LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124632.D
Acq On : 20 Jul 2021 17:23
Operator : JU/CG
Sample : M3076-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210578-COM-1

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: BF124632.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.251	23	28	32	rBB	14201	16326	7.79%	1.211%
2	5.145	517	520	524	rBB	2145	2861	1.37%	0.212%
3	5.522	579	584	587	rBB	165042	174368	83.25%	12.938%
4	6.522	749	754	757	rBV	154477	179438	85.67%	13.314%
5	6.904	816	819	821	rBB	39669	32875	15.70%	2.439%
6	7.463	909	914	917	rBB	109064	113850	54.36%	8.448%
7	8.081	1016	1019	1023	rBB	29313	23995	11.46%	1.780%
8	8.186	1033	1037	1040	rBB	54262	46268	22.09%	3.433%
9	9.263	1215	1220	1223	rBB	239019	209450	100.00%	15.541%
10	9.945	1332	1336	1339	rBB	63686	52050	24.85%	3.862%
11	10.733	1465	1470	1473	rBB	157338	130292	62.21%	9.668%
12	11.427	1585	1588	1592	rBB	57614	51022	24.36%	3.786%
13	11.951	1672	1677	1681	rBB	30800	26657	12.73%	1.978%
14	12.733	1803	1810	1815	rBB	13393	15103	7.21%	1.121%
15	13.021	1854	1859	1862	rBB	185311	177438	84.72%	13.166%
16	13.586	1952	1955	1957	rBV	3139	4032	1.93%	0.299%
17	13.904	2007	2009	2013	rBV	4816	5525	2.64%	0.410%
18	14.068	2034	2037	2040	rBV	36050	28332	13.53%	2.102%
19	14.245	2061	2067	2071	rBB2	3798	6825	3.26%	0.506%
20	14.792	2155	2160	2164	rBB	3499	5179	2.47%	0.384%
21	14.845	2164	2169	2174	rBB	3753	4438	2.12%	0.329%
22	15.192	2225	2228	2232	rBB	2780	3109	1.48%	0.231%
23	15.380	2256	2260	2264	rBB2	2492	3678	1.76%	0.273%
24	15.557	2285	2290	2293	rBV2	22749	26175	12.50%	1.942%
25	15.586	2293	2295	2298	rVB2	2290	2348	1.12%	0.174%
26	16.045	2368	2373	2380	rBB3	2842	6094	2.91%	0.452%

