LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071621\
Data File : BF124601.D
Acq On : 16 Jul 2021 17:48
Operator : JU/CG
Sample : M3029-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RVR-CF01-02

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: BF124601.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	25	29	33	rBB	9940	11746	7.54%	1.063%
2	5.163	520	523	526	rBB	2280	2505	1.61%	0.227%
3	5.539	582	587	590	rBB	147997	148995	95.67%	13.488%
4	6.539	752	757	760	rBB	145804	155735	100.00%	14.099%
5	6.922	819	822	825	rBB	49744	35669	22.90%	3.229%
6	7.486	913	918	920	rBB	105047	103074	66.19%	9.331%
7	8.104	1019	1023	1027	rBB	32509	26454	16.99%	2.395%
8	8.204	1036	1040	1043	rBB	64582	52113	33.46%	4.718%
9	9.280	1219	1223	1226	rBV	182153	151954	97.57%	13.756%
10	9.963	1336	1339	1342	rBV	79324	62039	39.84%	5.616%
11	10.751	1469	1473	1476	rBB	130552	108511	69.68%	9.823%
12	11.451	1589	1592	1595	rBV	78167	61533	39.51%	5.571%
13	11.474	1595	1596	1598	rVB	4067	2097	1.35%	0.190%
14	11.968	1677	1680	1682	rBB	9097	6250	4.01%	0.566%
15	12.663	1796	1798	1800	rBB	7530	5164	3.32%	0.467%
16	12.757	1811	1814	1816	rBB	6912	5384	3.46%	0.487%
17	12.892	1835	1837	1840	rBB	5901	3920	2.52%	0.355%
18	13.039	1858	1862	1865	rBB	111888	84170	54.05%	7.620%
19	13.104	1871	1873	1876	rBB	4460	2969	1.91%	0.269%
20	13.939	2011	2015	2021	rBB	5312	7072	4.54%	0.640%
21	14.092	2038	2041	2044	rVB	34693	27321	17.54%	2.473%
22	14.557	2118	2120	2124	rBV	3845	3576	2.30%	0.324%
23	15.227	2231	2234	2237	rBB	8204	8883	5.70%	0.804%
24	15.592	2291	2296	2299	rBV	22269	27486	17.65%	2.488%

