LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124971.D
Acq On : 7 Aug 2021 13:03
Operator : JU/CG
Sample : M3281-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TWP02

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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124971.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.357	382	386	390	rBB	17464	18062	7.63%	1.240%
2	5.440	567	570	575	rBB	57752	47469	20.05%	3.258%
3	6.451	740	742	746	rBB	40698	31380	13.26%	2.154%
4	6.828	803	806	809	rBB	40613	28945	12.23%	1.987%
5	6.987	829	833	835	rBV	168918	146486	61.88%	10.054%
6	7.010	835	837	839	rVB	45248	32313	13.65%	2.218%
7	7.392	897	902	905	rBB	131577	116861	49.36%	8.021%
8	7.763	963	965	967	rBB	4106	2750	1.16%	0.189%
9	8.010	1005	1007	1014	rBB	27433	23058	9.74%	1.583%
10	8.110	1021	1024	1026	rBV	49037	49178	20.77%	3.375%
11	8.134	1026	1028	1031	rVB	205063	156572	66.14%	10.746%
12	8.181	1031	1036	1039	rBB	7070	5585	2.36%	0.383%
13	8.922	1159	1162	1164	rBB	6749	5273	2.23%	0.362%
14	9.186	1203	1207	1210	rVB	279830	225376	95.20%	15.469%
15	9.863	1319	1322	1325	rBB	66288	46994	19.85%	3.225%
16	9.898	1325	1328	1330	rBB	30636	25310	10.69%	1.737%
17	10.069	1354	1357	1359	rBB	9070	7230	3.05%	0.496%
18	10.410	1412	1415	1417	rBB	14116	9740	4.11%	0.669%
19	10.651	1453	1456	1459	rBV	113198	86660	36.61%	5.948%
20	11.351	1571	1575	1577	rBV	59948	47314	19.99%	3.247%
21	11.375	1577	1579	1581	rVB	4808	3187	1.35%	0.219%
22	11.580	1612	1614	1616	rBB	4283	2826	1.19%	0.194%
23	11.880	1661	1665	1671	rBB	20835	21476	9.07%	1.474%
24	12.663	1794	1798	1804	rBV	12893	14403	6.08%	0.989%
25	12.933	1840	1844	1847	rBV	256880	236730	100.00%	16.248%
26	13.851	1995	2000	2003	rBB2	2528	3249	1.37%	0.223%
27	13.986	2020	2023	2026	rBB	39733	30313	12.80%	2.081%