Sum of corrected areas: 1347728

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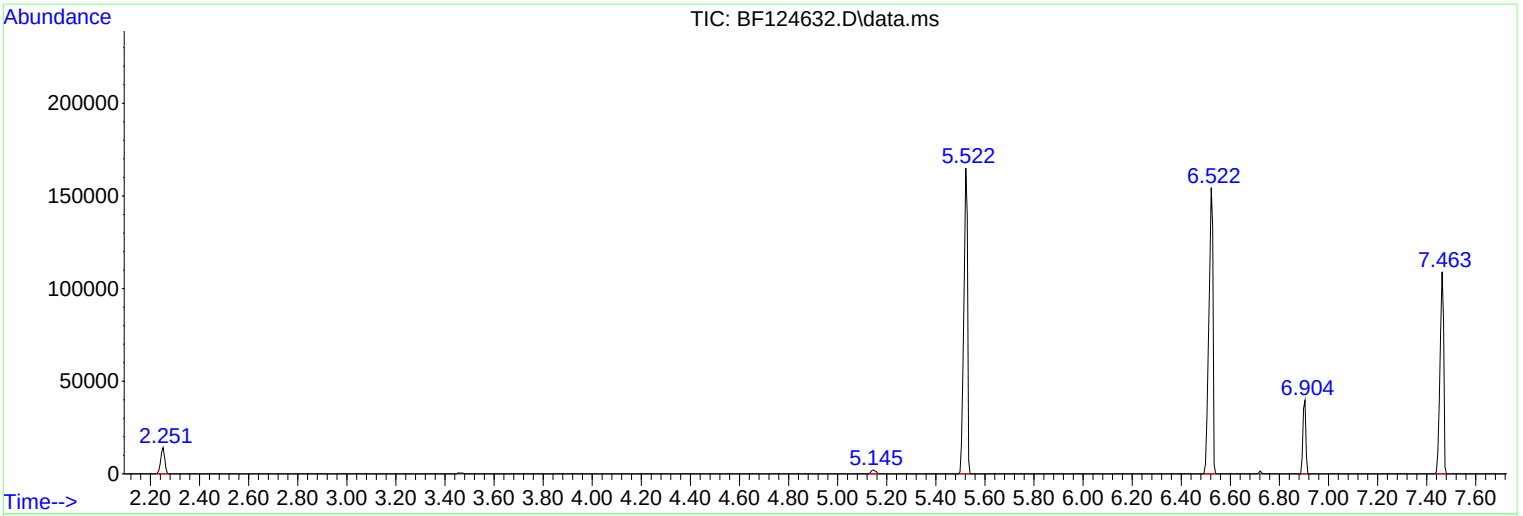
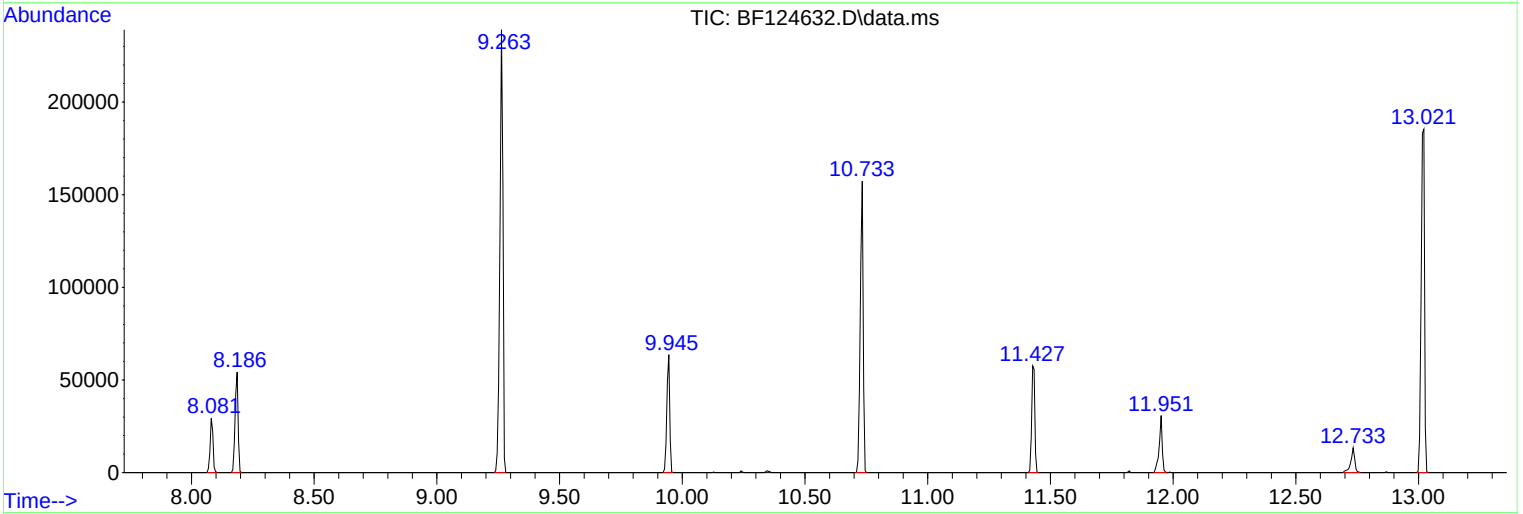
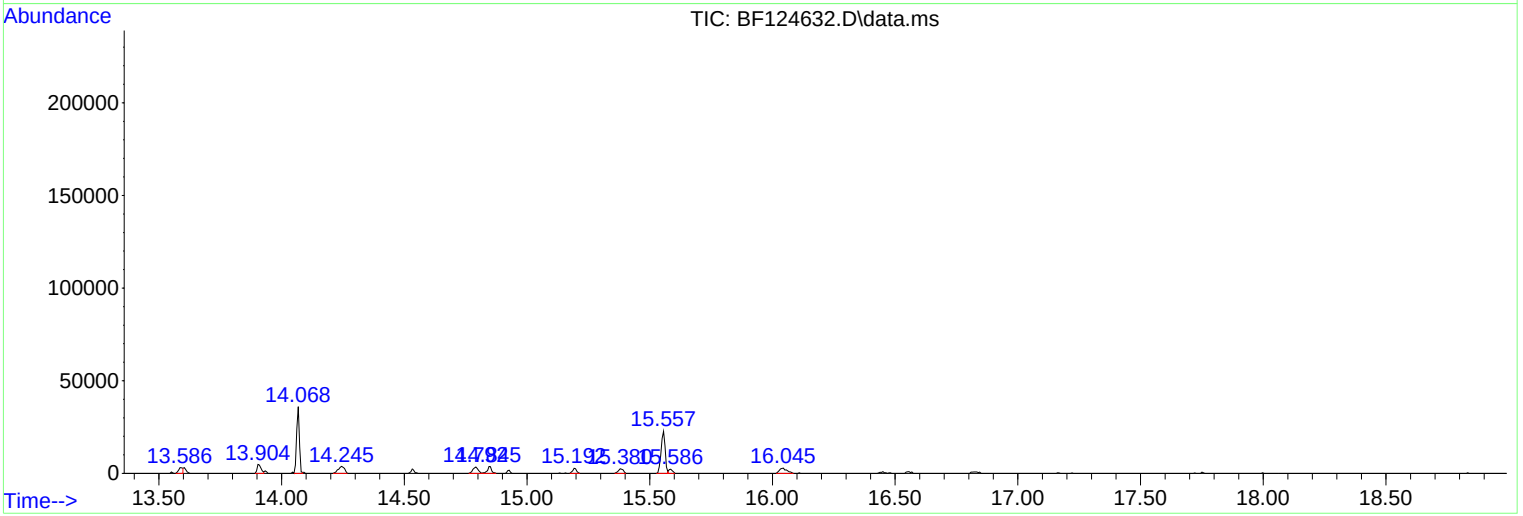
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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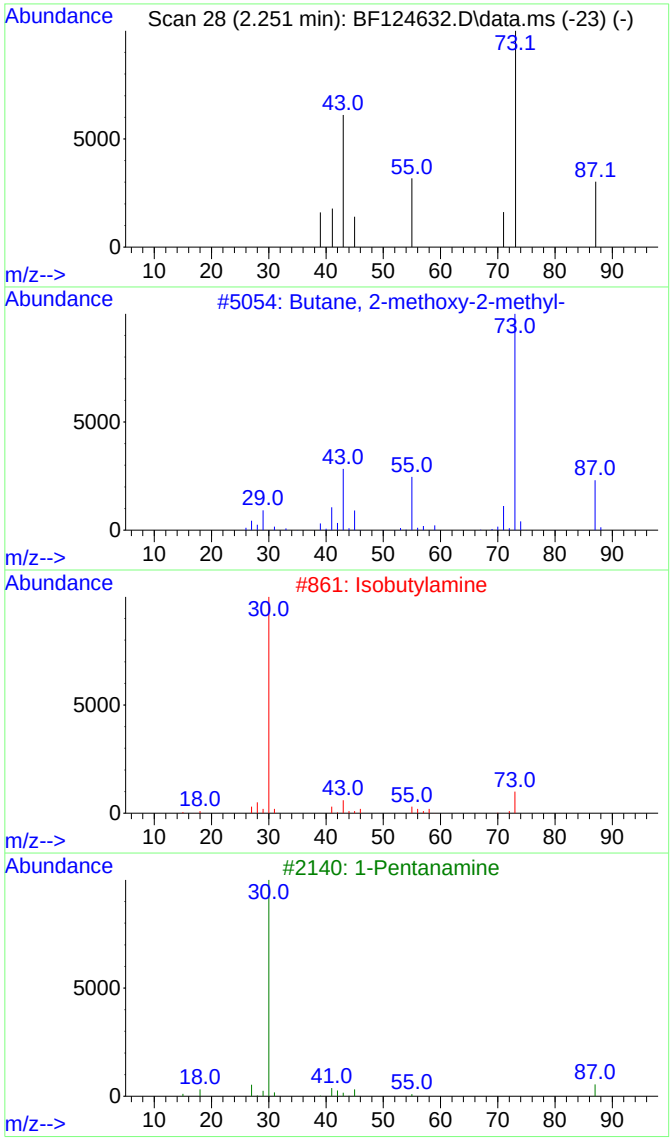
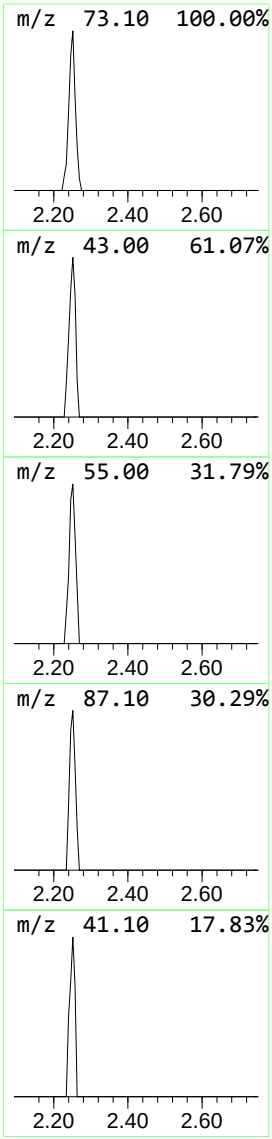
Peak Number 1 unknown2.251 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.251	9.93 ng	16326	1,4-Dichlorobenzene-d4	6.904

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	5
3	1-Pentanamine	87	C5H13N	000110-58-7	4
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	4
5	2-Pentanol, acetate	130	C7H14O2	000626-38-0	4





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Operator : JU/CG
Sample : M3076-01
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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210578-COM-1