Sum of corrected areas: 1104620

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Misc :
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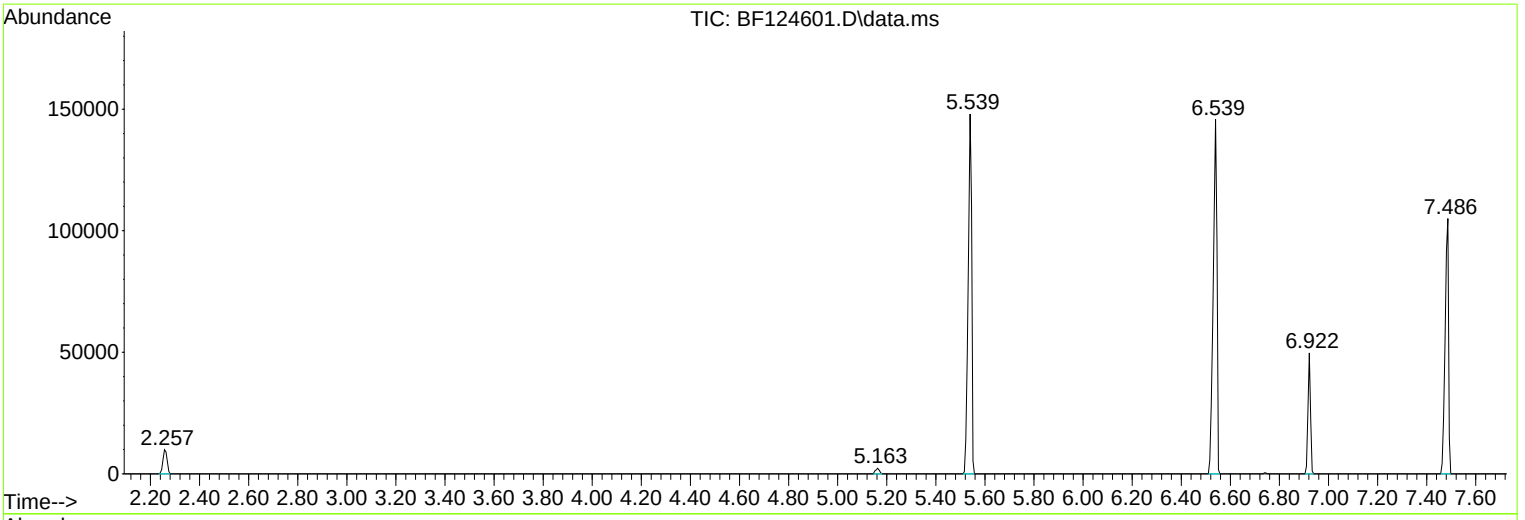
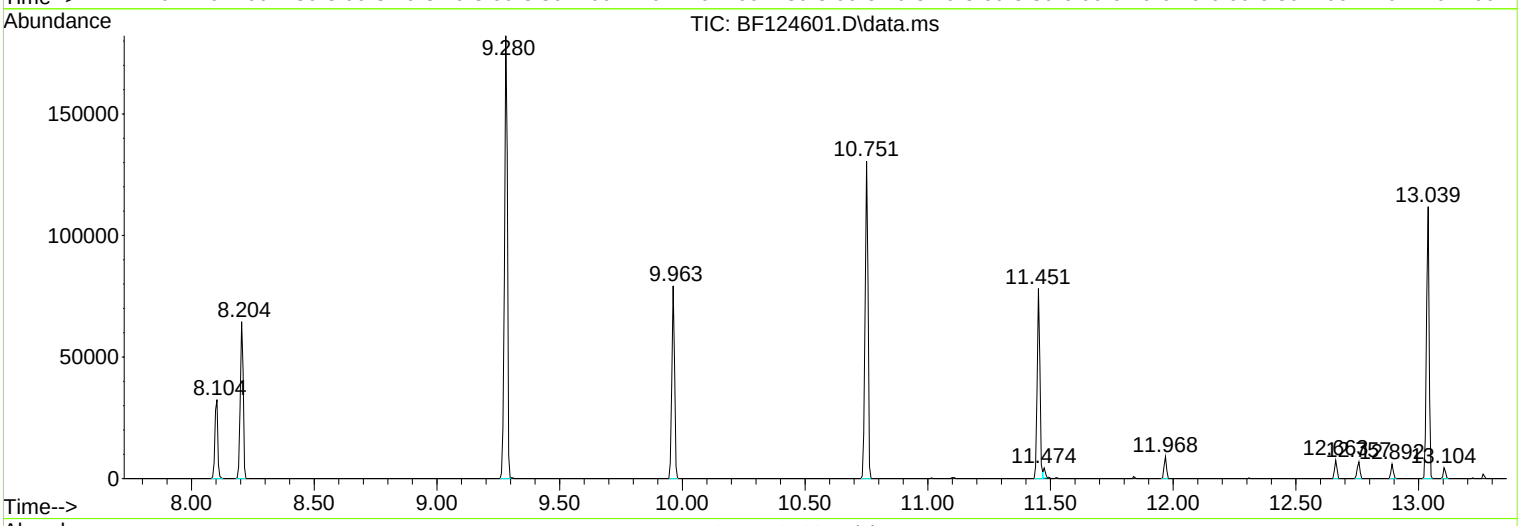
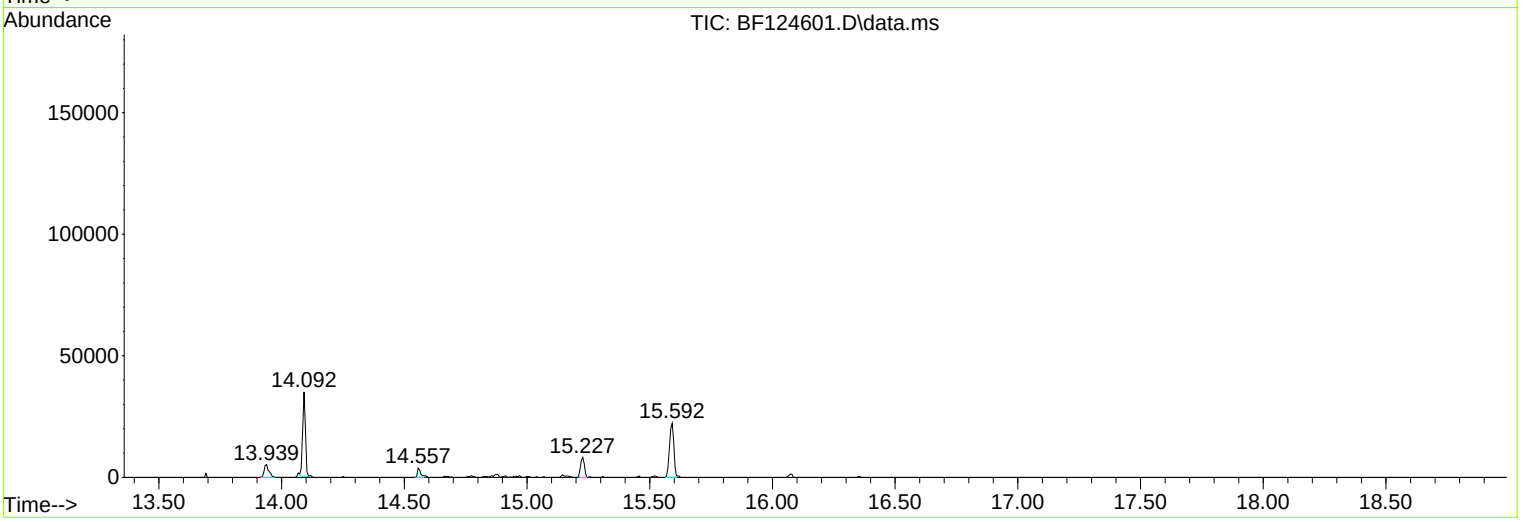
Instrument :
BNA_F
ClientSampleId :
RVR-CF01-02