28	14.657	2132	2137	2142	rBB	1736	3528	1.49%	0.242%
29	15.445	2267	2271	2275	rBB	23929	28706	12.13%	1.970%

Sum of corrected areas: 1456974

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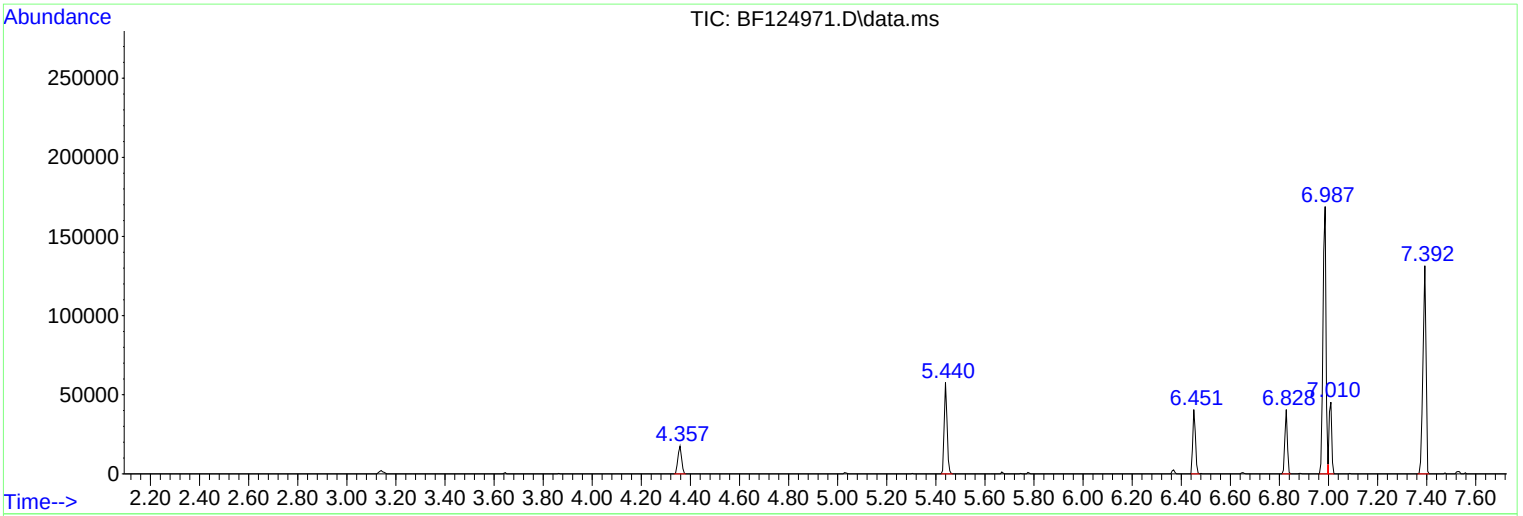
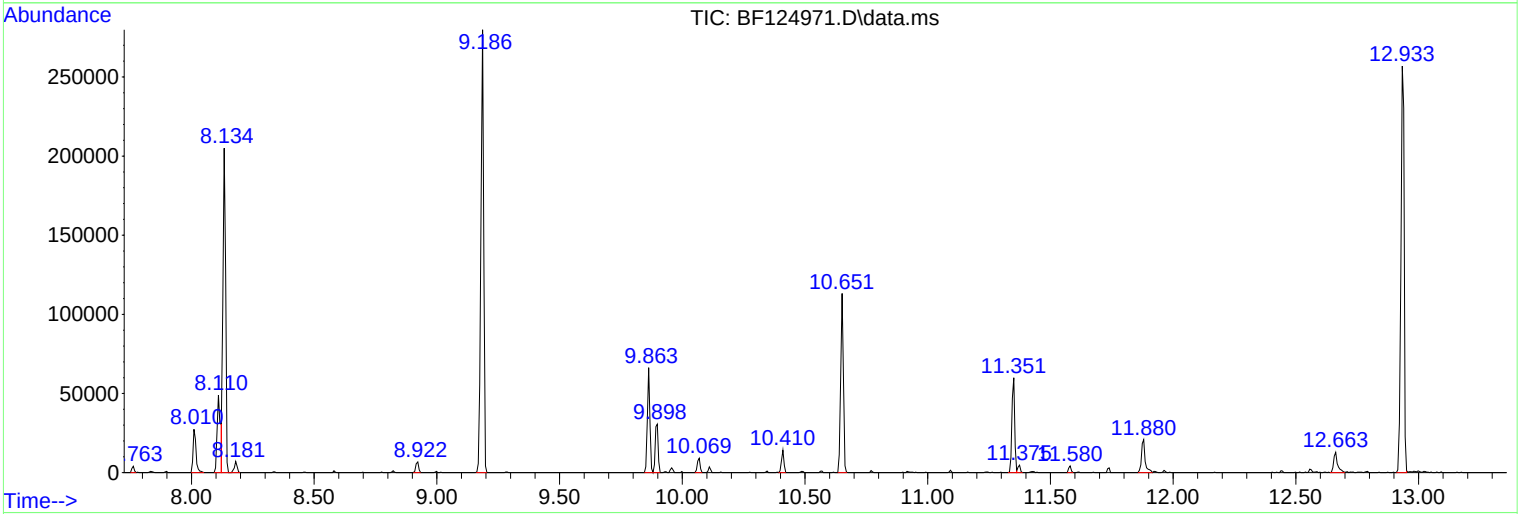
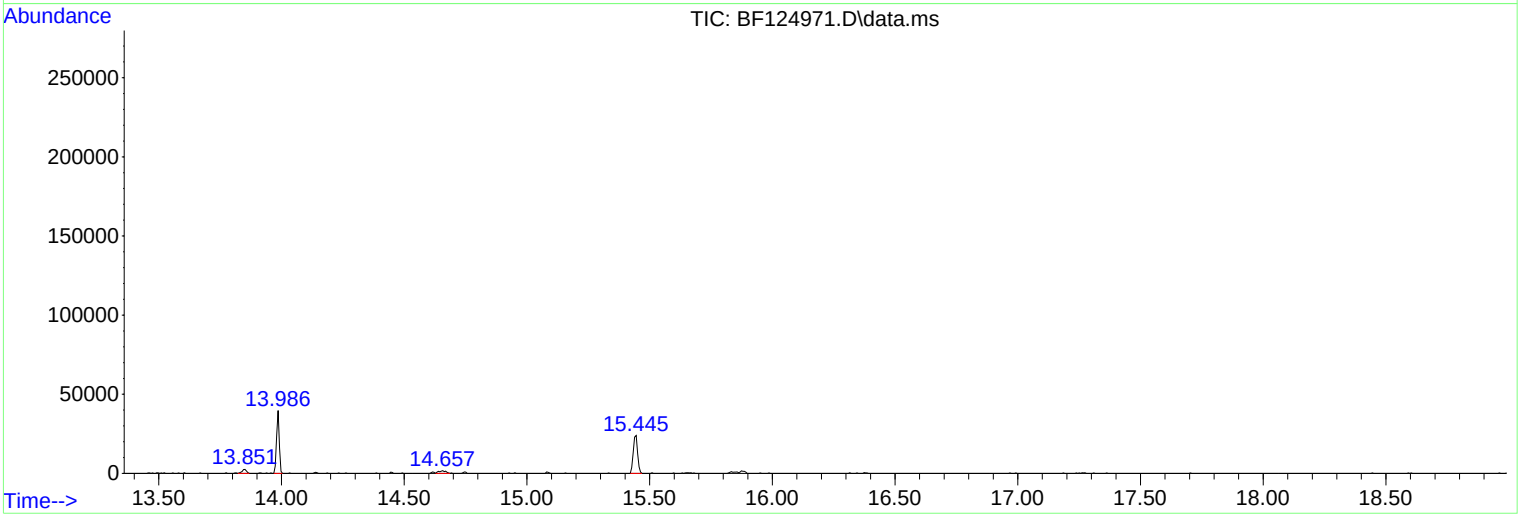
Instrument :
BNA_F
ClientSampleId :
TWP02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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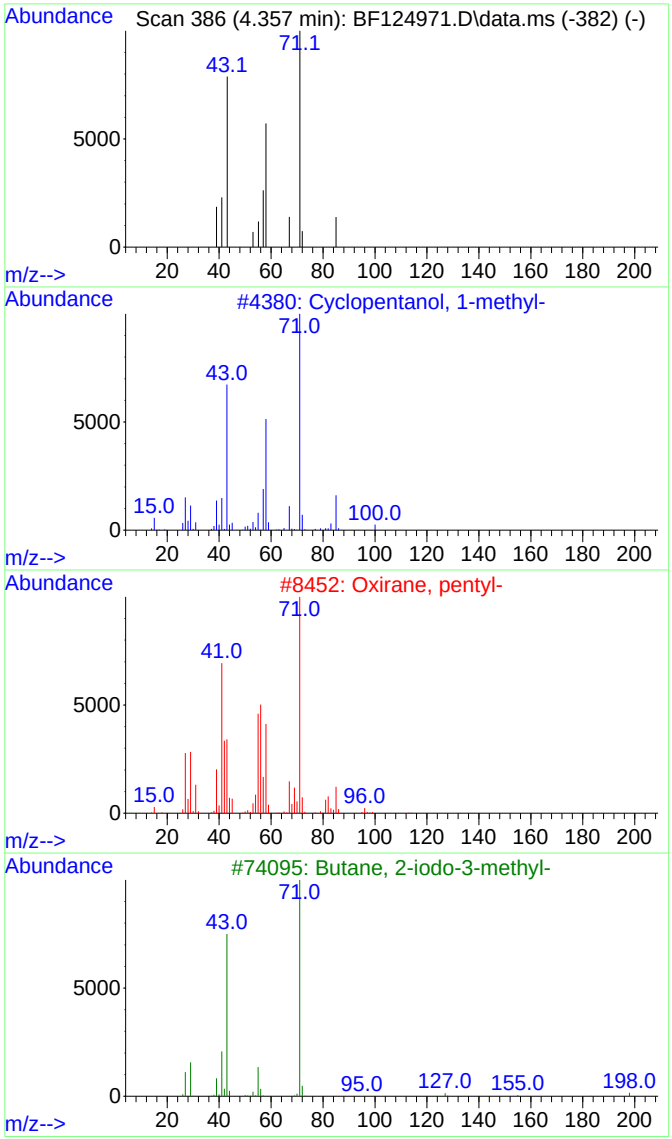
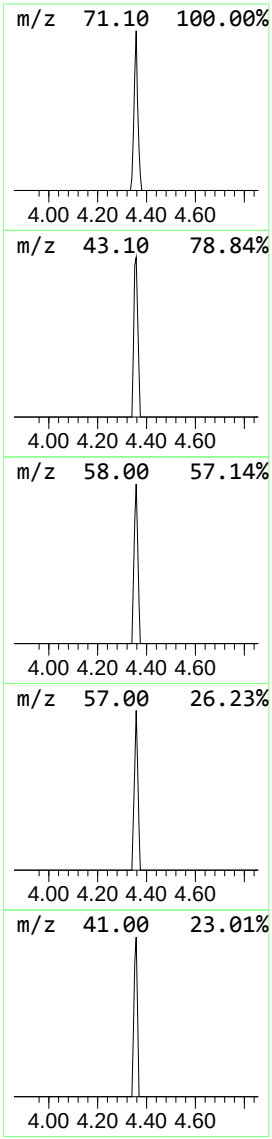
****

Peak Number 1 Cyclopentanol, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.357	12.48 ng	18062	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanol, 1-methyl-	100	C6H12O	001462-03-9	83
2	Oxirane, pentyl-	114	C7H14O	005063-65-0	43
3	Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	9
4	1-Penten-3-ol, 3-methyl-	100	C6H12O	000918-85-4	9