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

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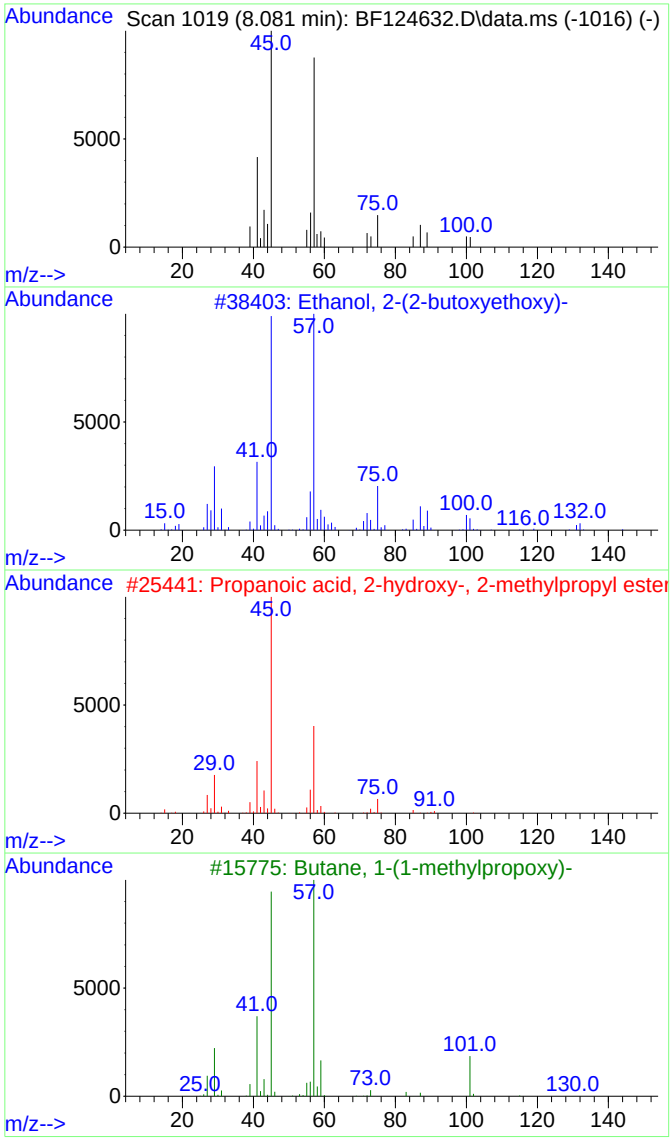
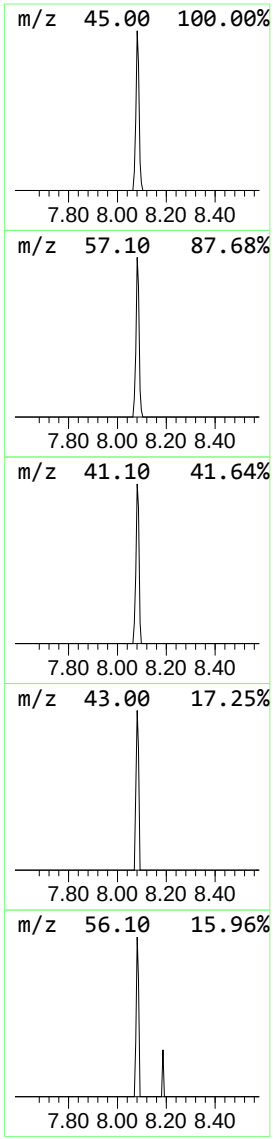
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	10.37 ng	23995	Naphthalene-d8	8.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	42
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	42
4	Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	39
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	39





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Misc :
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Instrument : BNA_F
ClientSampleId : 20210578-COM-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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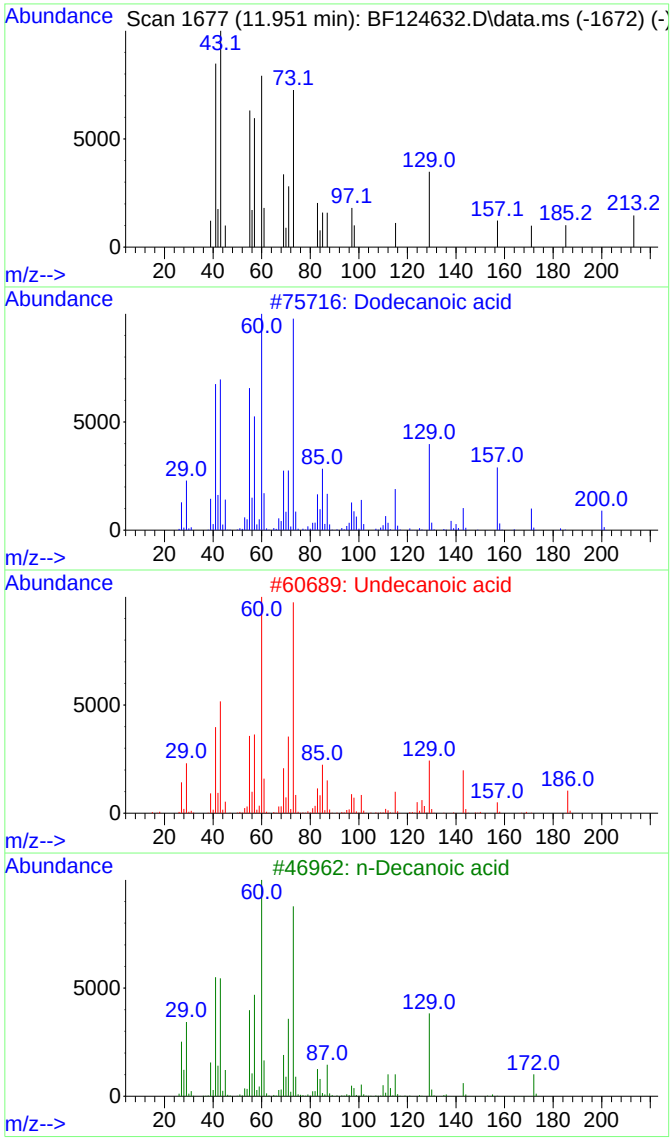
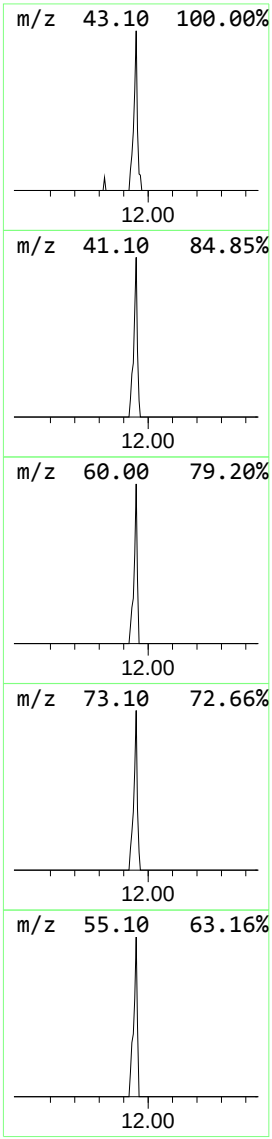
Peak Number 3 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	10.45 ng	26657	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	59
2	Undecanoic acid	186	C11H22O2	000112-37-8	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	47
5	Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	47