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

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Data File : BF124601.D
Acq On : 16 Jul 2021 17:48
Operator : JU/CG
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Instrument :
BNA_F
ClientSampleId :
RVR-CF01-02

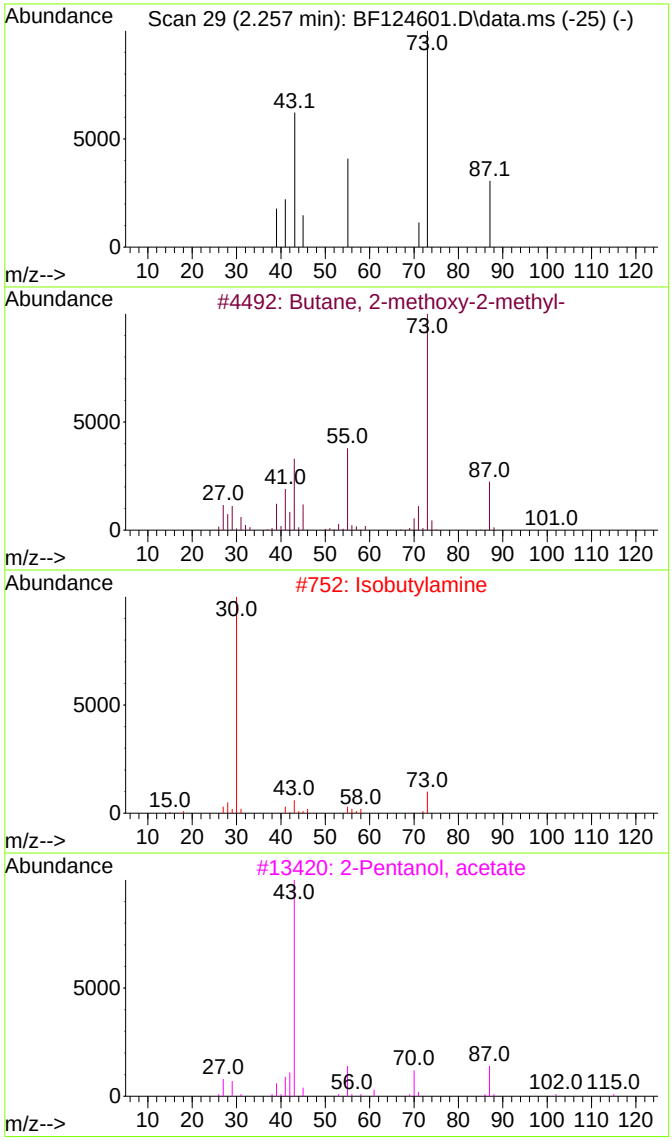
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

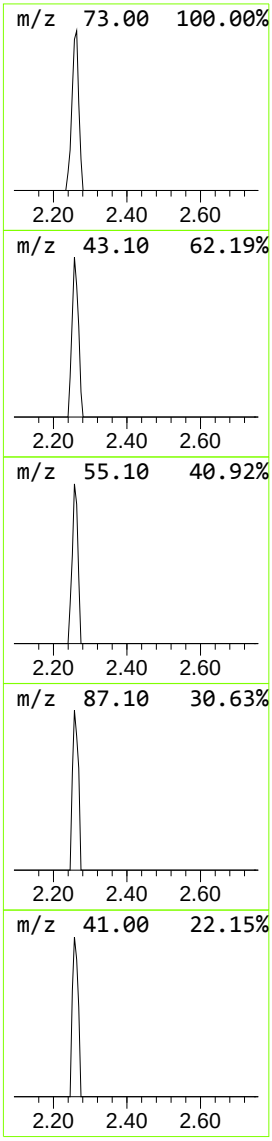
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	6.59 ng	11746	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	Isobutylamine	73	C4H11N	000078-81-9	5
3	2-Pentanol, acetate	130	C7H14O2	000626-38-0	4
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071621\
Data File : BF124601.D
Acq On : 16 Jul 2021 17:48
Operator : JU/CG
Sample : M3029-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RVR-CF01-02