5	1,7-Octadiene, 3-methoxy-	140	C9H16O	020202-62-4	9





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Data File : BF124971.D
Acq On : 7 Aug 2021 13:03
Operator : JU/CG
Sample : M3281-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TWP02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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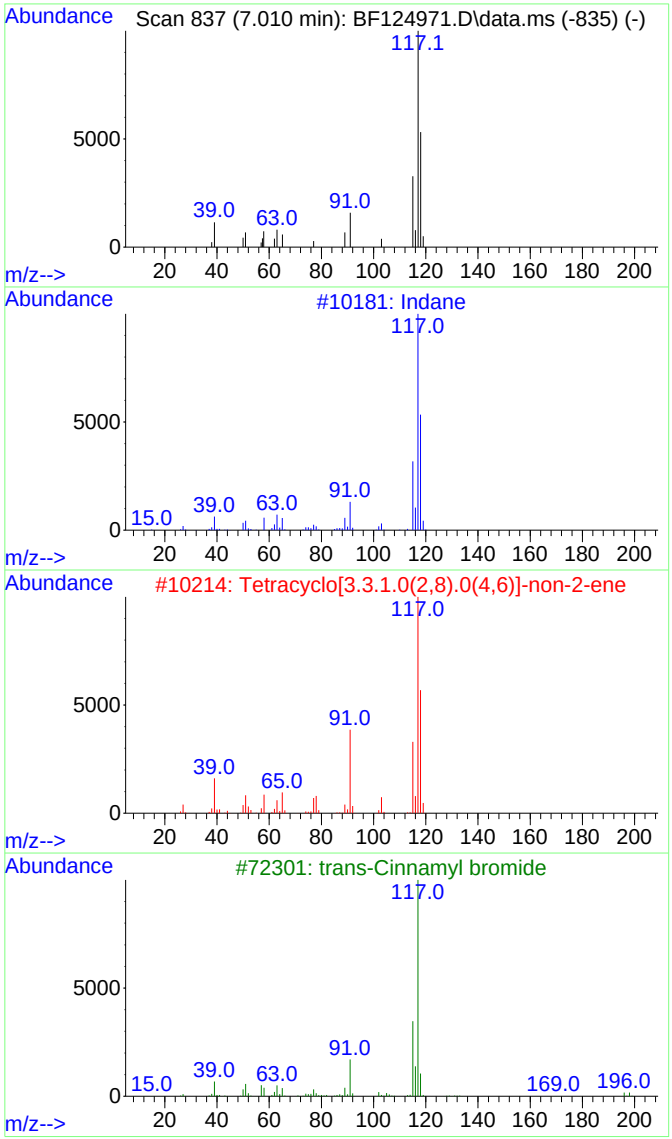
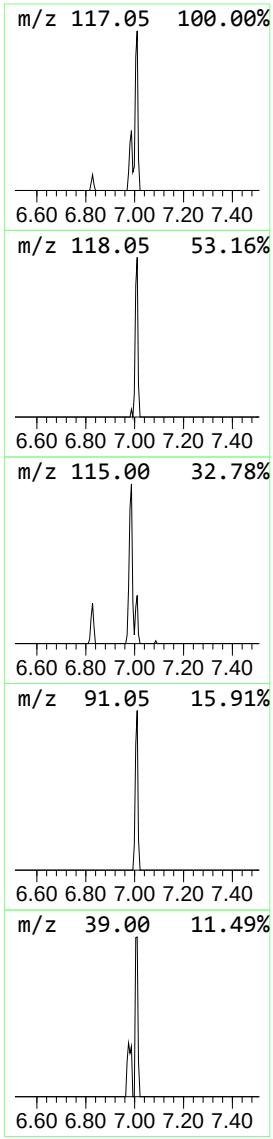
Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.010	22.33 ng	32313	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
3	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
4	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	53
5	Deltacyclene	118	C9H10	007785-10-6	53





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Data File : BF124971.D
Acq On : 7 Aug 2021 13:03
Operator : JU/CG
