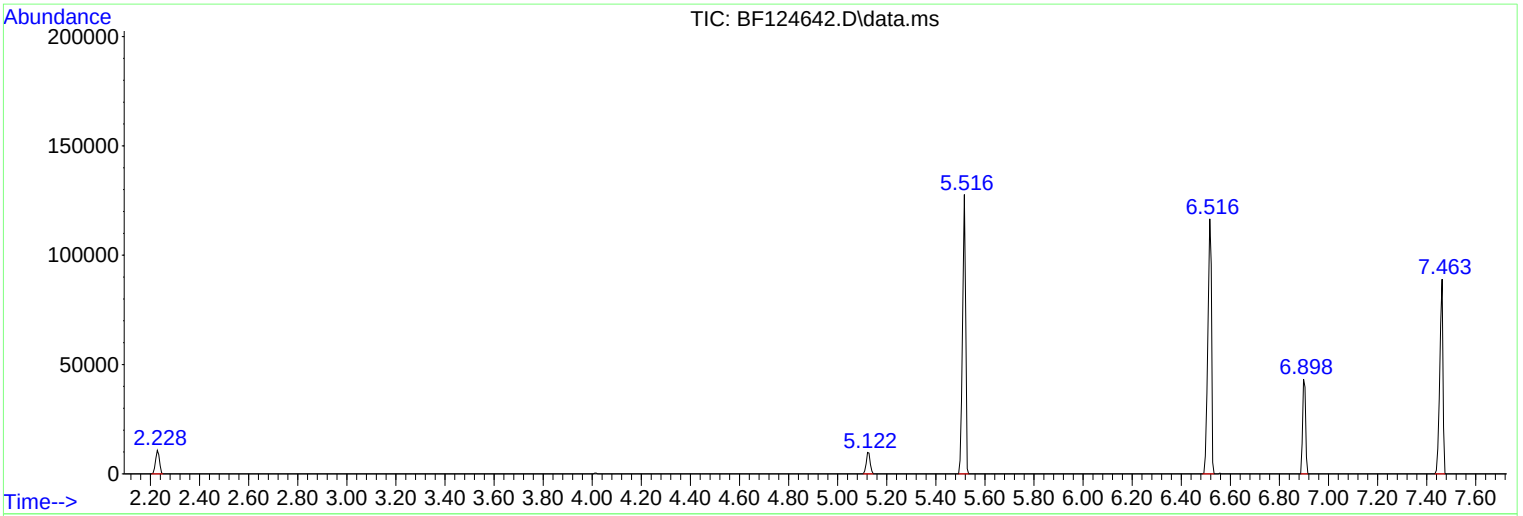
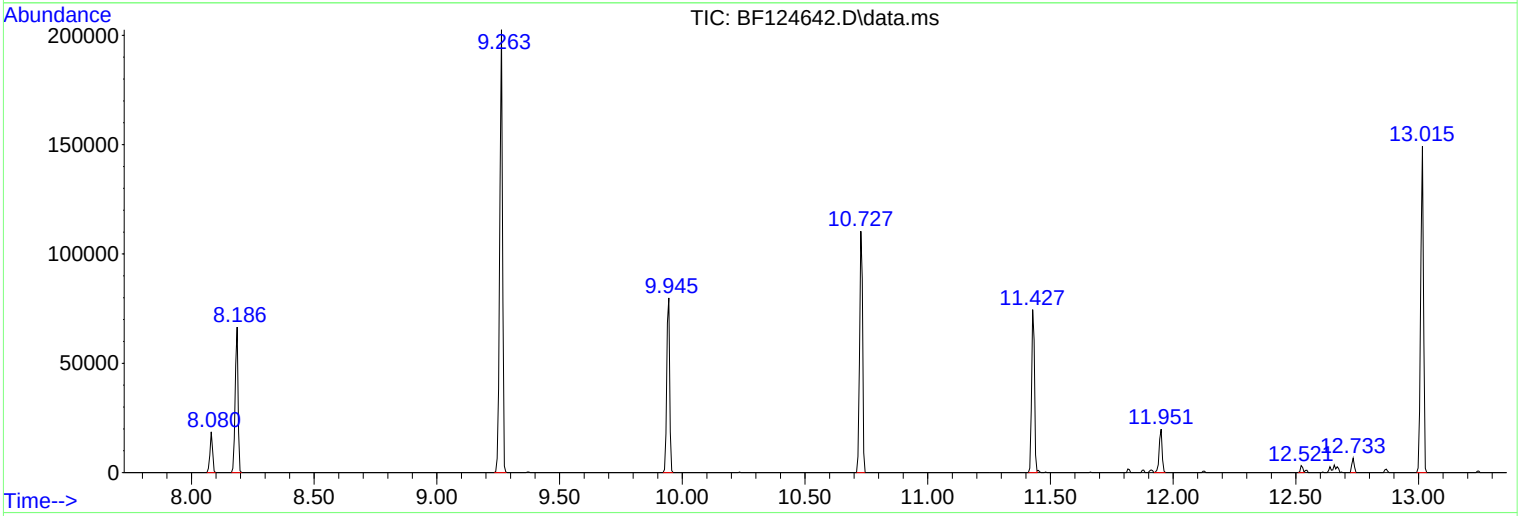
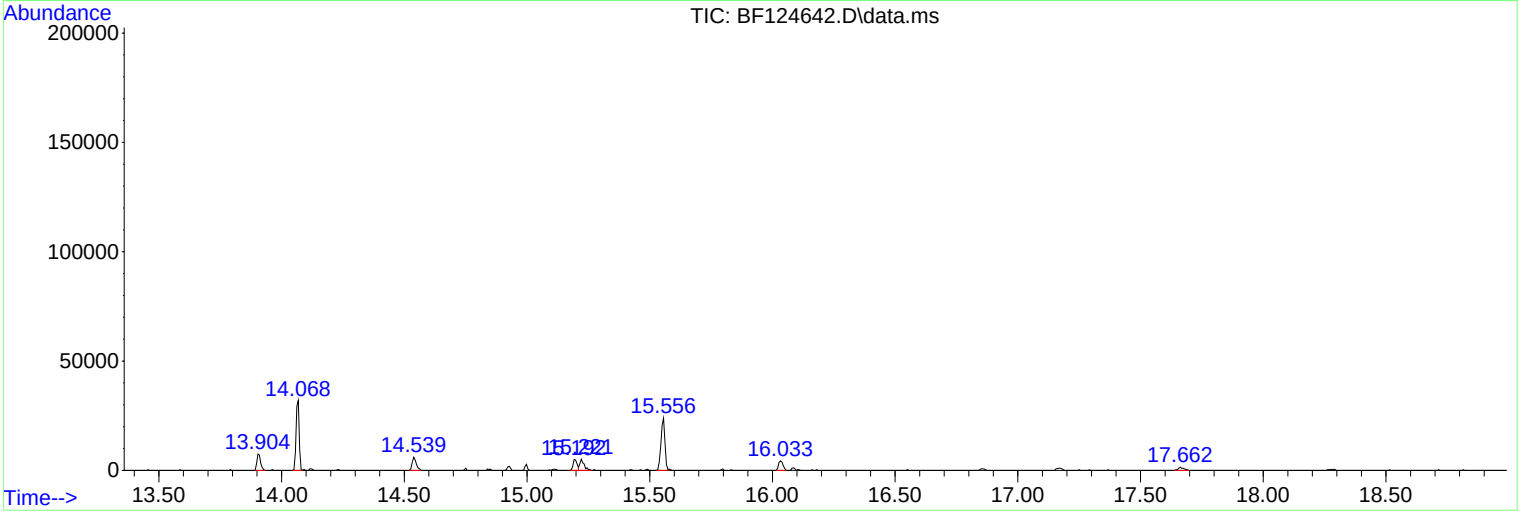
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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TIC Library : C:\Database\NIST20.L
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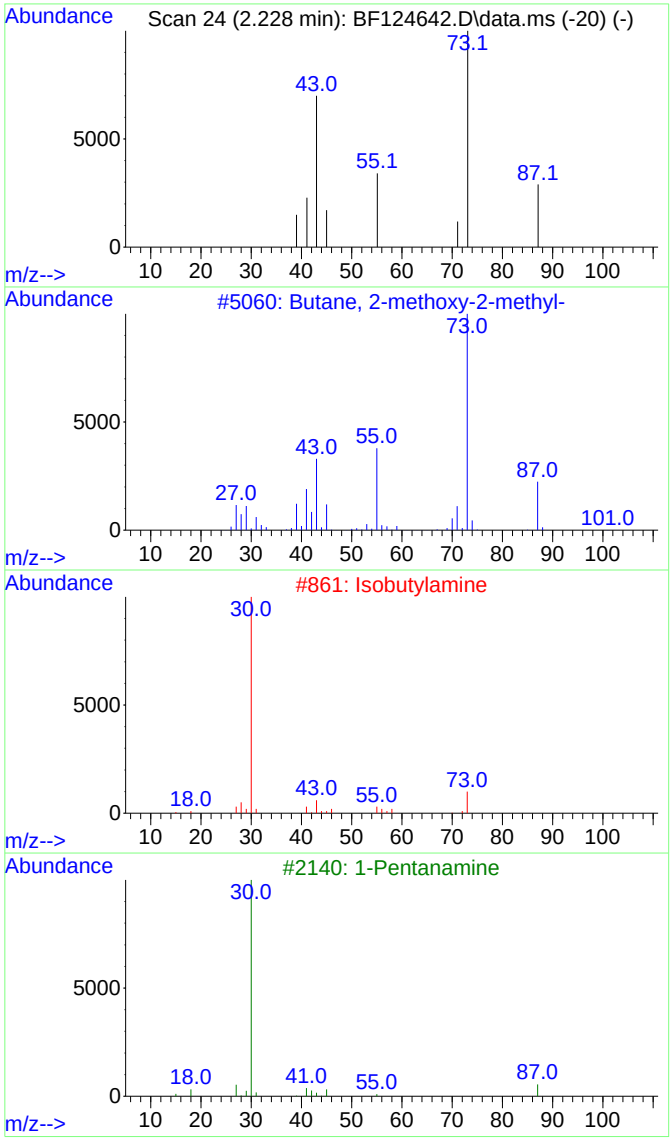
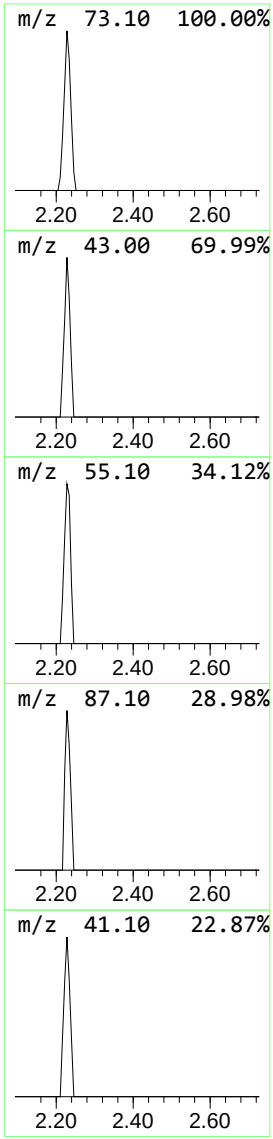
Peak Number 1 unknown2.228 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	6.43 ng	11877	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
2	Isobutylamine	73	C4H11N	000078-81-9	4
3	1-Pentanamine	87	C5H13N	000110-58-7	4
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4
5	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4





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Data File : BF124642.D