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

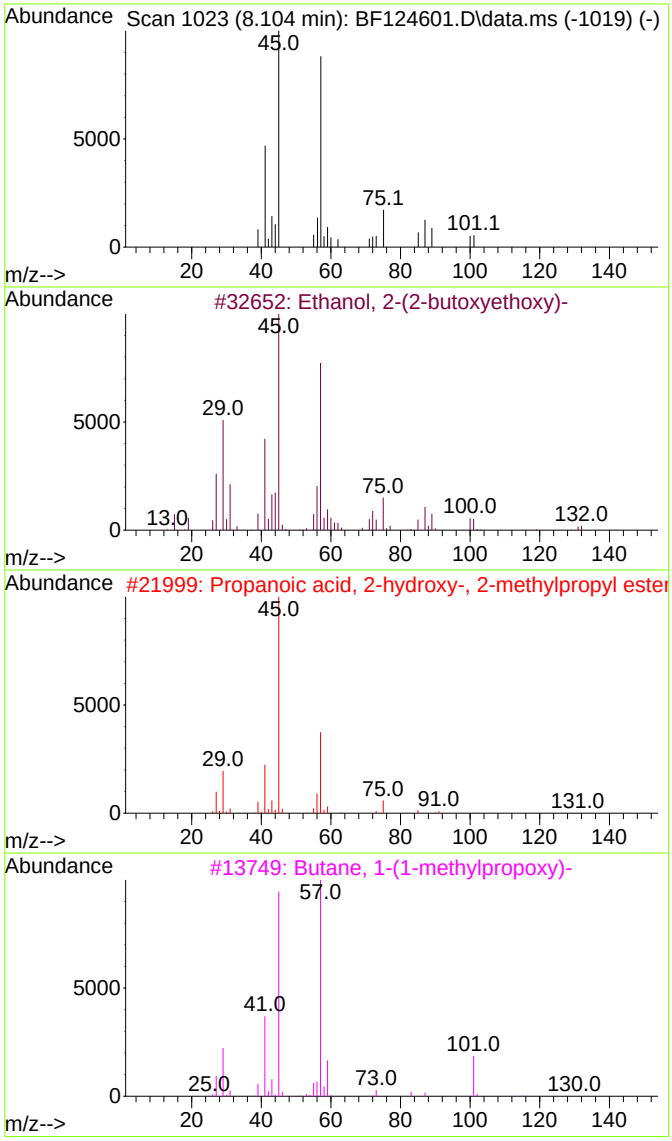
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

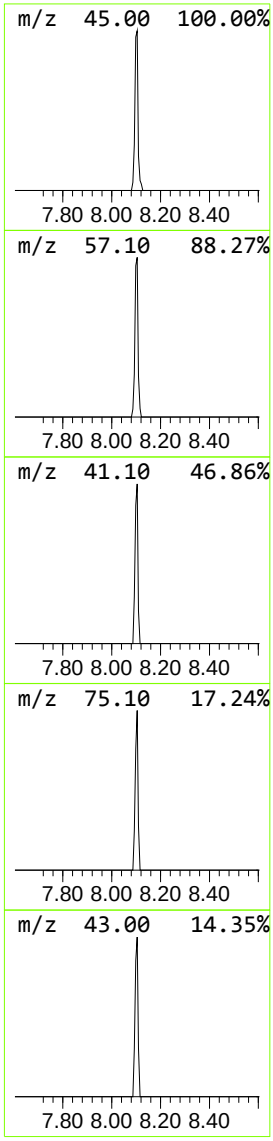
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	10.15 ng	26454	Naphthalene-d8	8.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	45
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	42
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	37
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	37





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Acq On : 16 Jul 2021 17:48
Operator : JU/CG
Sample : M3029-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVR-CF01-02