Sample : M3281-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TWP02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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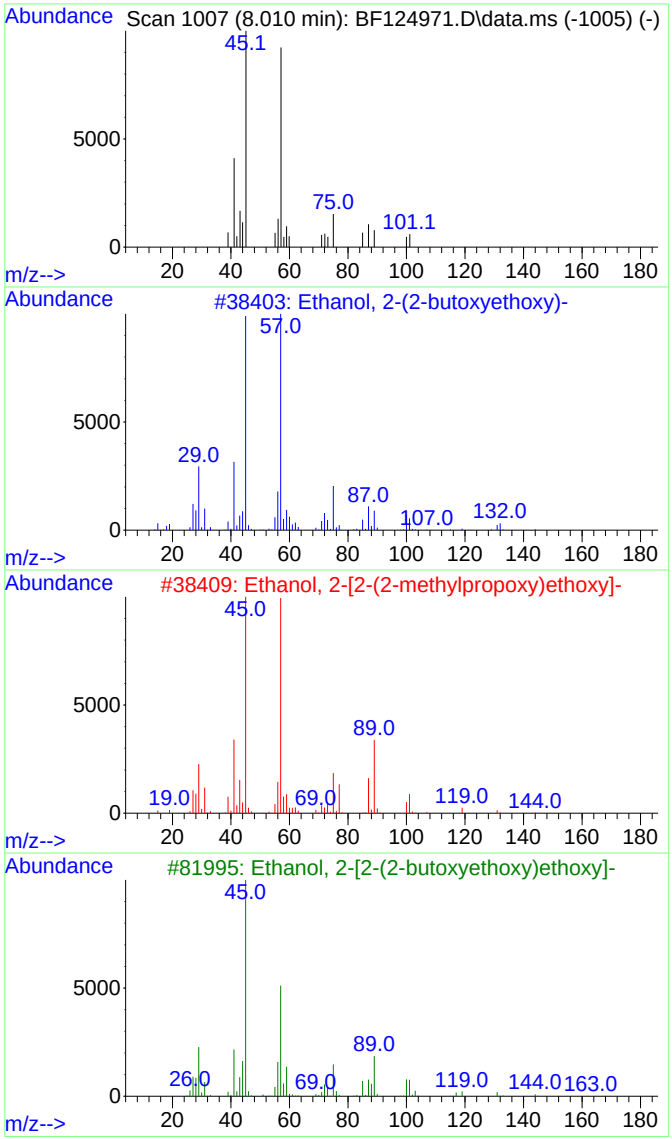
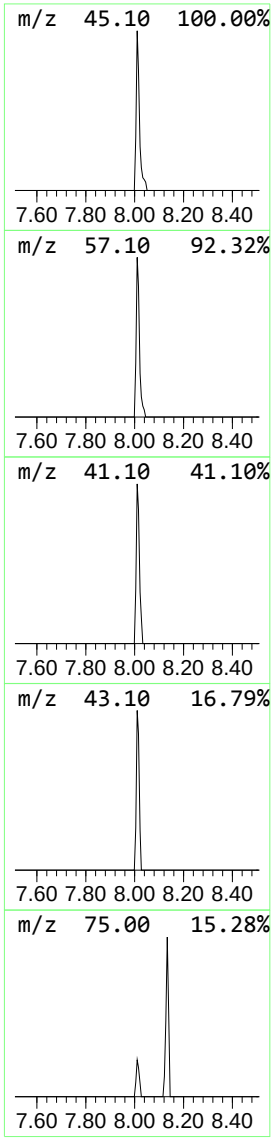
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.010	9.38 ng	23058	Naphthalene-d8	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	42





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Acq On : 7 Aug 2021 13:03
Operator : JU/CG
Sample : M3281-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TWP02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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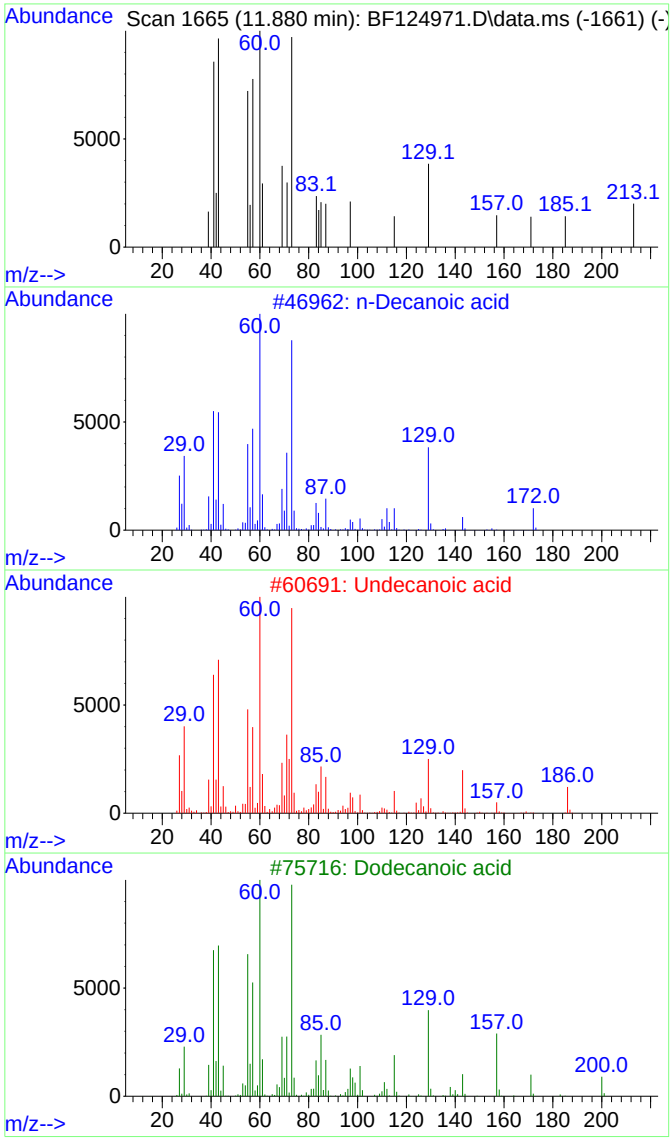
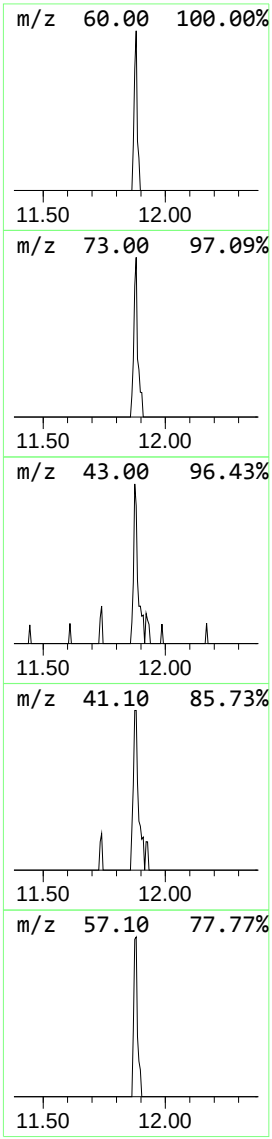
Peak Number 5 n-Decanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	9.08 ng	21476	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	50