Acq On : 20 Jul 2021 23:13
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Sample : M3096-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-071921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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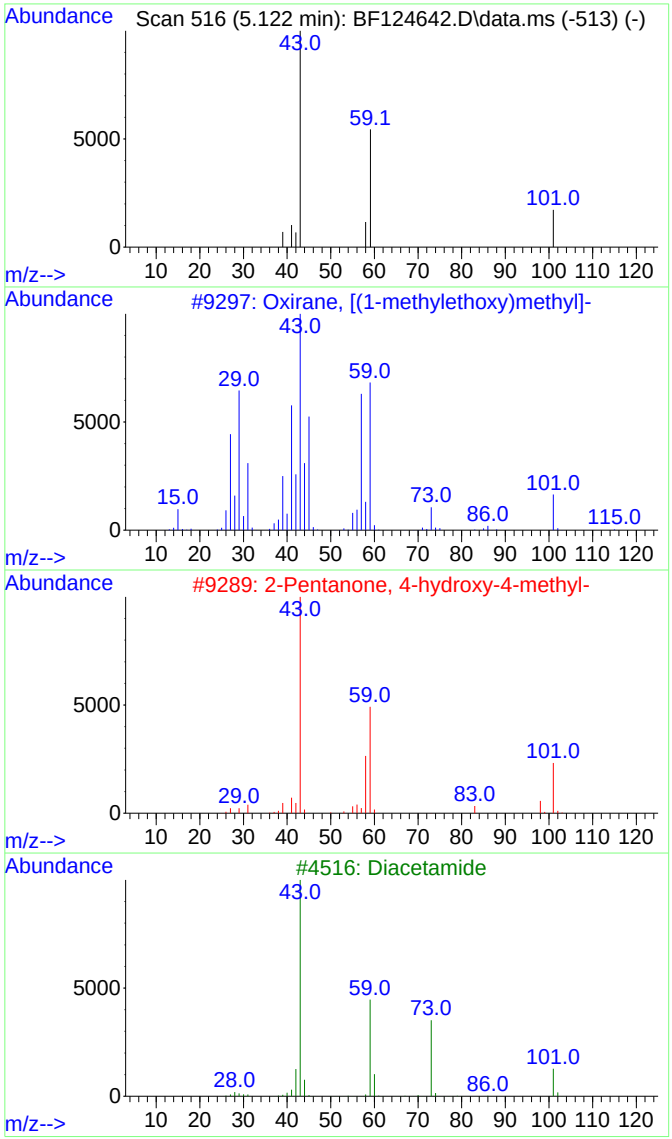
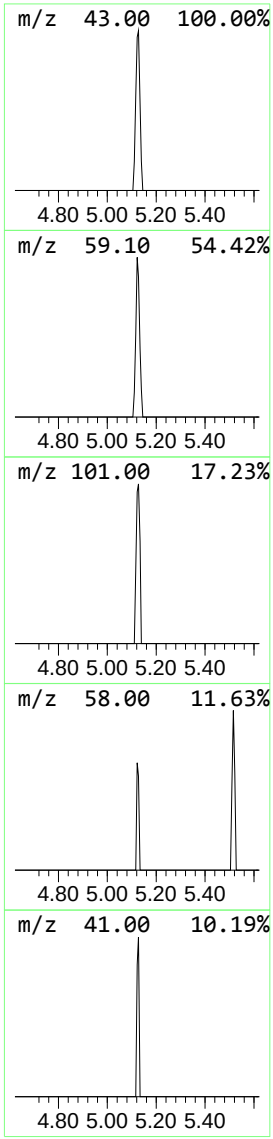
Peak Number 2 unknown5.122 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	5.91 ng	10914	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	9
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
3	Diacetamide	101	C4H7NO2	000625-77-4	7
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	4





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-071921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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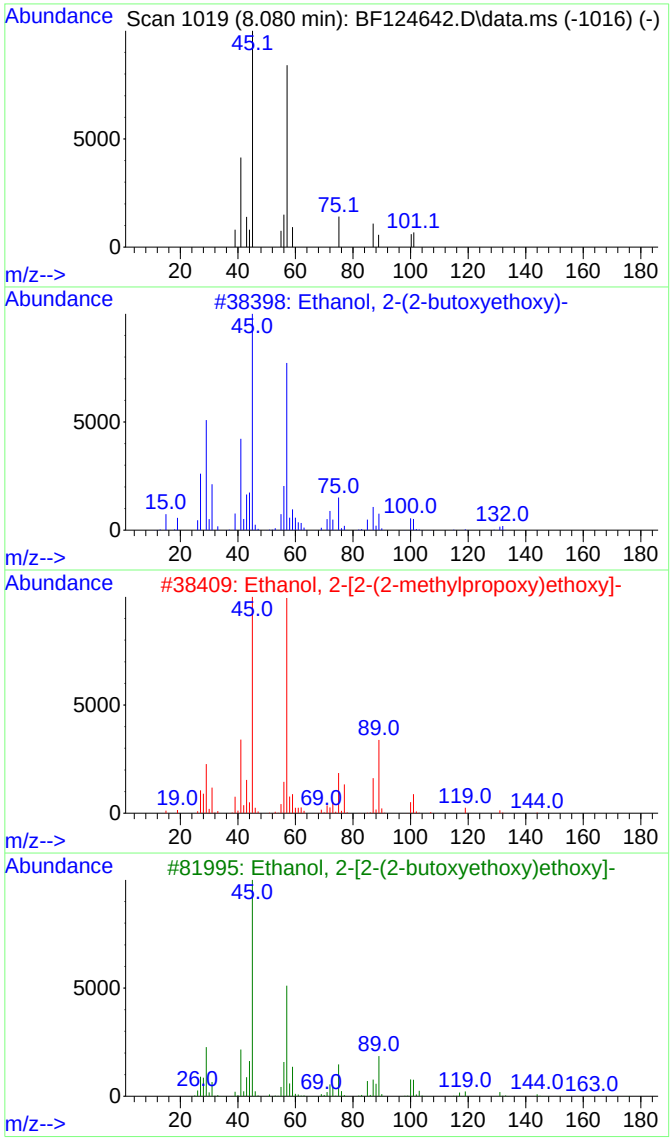