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

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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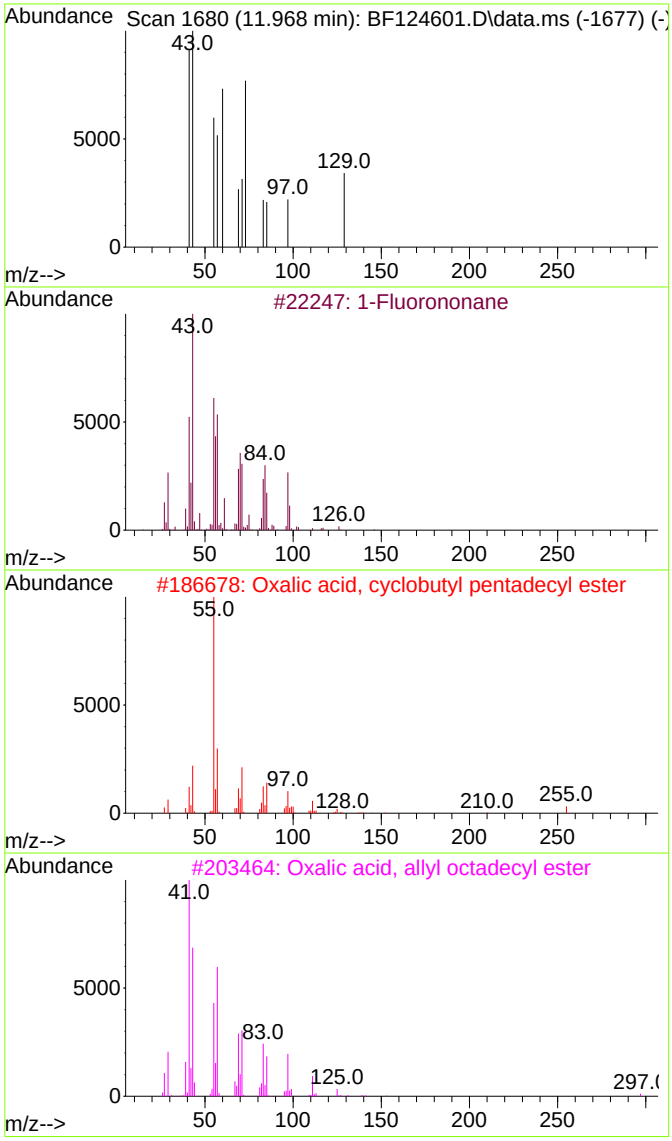
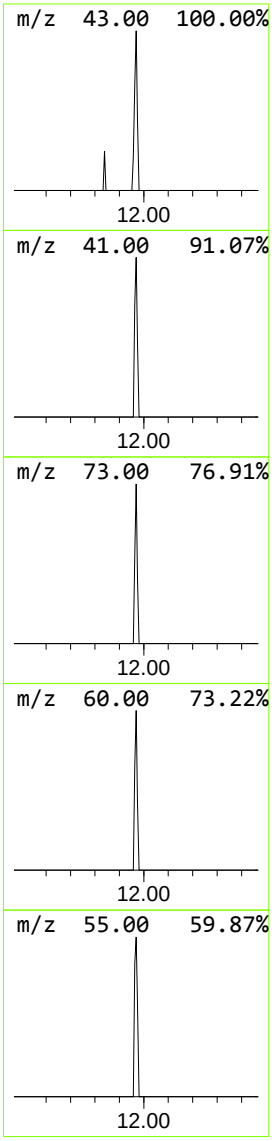
Peak Number 3 unknown11.969 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	2.03 ng	6250	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Fluorononane	146	C9H19F	000463-18-3	27
2	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	16
3	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	16
4	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	12
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	12





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Data File : BF124601.D
Acq On : 16 Jul 2021 17:48
Operator : JU/CG
Sample : M3029-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVR-CF01-02

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

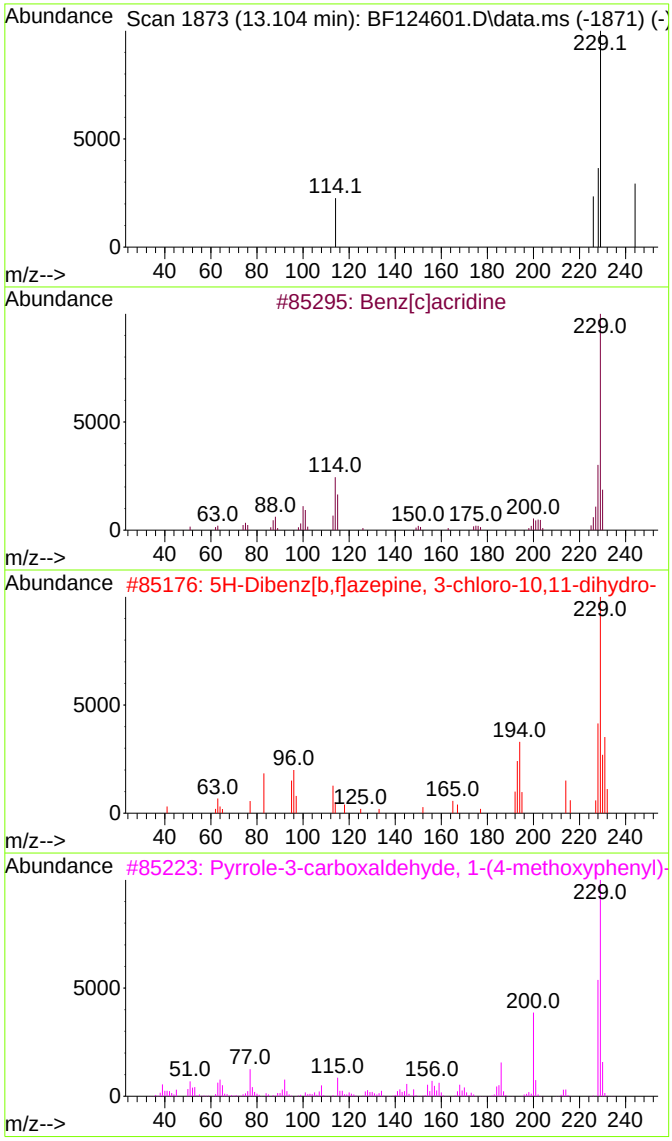
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