2	Undecanoic acid	186	C11H22O2	000112-37-8	50
3	Dodecanoic acid	200	C12H24O2	000143-07-7	50
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	45
5	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	43





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Sample : M3281-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TWP02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
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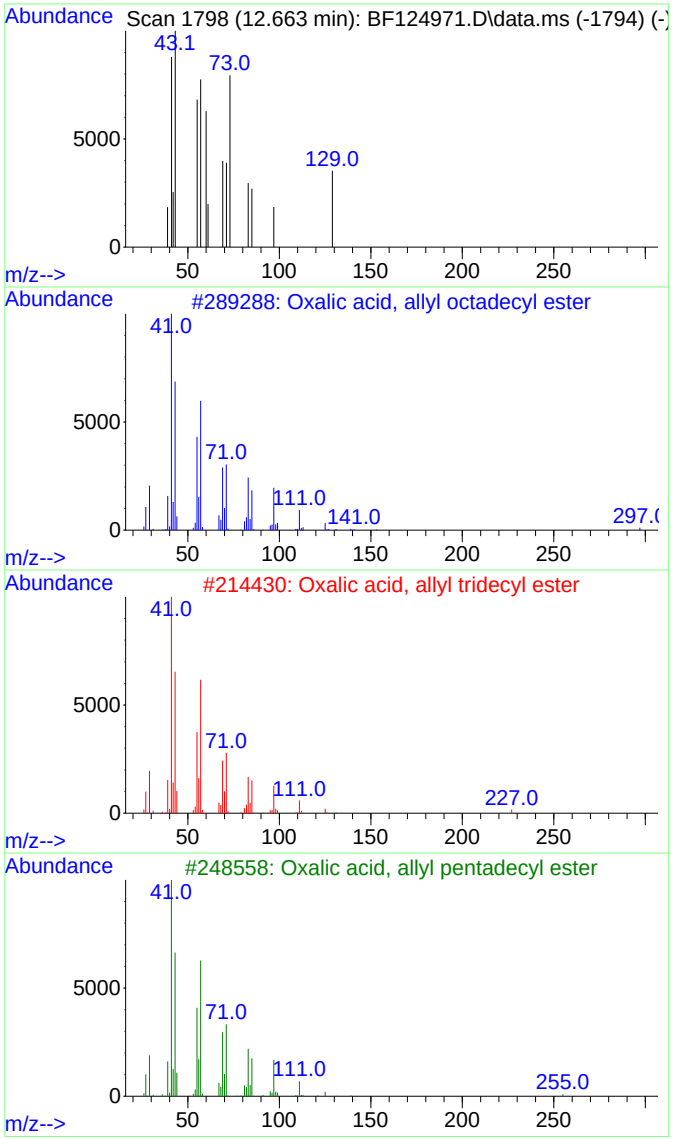
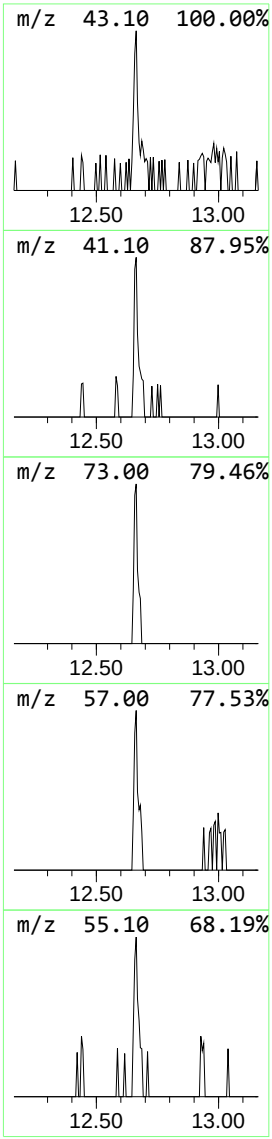
Peak Number 6 unknown12.663 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	6.09 ng	14403	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	38
2	Oxalic acid, allyl tridecyl ester	312	C18H32O4	1000309-24-1	38
3	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	38
4	Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	38
5	1-Fluorononane	146	C9H19F	000463-18-3	38