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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210578-COM-1

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TIC Library : C:\Database\NIST20.L
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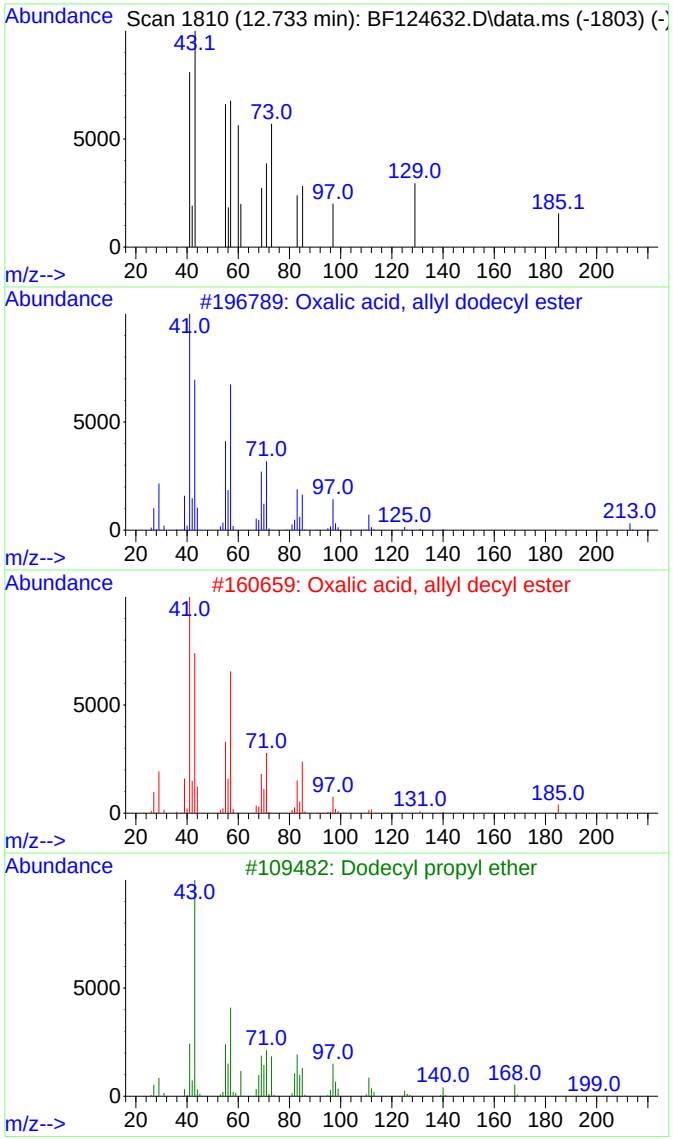
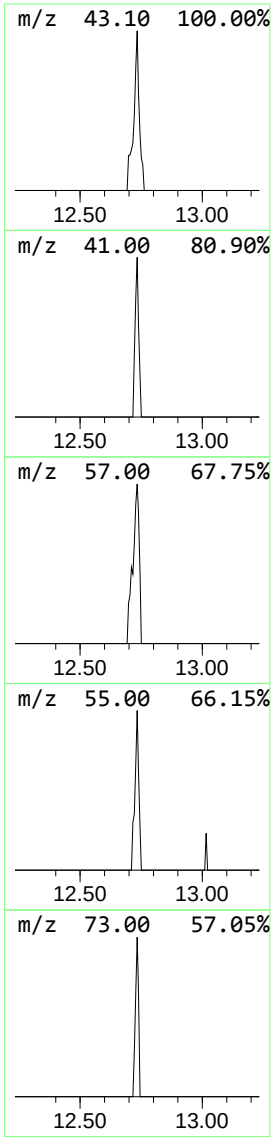
Peak Number 4 unknown12.733 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	5.92 ng	15103	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	38
2	Oxalic acid, allyl decyl ester	270	C15H26O4	1010309-23-8	38
3	Dodecyl propyl ether	228	C15H32O	1000406-27-7	37
4	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	35
5	Oxalic acid, cyclobutyl decyl ester	284	C16H28O4	1000309-70-1	35





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Instrument :
BNA_F
ClientSampleId :
20210578-COM-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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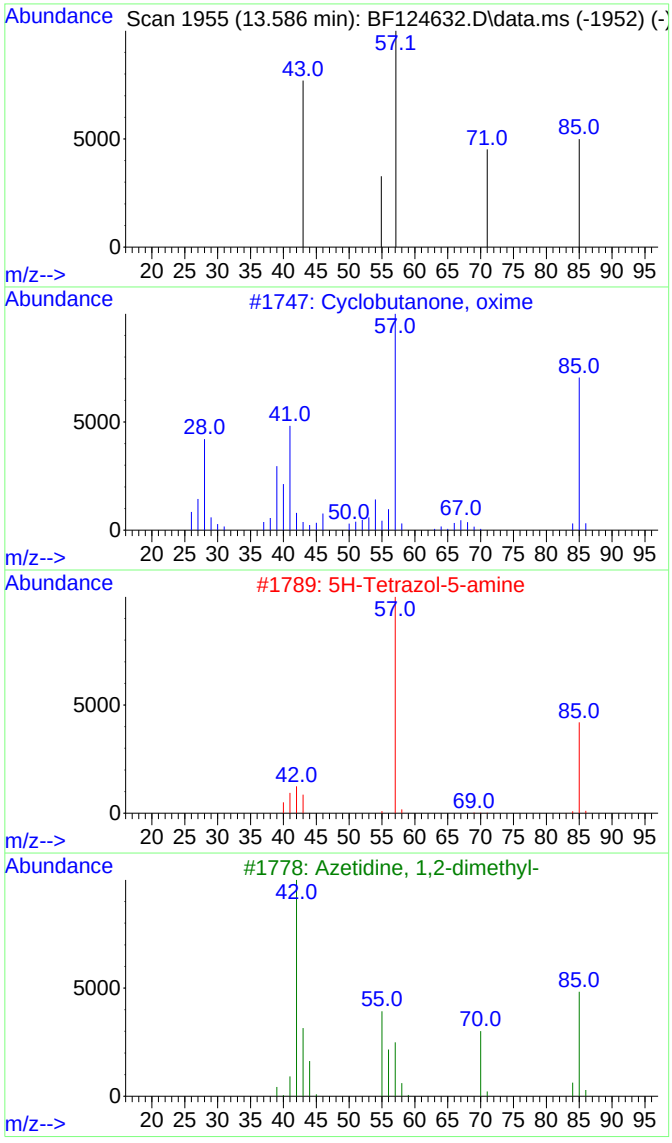
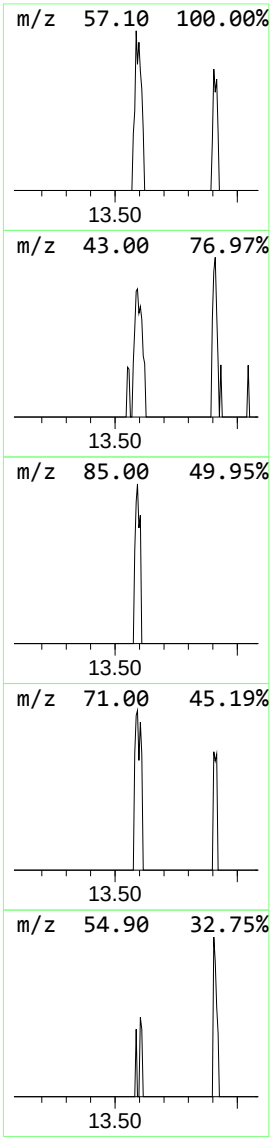
Peak Number 5 unknown13.586 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.586	2.85 ng	4032	Chrysene-d12	14.068