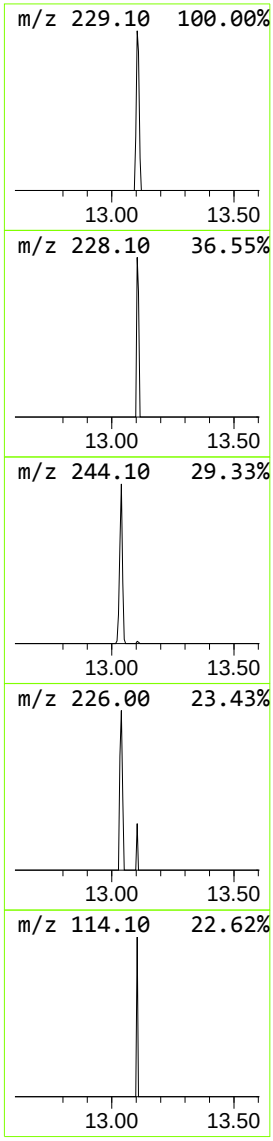
****

Peak Number 4 unknown13.104 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.104	2.17 ng	2969	Chrysene-d12	14.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[c]acridine	229	C17H11N	000225-51-4	9
2	5H-Dibenz[b,f]azepine, 3-chloro-...	229	C14H12ClN	032943-25-2	5
3	Pyrrole-3-carboxaldehyde, 1-(4-m...	229	C14H15NO2	347331-30-0	5
4	Naphtho(2,3-h)quinoline	229	C17H11N	000084-56-0	5
5	Benzo(a)acridine	229	C17H11N	000225-11-6	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071621\
Data File : BF124601.D
Acq On : 16 Jul 2021 17:48
Operator : JU/CG
Sample : M3029-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVR-CF01-02

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

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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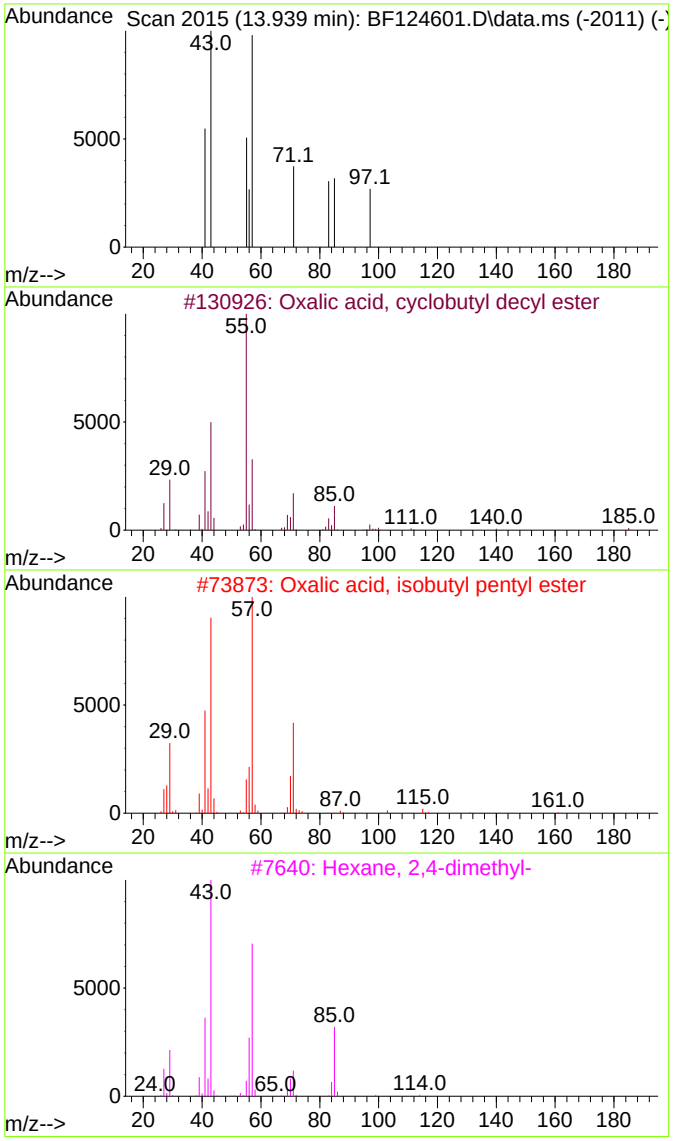
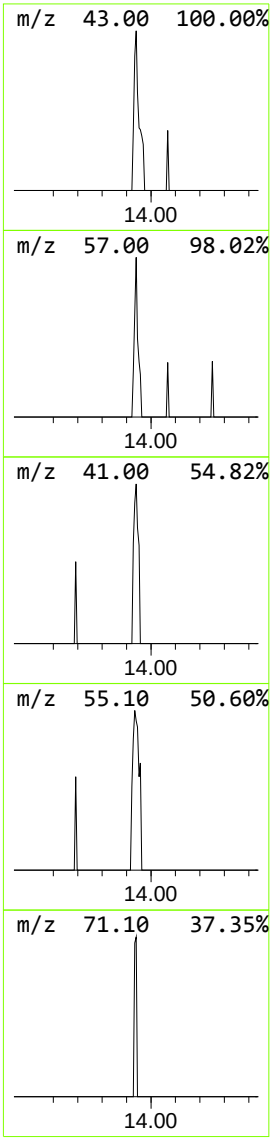
Peak Number 5 unknown13.939 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	5.18 ng	7072	Chrysene-d12	14.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclobutyl decyl ester	284	C16H28O4	1000309-70-1	39
2	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	23
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	9
4	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	9
5	Oxalic acid, cyclobutyl nonyl ester	270	C15H26O4	1000309-70-0	9