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Instrument : BNA_F
ClientSampleId : TWP02

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TIC Library : C:\Database\NIST20.L
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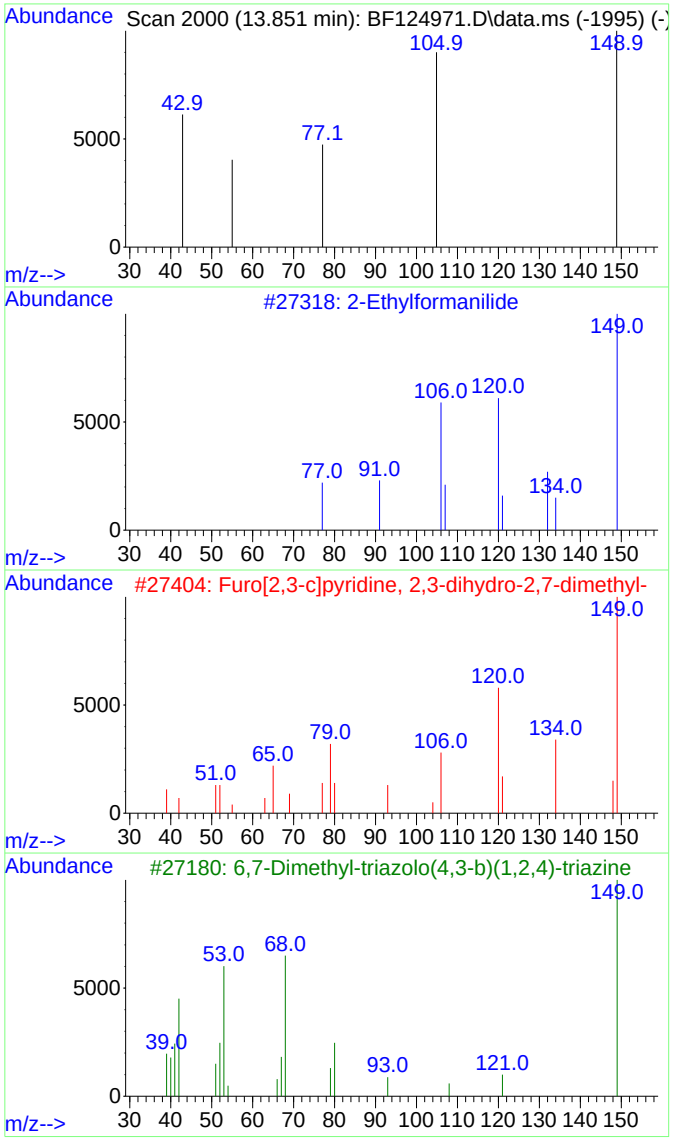
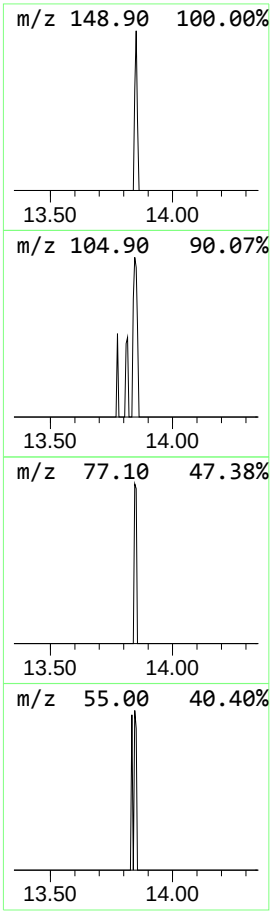
Peak Number 7 unknown13.851 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	2.14 ng	3249	Chrysene-d12	13.986

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylformanilide	149	C9H11NO	002860-30-2	2
2	Furo[2,3-c]pyridine, 2,3-dihydro...	149	C9H11NO	069022-82-8	2
3	6,7-Dimethyl-triazolo(4,3-b)(1,2...	149	C6H7N5	061139-73-9	2
4	Mercaptamine	77	C2H7NS	000060-23-1	2
5	3(2H)-Thiophenone, dihydro-, oxi...	149	C4H7NO3S	1010327-57-0	2





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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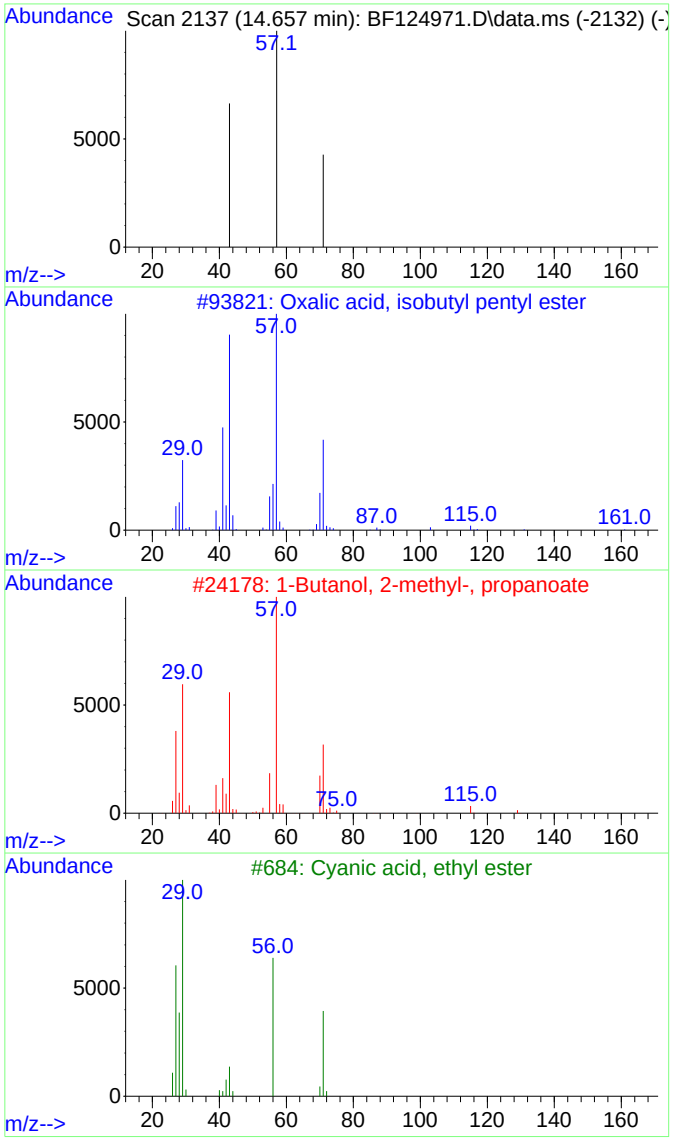