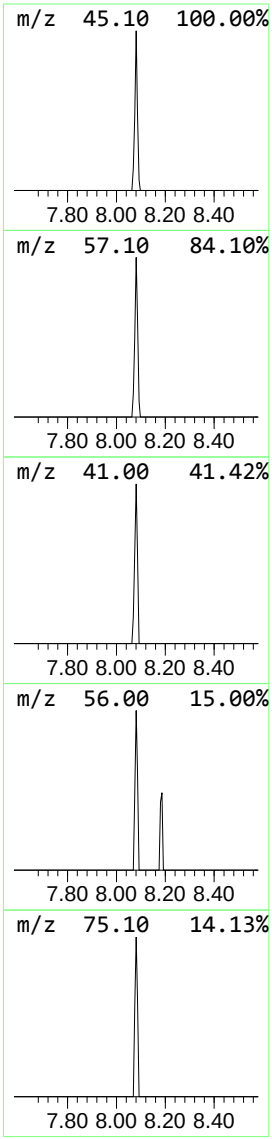
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.080	5.13 ng	13824	Naphthalene-d8	8.186

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	64
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	39
4	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	23
5	Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	17





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BNA_F
ClientSampleId :
SU-04-071921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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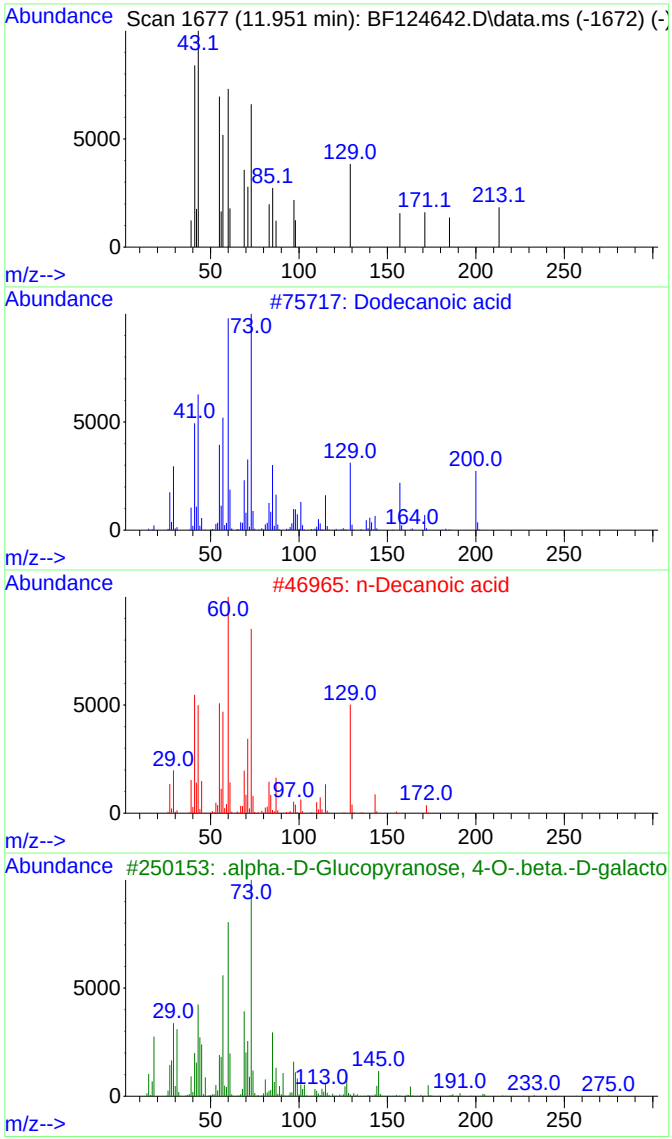
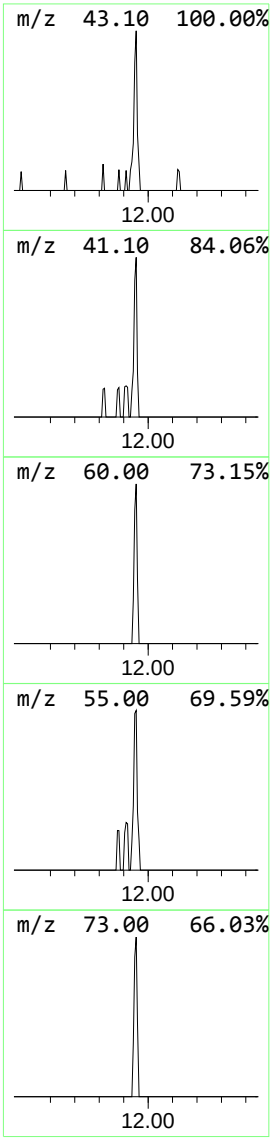
Peak Number 4 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	5.39 ng	16594	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	53