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	Azetidine, 1,2-dimethyl-	85	C5H11N	051764-32-0	4
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	4
5	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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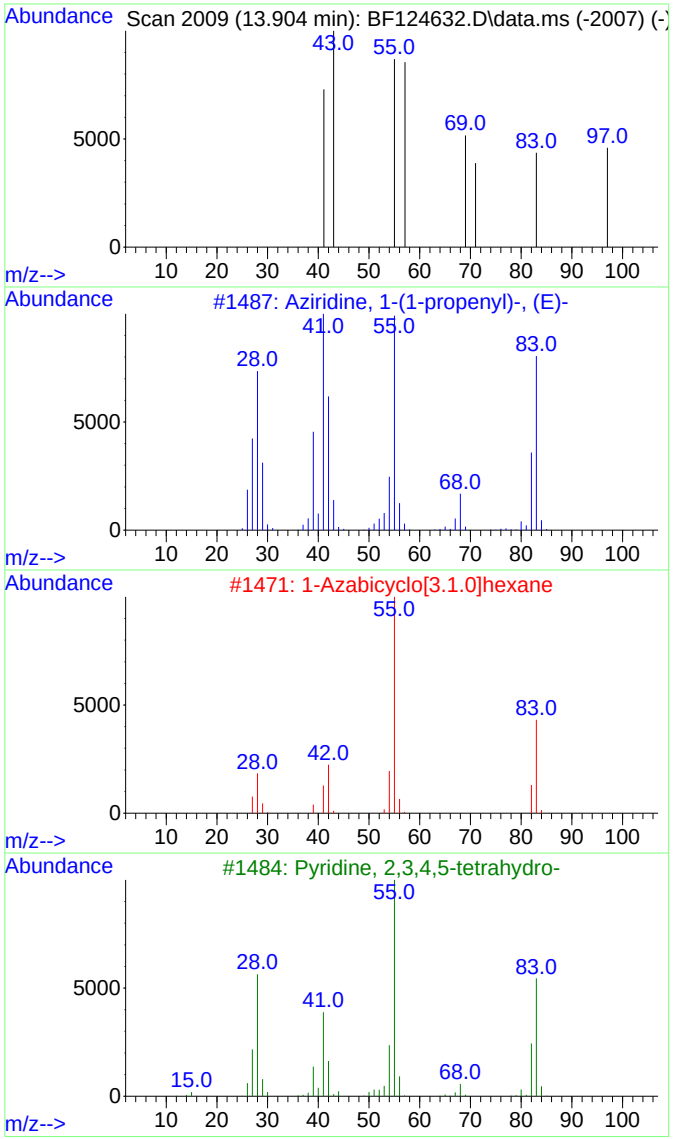
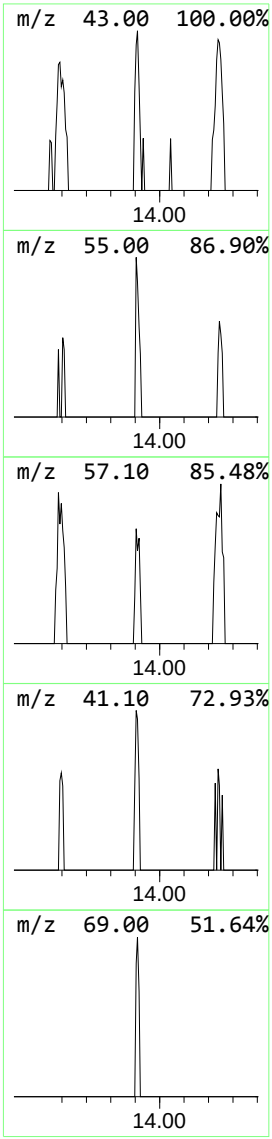
Peak Number 6 unknown13.904 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.90 ng	5525	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	4
2	1-Azabicyclo[3.1.0]hexane	83	C5H9N	000285-76-7	4
3	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	4
4	1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	4
5	3-Hexyn-2-ol, 5-methyl-	112	C7H12O	023293-50-7	2





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ClientSampleId :
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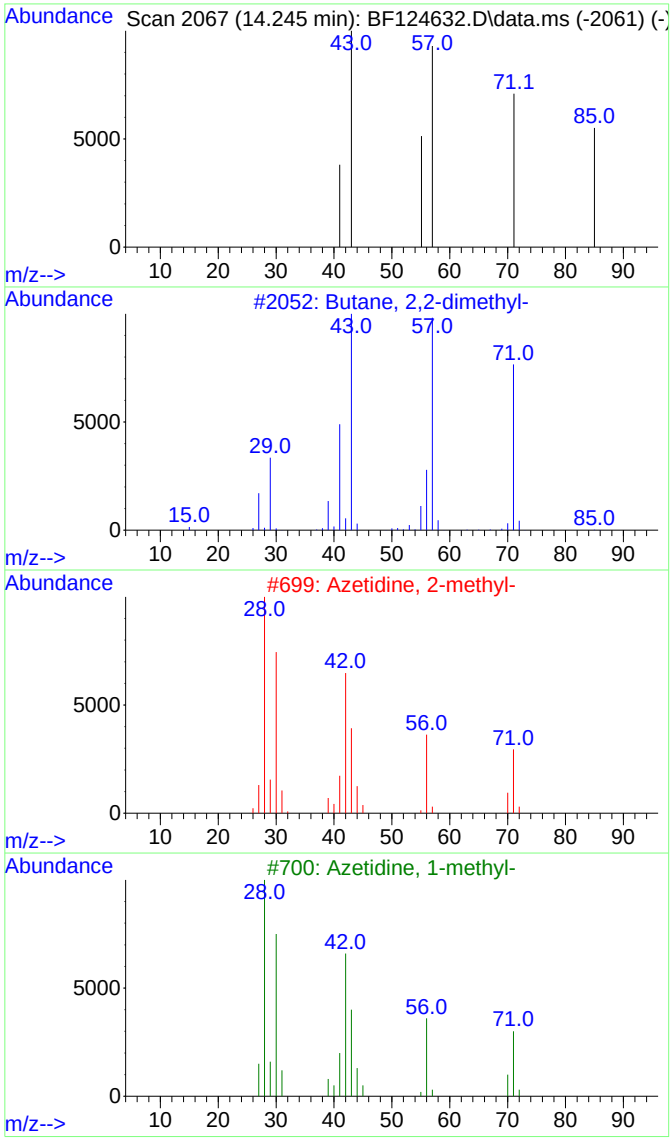
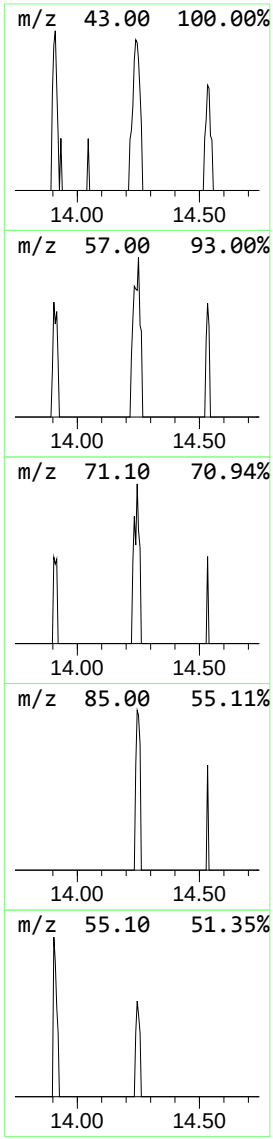
Peak Number 7 unknown14.245 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	4.82 ng	6825	Chrysene-d12	14.068