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Operator : JU/CG
Sample : M3029-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVR-CF01-02

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

TIC Library : C:\DATABASE\NIST11.L
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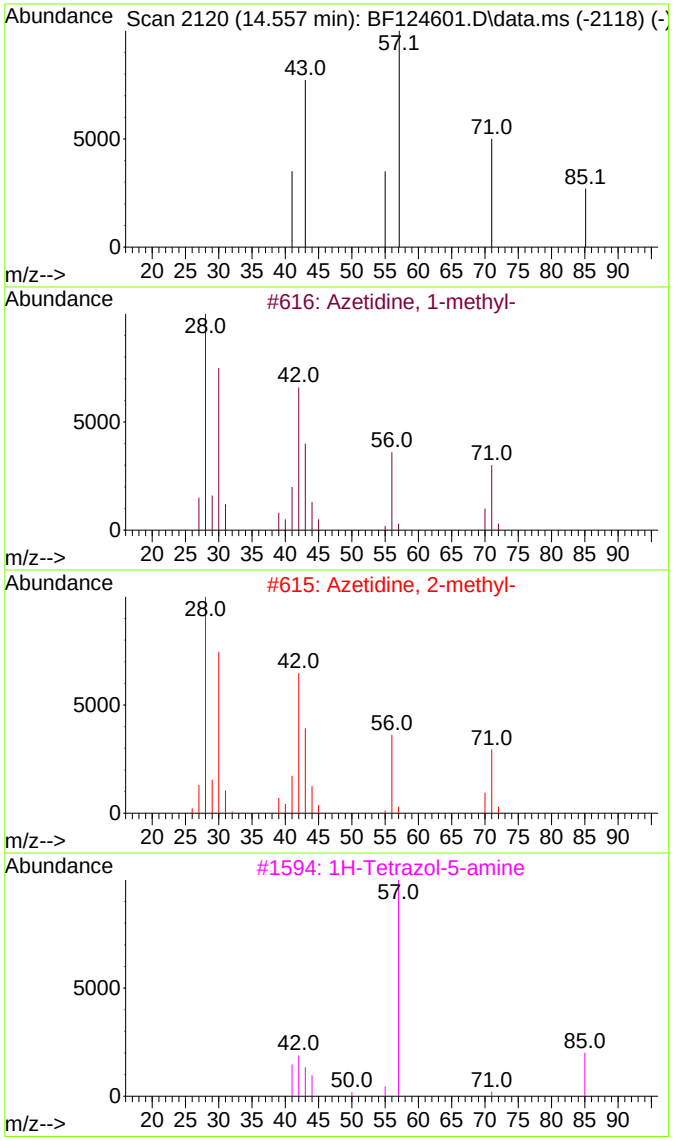
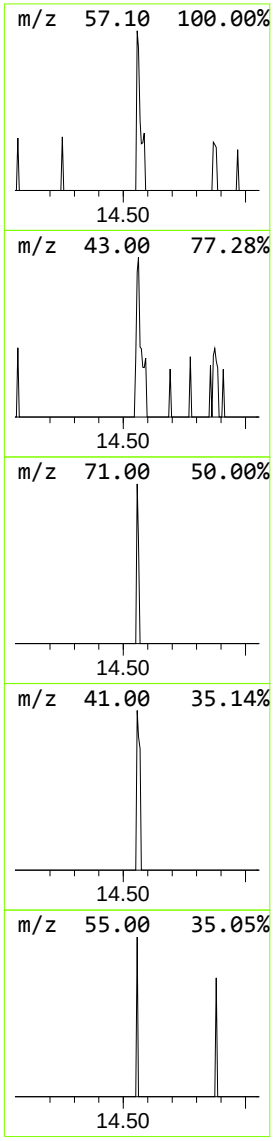
****