2	n-Decanoic acid	172	C10H20O2	000334-48-5	47
3	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	38
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38
5	Trehalose	342	C12H22O11	000099-20-7	38





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Sample : M3096-01
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Instrument : BNA_F
ClientSampleId : SU-04-071921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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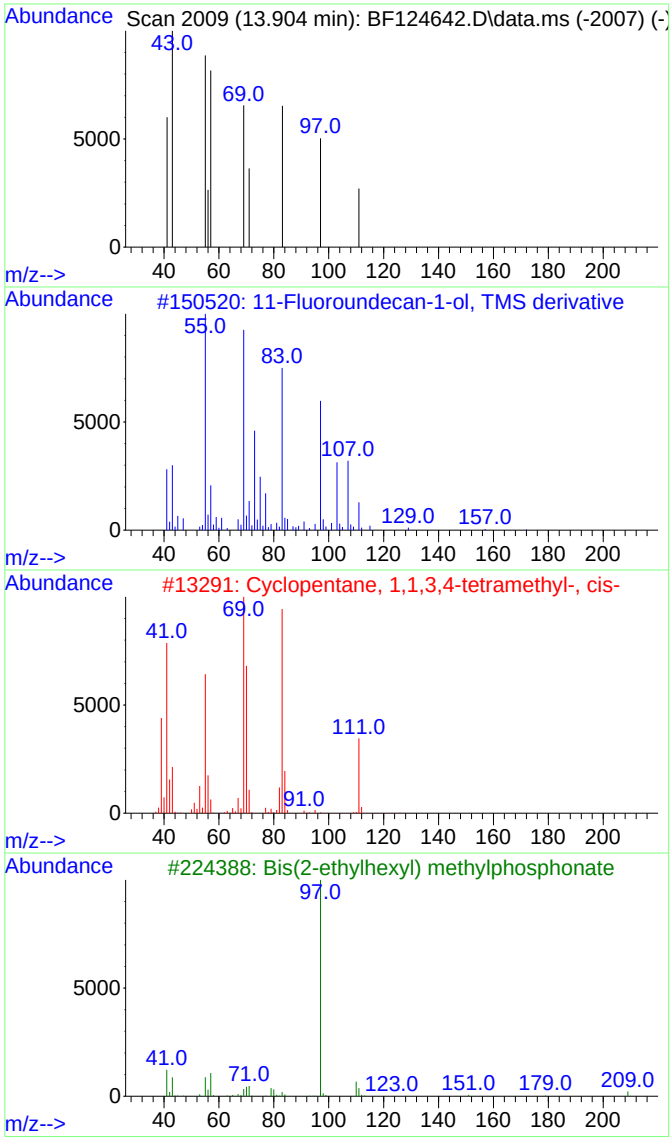
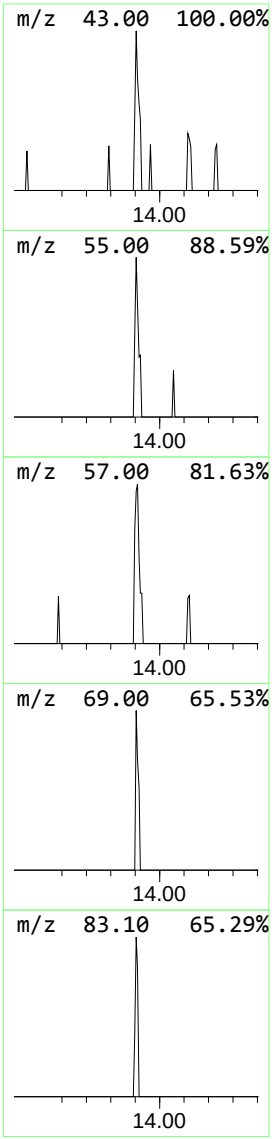
Peak Number 5 unknown13.904 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	5.58 ng	7843	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Fluoroundecan-1-ol, TMS deriv...	262	C14H31FOSi	026305-81-7	28