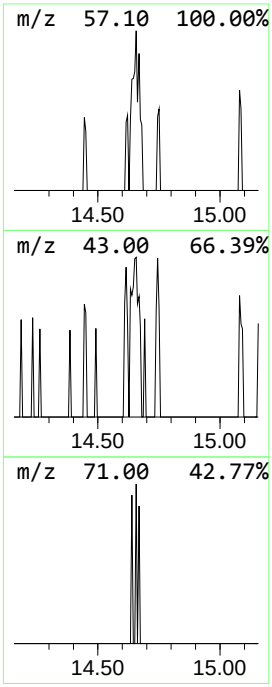
Peak Number 8 unknown14.657 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.657	2.33 ng	3528	Chrysene-d12	13.986

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	2
2	1-Butanol, 2-methyl-, propanoate	144	C8H16O2	002438-20-2	2
3	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	2
4	Azetidine	57	C3H7N	000503-29-7	1
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	1





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentanol, ...	4.357	12.5	ng	18062	1	6.828	28945	20.0
Indane	7.010	22.3	ng	32313	1	6.828	28945	20.0
Ethanol, 2-(2-b...	8.010	9.4	ng	23058	2	8.110	49178	20.0
n-Decanoic acid	11.880	9.1	ng	21476	4	11.351	47314	20.0
unknown12.663	12.663	6.1	ng	14403	4	11.351	47314	20.0
unknown13.851	13.851	2.1	ng	3249	5	13.986	30313	20.0
unknown14.657	14.657	2.3	ng	3528	5	13.986	30313	20.0