Peak Number 6 unknown14.557 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	2.62 ng	3576	Chrysene-d12	14.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
2	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
3	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
4	Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	4
5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	4





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Sample : M3029-04
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Instrument :
BNA_F
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

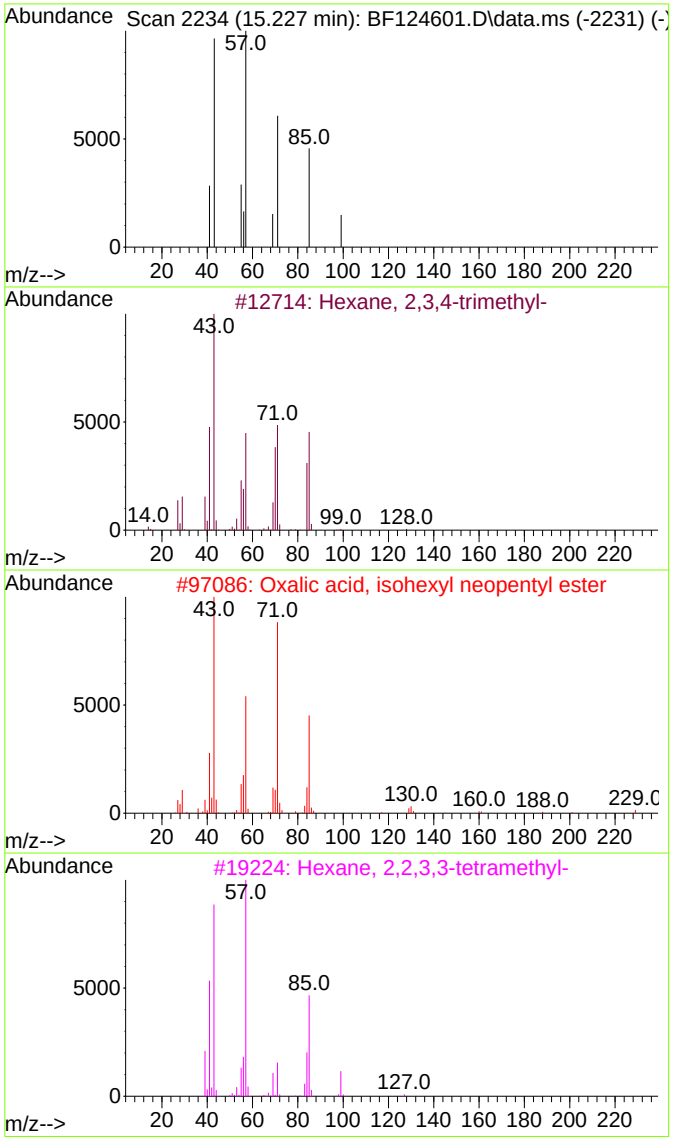
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

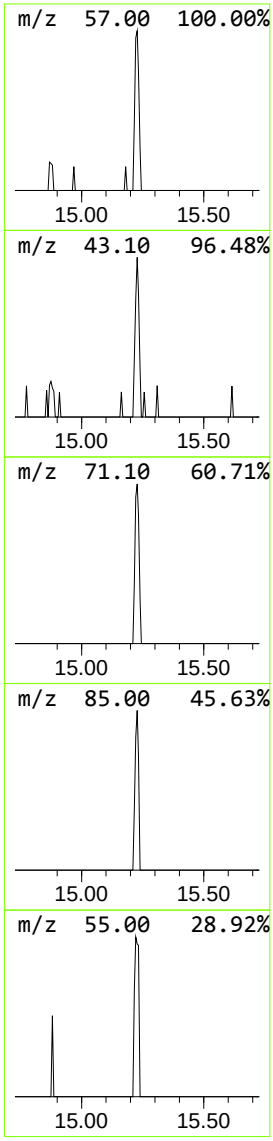
****

Peak Number 7 Hexane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	6.46 ng	8883	Perylene-d12	15.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	72
2	Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	39
3	Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	38
4	Sulfurous acid, hexyl heptyl ester	264	C13H28O3S	1000309-12-9	36
5	Pentane, 3-ethyl-2,3-dimethyl-	128	C9H20	016747-33-4	36





Tentatively Identified Compound (LSC) summary

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Data File : BF124601.D
Acq On : 16 Jul 2021 17:48
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.257	6.6	ng	11746	1	6.922	35669	20.0
Ethanol, 2-(2-b...	8.104	10.2	ng	26454	2	8.204	52113	20.0
unknown11.969	11.969	2.0	ng	6250	4	11.451	61533	20.0
unknown13.104	13.104	2.2	ng	2969	5	14.092	27321	20.0
unknown13.939	13.939	5.2	ng	7072	5	14.092	27321	20.0
unknown14.557	14.557	2.6	ng	3576	5	14.092	27321	20.0
Hexane, 2,3,4-t...	15.227	6.5	ng	8883	6	15.592	27486	20.0