2	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	053907-60-1	17
3	Bis(2-ethylhexyl) methylphosphonate	320	C17H37O3P	1000298-35-3	9
4	Ether, 6-methylheptyl vinyl	156	C10H20O	010573-35-0	9
5	Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	9





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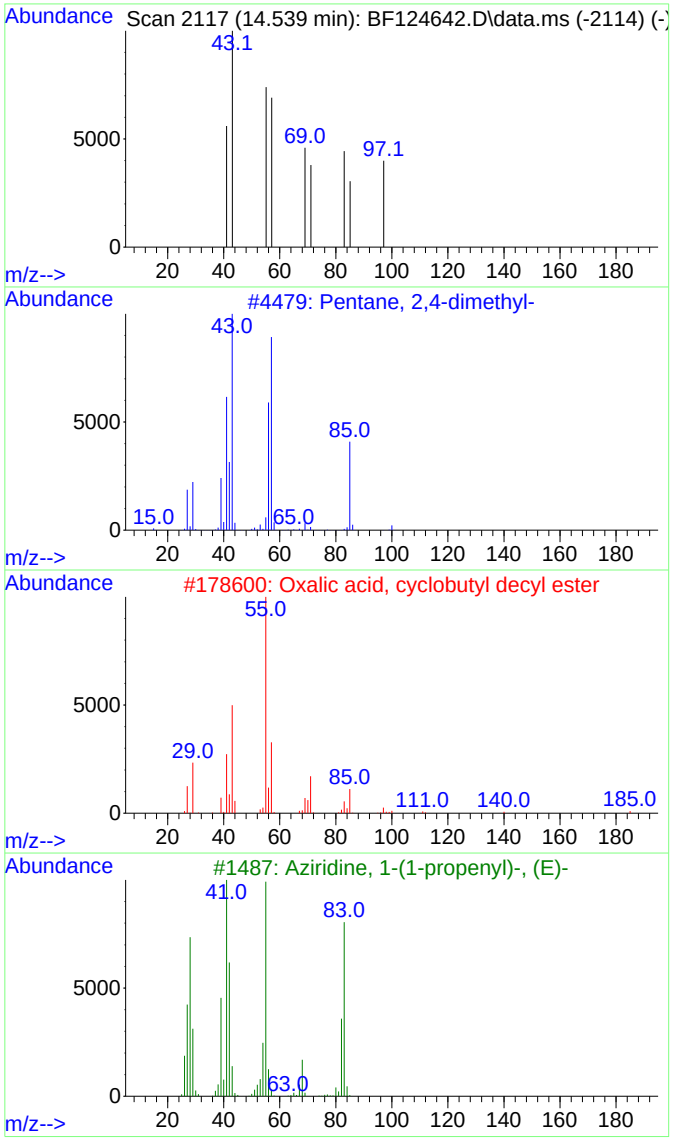
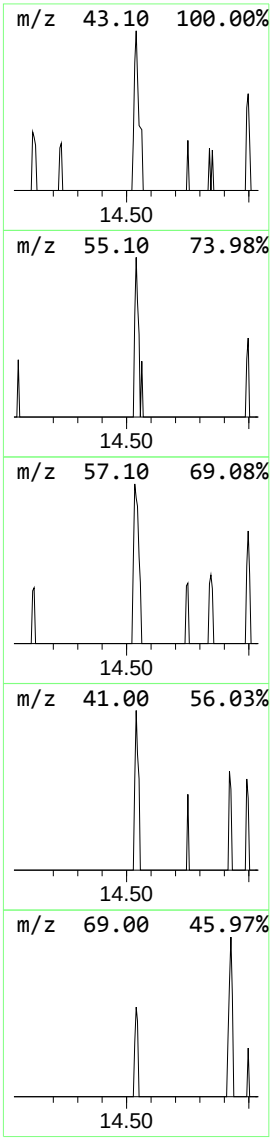
Peak Number 6 unknown14.539 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	4.98 ng	7004	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	9
2	Oxalic acid, cyclobutyl decyl ester	284	C16H28O4	1000309-70-1	9
3	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7
4	Oxazole, 4,5-dihydro-2-methyl-	85	C4H7NO	001120-64-5	4
5	1-Azabicyclo[3.1.0]hexane	83	C5H9N	000285-76-7	4