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	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	4





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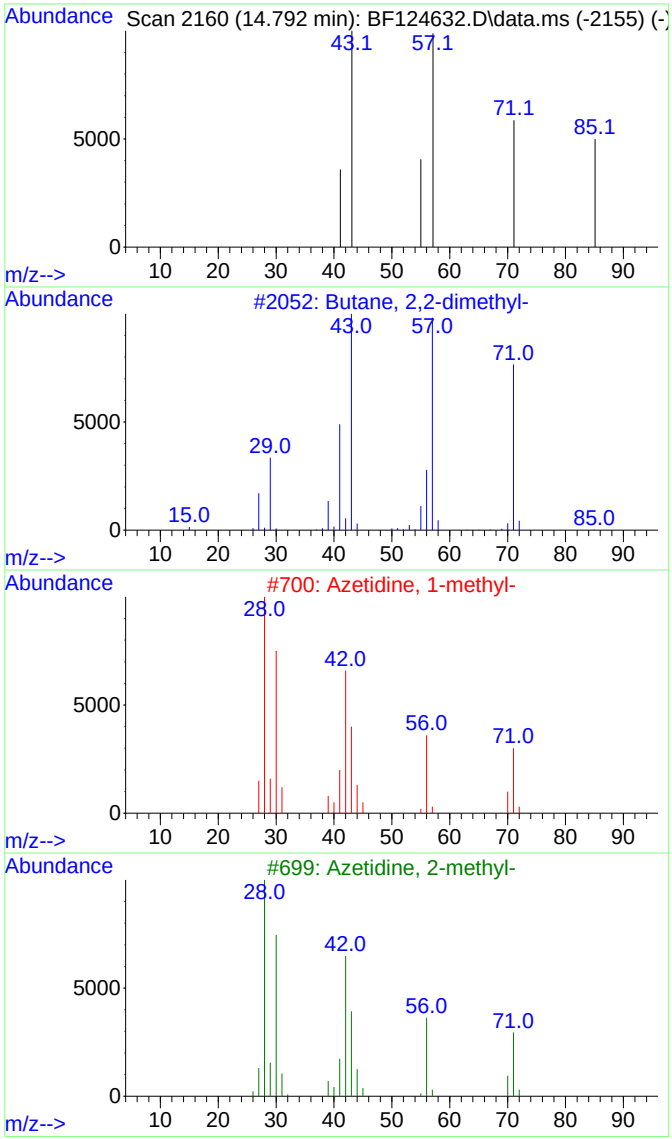
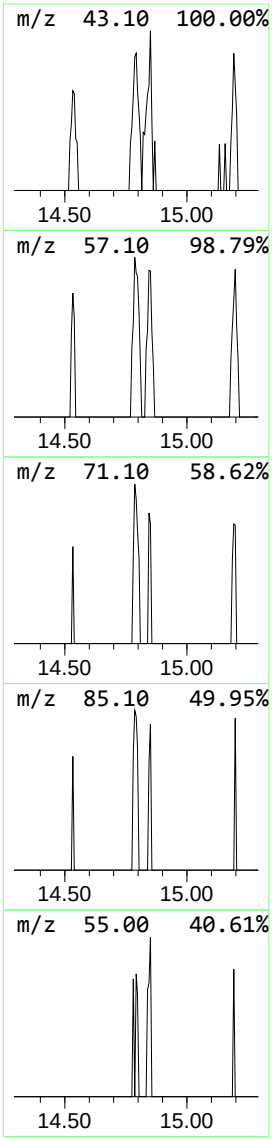
Peak Number 8 unknown14.792 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	3.66 ng	5179	Chrysene-d12	14.068

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	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
5	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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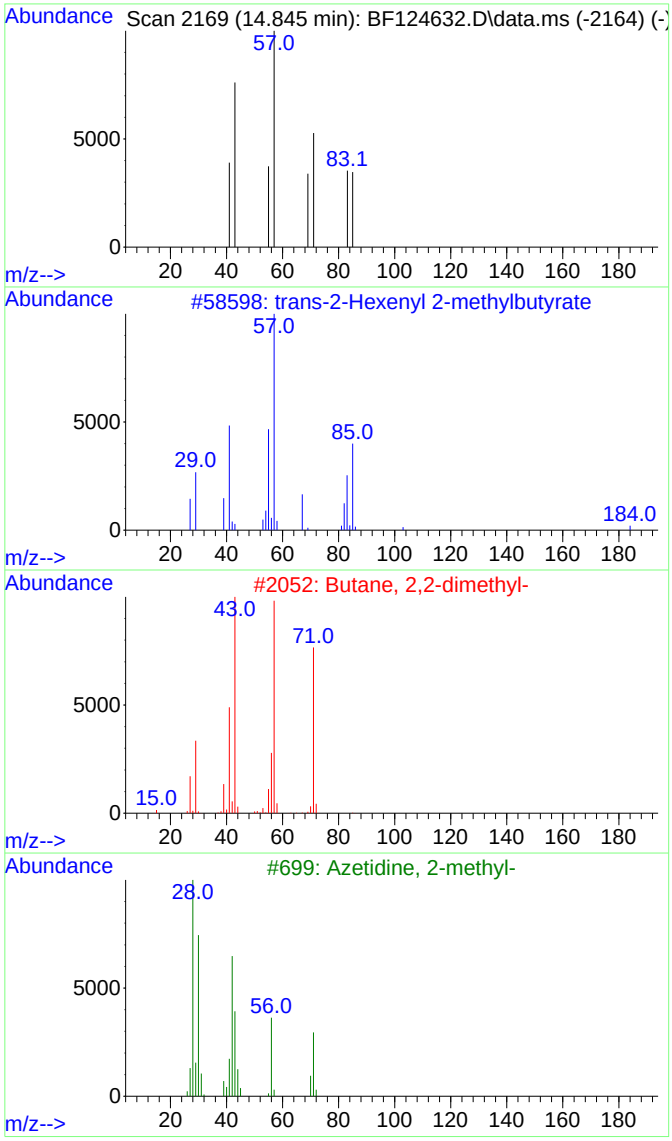
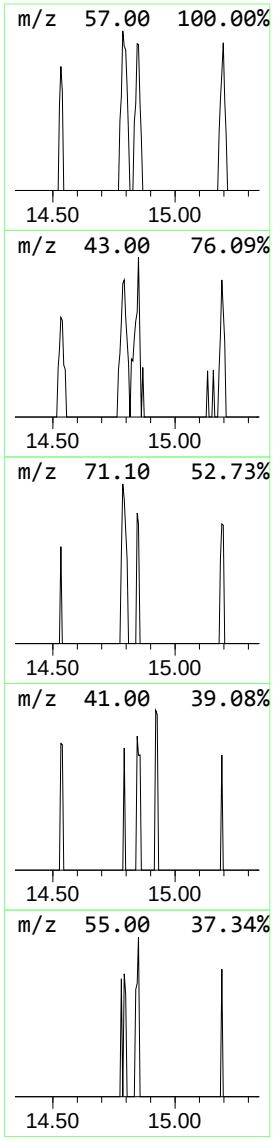
Peak Number 9 unknown14.845 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	3.39 ng	4438	Perylene-d12	15.557