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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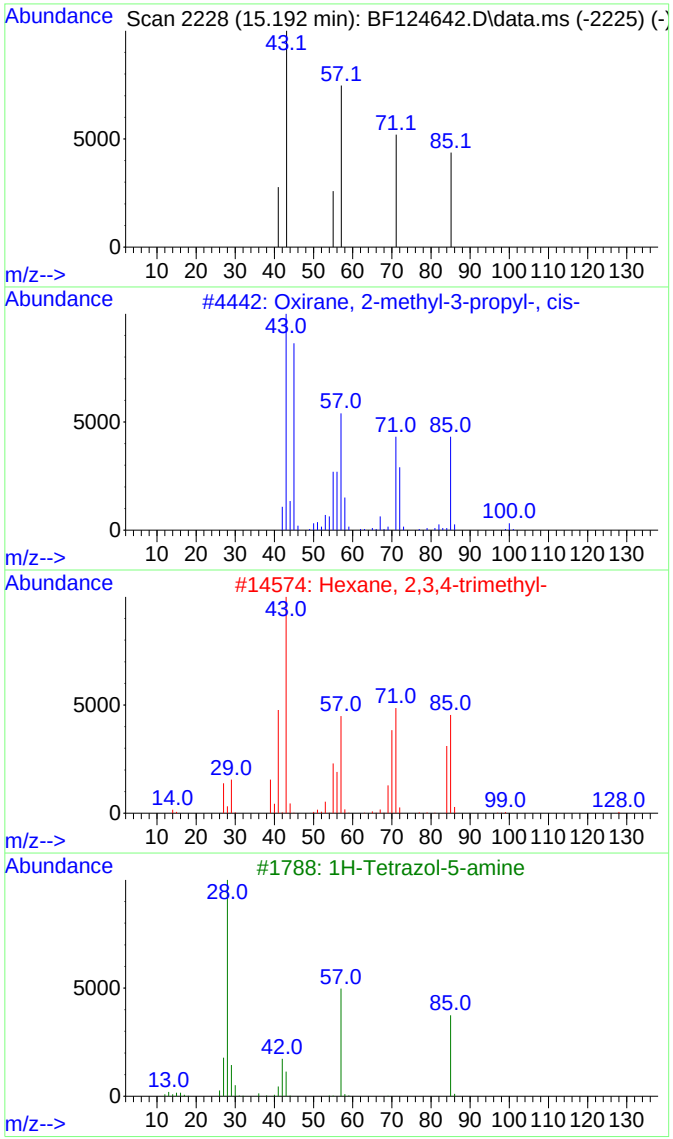
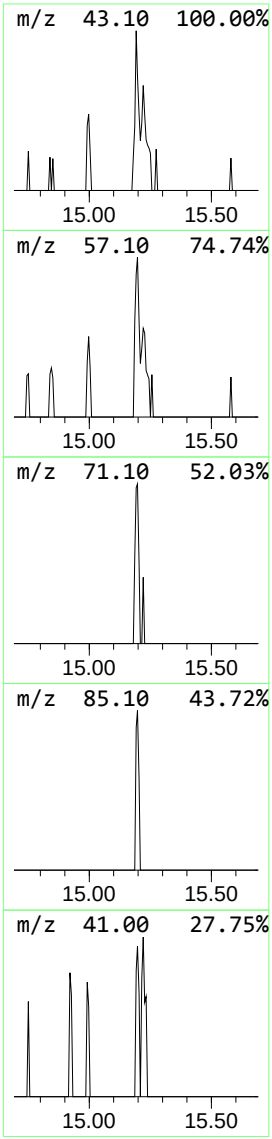
Peak Number 7 unknown15.192 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	4.30 ng	5722	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, 2-methyl-3-propyl-, cis-	100	C6H12O	006124-90-9	9
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	9
3	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
4	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
5	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4





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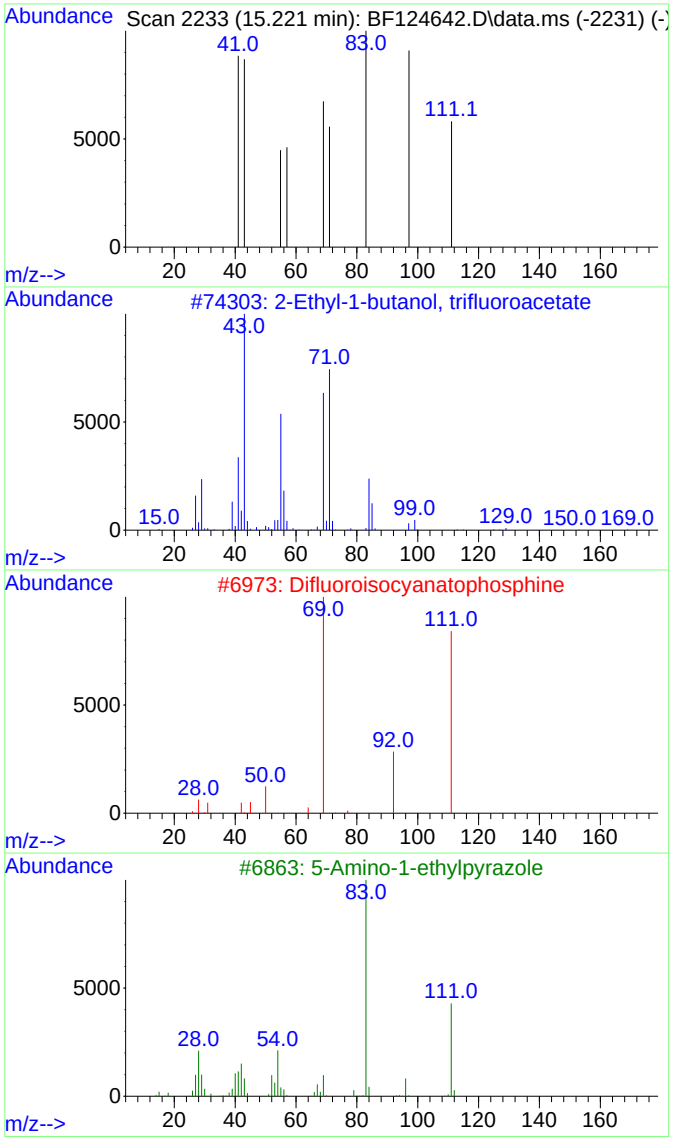
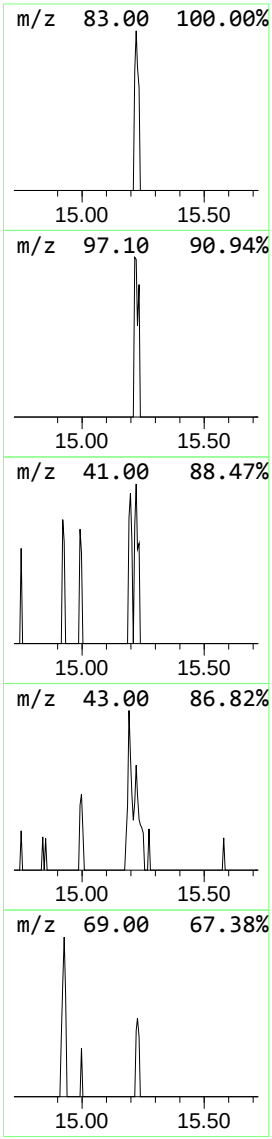
Peak Number 8 unknown15.221 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.221	4.59 ng	6104	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-1-butanol, trifluoroacetate	198	C8H13F3O2	116464-98-3	9
2	Difluoroisocyanatophosphine	111	CF2NOP	1000306-12-1	5
3	5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	5
4	Oxazole, 4,5-dimethyl-	97	C5H7NO	020662-83-3	4
5	2-Furanmethanamine	97	C5H7NO	000617-89-0	4





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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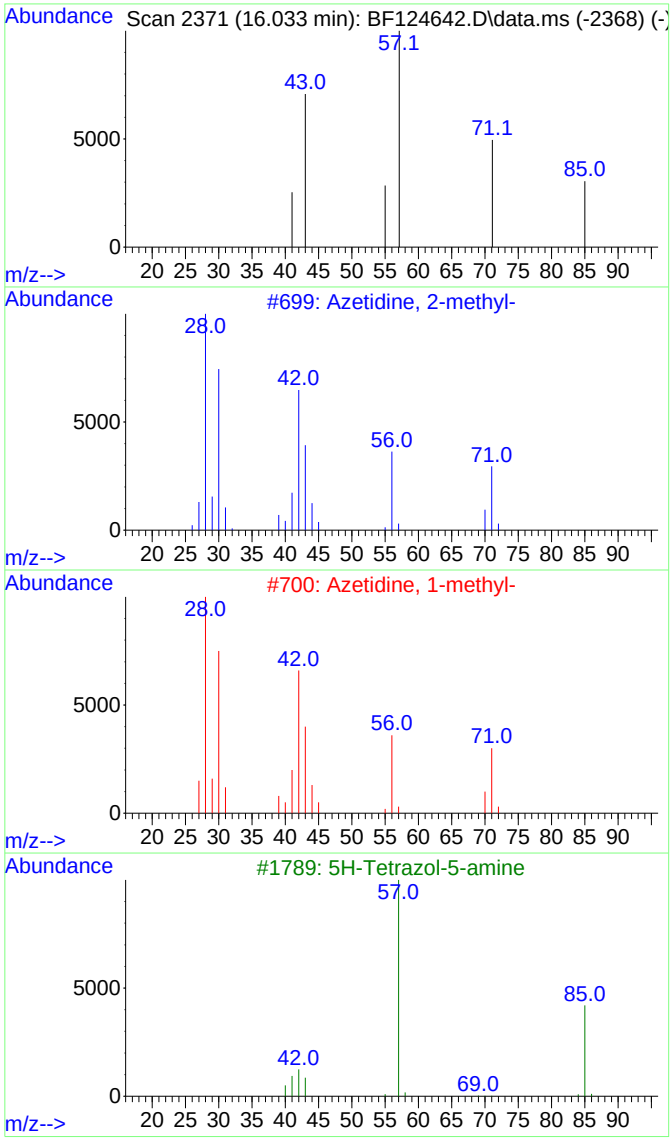
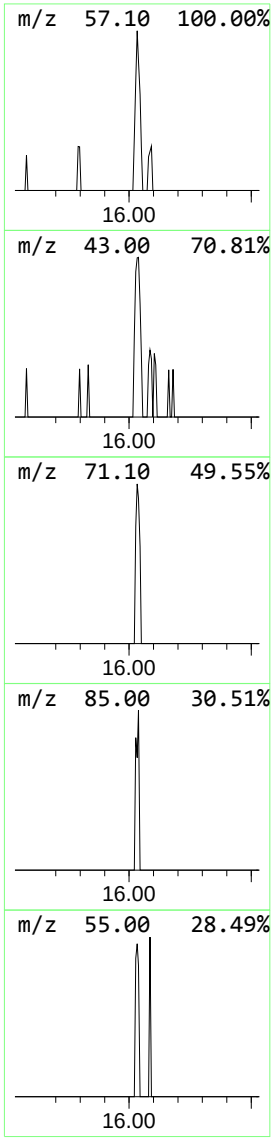
Peak Number 9 unknown16.033 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	4.16 ng	5527	Perylene-d12	15.557

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	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
5	Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	4





Tentatively Identified Compound (LSC) summary

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Acq On : 20 Jul 2021 23:13
Operator : JU/CG
Sample : M3096-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-071921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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
unknown2.228	2.228	6.4	ng	11877	1	6.898	36947	20.0
unknown5.122	5.122	5.9	ng	10914	1	6.898	36947	20.0
Ethanol, 2-(2-b...	8.080	5.1	ng	13824	2	8.186	53921	20.0
Dodecanoic acid	11.951	5.4	ng	16594	4	11.427	61576	20.0
unknown13.904	13.904	5.6	ng	7843	5	14.068	28131	20.0
unknown14.539	14.539	5.0	ng	7004	5	14.068	28131	20.0
unknown15.192	15.192	4.3	ng	5722	6	15.557	26584	20.0
unknown15.221	15.221	4.6	ng	6104	6	15.557	26584	20.0
unknown16.033	16.033	4.2	ng	5527	6	15.557	26584	20.0