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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Data File : BF124632.D
Acq On : 20 Jul 2021 17:23
Operator : JU/CG
Sample : M3076-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210578-COM-1

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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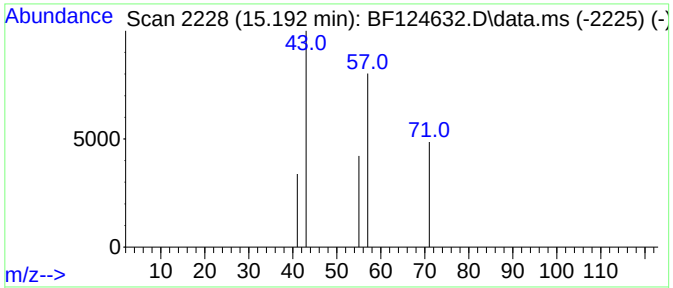
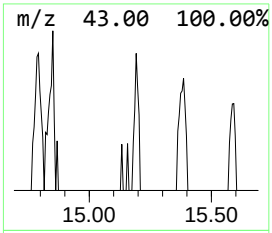
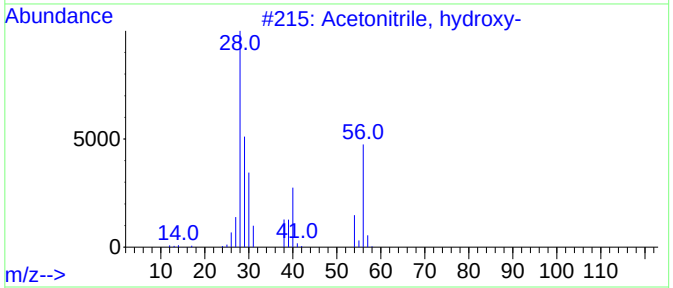
Peak Number 10 unknown15.192 Concentration Rank 12

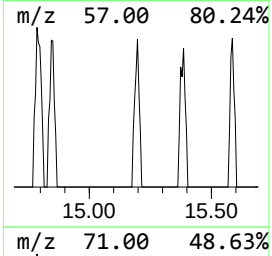
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	2.38 ng	3109	Perylene-d12	15.557

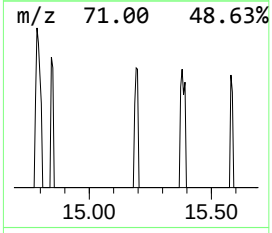
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	4
2	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
3	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	2
4	Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	2
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	2

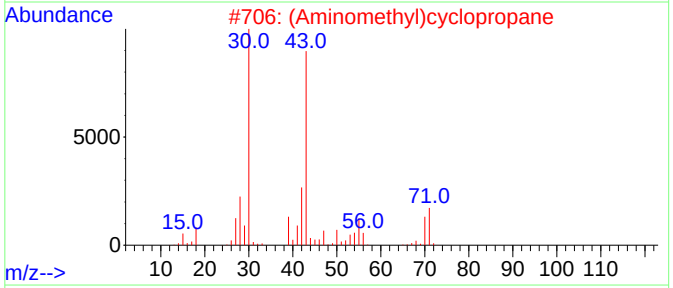


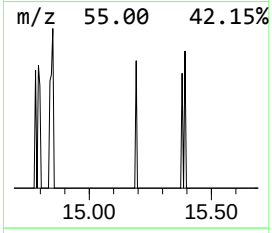


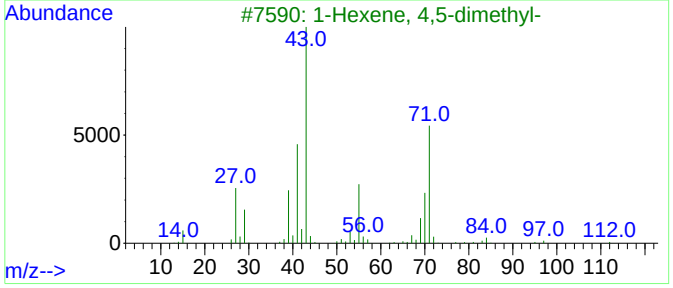


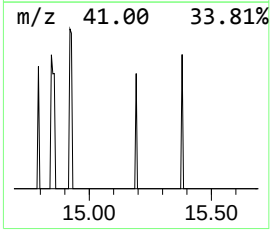












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Data File : BF124632.D
Acq On : 20 Jul 2021 17:23
Operator : JU/CG
Sample : M3076-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210578-COM-1

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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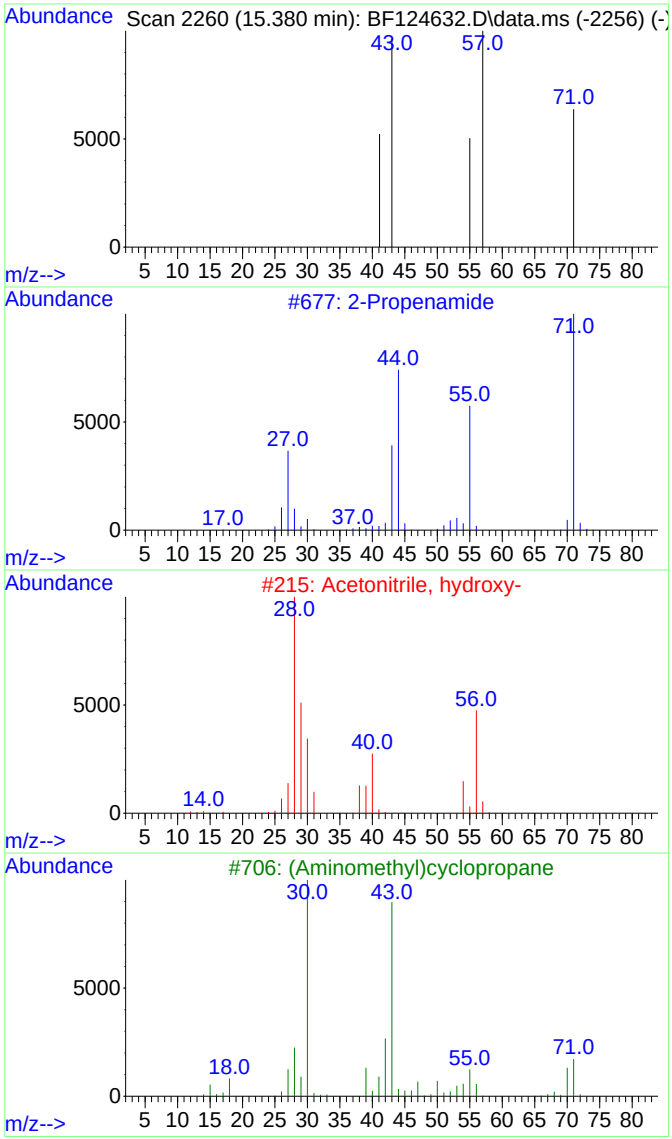
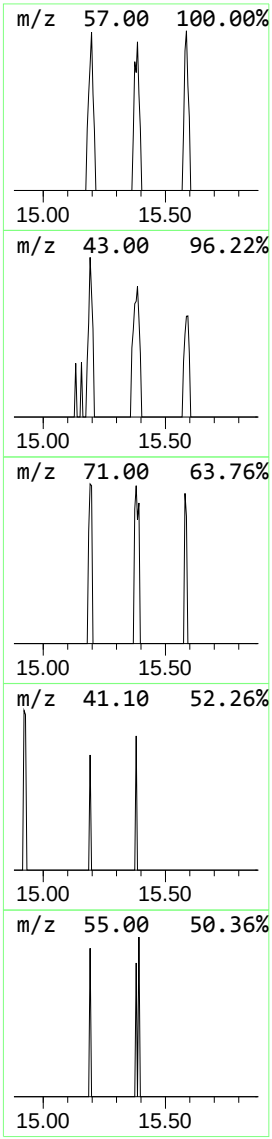
Peak Number 11 unknown15.380 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	2.81 ng	3678	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide	71	C3H5NO	000079-06-1	4
2	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
3	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
4	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	2
5	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	2





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Data File : BF124632.D
Acq On : 20 Jul 2021 17:23
Operator : JU/CG
Sample : M3076-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210578-COM-1

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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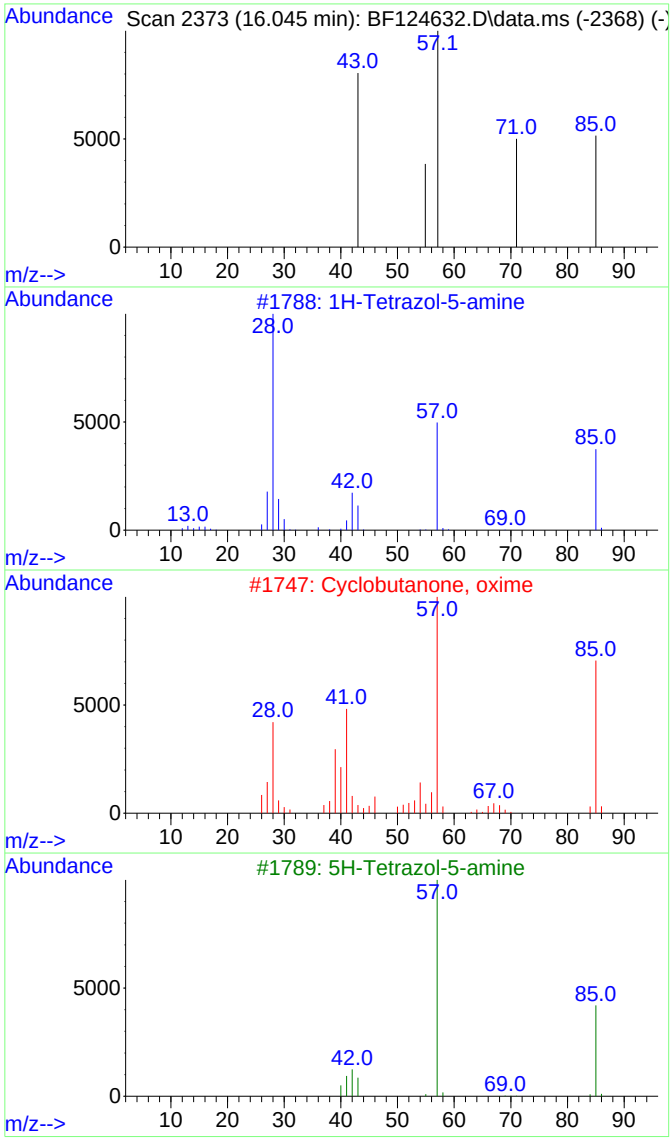
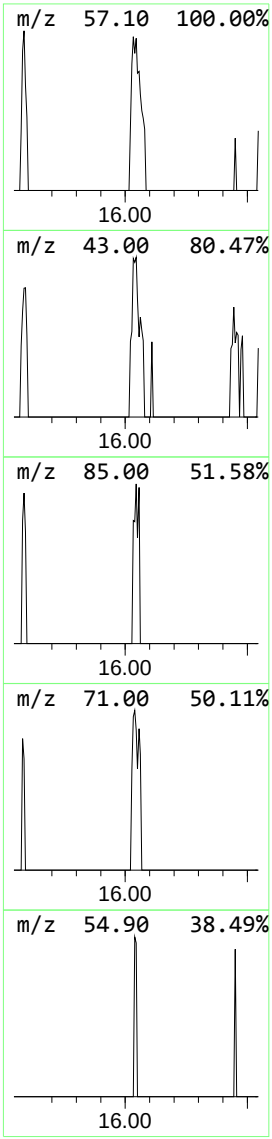
Peak Number 12 unknown16.045 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.045	4.66 ng	6094	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
2	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
3	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4	2-Propenamide	71	C3H5NO	000079-06-1	4
5	Azetidine, 1,2-dimethyl-	85	C5H11N	051764-32-0	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124632.D
Acq On : 20 Jul 2021 17:23
Operator : JU/CG
Sample : M3076-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210578-COM-1

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
unknown2.251	2.251	9.9	ng	16326	1	6.904	32875	20.0
Ethanol, 2-(2-b...	8.081	10.4	ng	23995	2	8.186	46268	20.0
Dodecanoic acid	11.951	10.4	ng	26657	4	11.427	51022	20.0
unknown12.733	12.733	5.9	ng	15103	4	11.427	51022	20.0
unknown13.586	13.586	2.9	ng	4032	5	14.068	28332	20.0
unknown13.904	13.904	3.9	ng	5525	5	14.068	28332	20.0
unknown14.245	14.245	4.8	ng	6825	5	14.068	28332	20.0
unknown14.792	14.792	3.7	ng	5179	5	14.068	28332	20.0
unknown14.845	14.845	3.4	ng	4438	6	15.557	26175	20.0
unknown15.192	15.192	2.4	ng	3109	6	15.557	26175	20.0
unknown15.380	15.380	2.8	ng	3678	6	15.557	26175	20.0
unknown16.045	16.045	4.7	ng	6094	6	15.557	26175	20.0