LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081021\
Data File : BF125049.D
Acq On : 11 Aug 2021 1:30
Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

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: BF125049.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.387	389	391	394	rBB	2874	2048	1.14%	0.181%
2	5.028	494	500	507	rBB	95675	125952	69.97%	11.129%
3	5.434	565	569	573	rBV	158888	161990	89.99%	14.313%
4	5.828	633	636	639	rBB	21746	18504	10.28%	1.635%
5	6.451	737	742	745	rBV	190562	180016	100.00%	15.906%
6	6.810	800	803	806	rBB	49964	35915	19.95%	3.173%
7	7.381	895	900	903	rBV	133402	120974	67.20%	10.689%
8	7.998	1002	1005	1008	rBV	54975	41289	22.94%	3.648%
9	8.092	1018	1021	1024	rBV	59331	45741	25.41%	4.042%
10	9.169	1200	1204	1207	rBV	166356	127957	71.08%	11.306%
11	9.845	1316	1319	1322	rBB	38523	28383	15.77%	2.508%
12	10.633	1450	1453	1456	rBB	72334	59306	32.94%	5.240%
13	11.333	1569	1572	1574	rBV	28431	21861	12.14%	1.932%
14	11.857	1658	1661	1663	rBB	5430	4159	2.31%	0.367%
15	12.545	1775	1778	1780	rBB	3843	3004	1.67%	0.265%
16	12.768	1814	1816	1819	rBB	4258	3442	1.91%	0.304%
17	12.915	1837	1841	1844	rBB	126985	95895	53.27%	8.473%
18	13.810	1990	1993	1997	rBB	4242	4764	2.65%	0.421%
19	13.968	2016	2020	2023	rBV	28129	22665	12.59%	2.003%
20	14.998	2193	2195	2201	rBB	2615	3803	2.11%	0.336%
21	15.057	2202	2205	2207	rBV2	1739	1954	1.09%	0.173%
22	15.298	2243	2246	2251	rVB2	1690	2089	1.16%	0.185%
23	15.362	2254	2257	2261	rBB	1875	2465	1.37%	0.218%
24	15.421	2262	2267	2271	rBB2	14388	17580	9.77%	1.553%

Sum of corrected areas: 1131756

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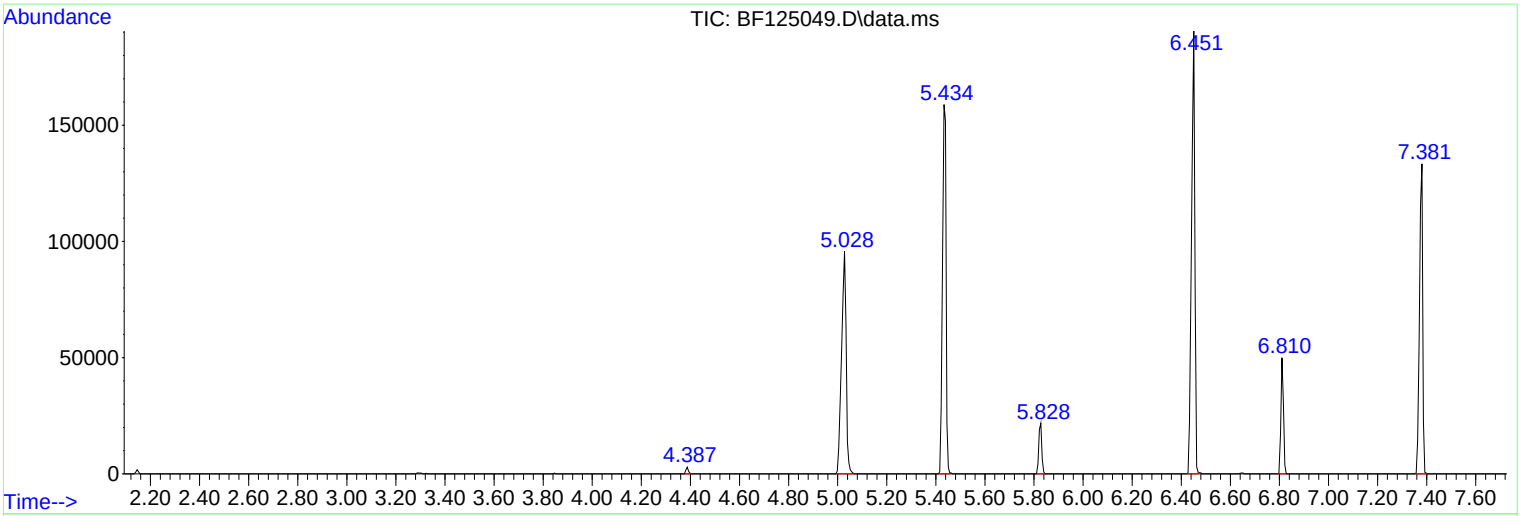
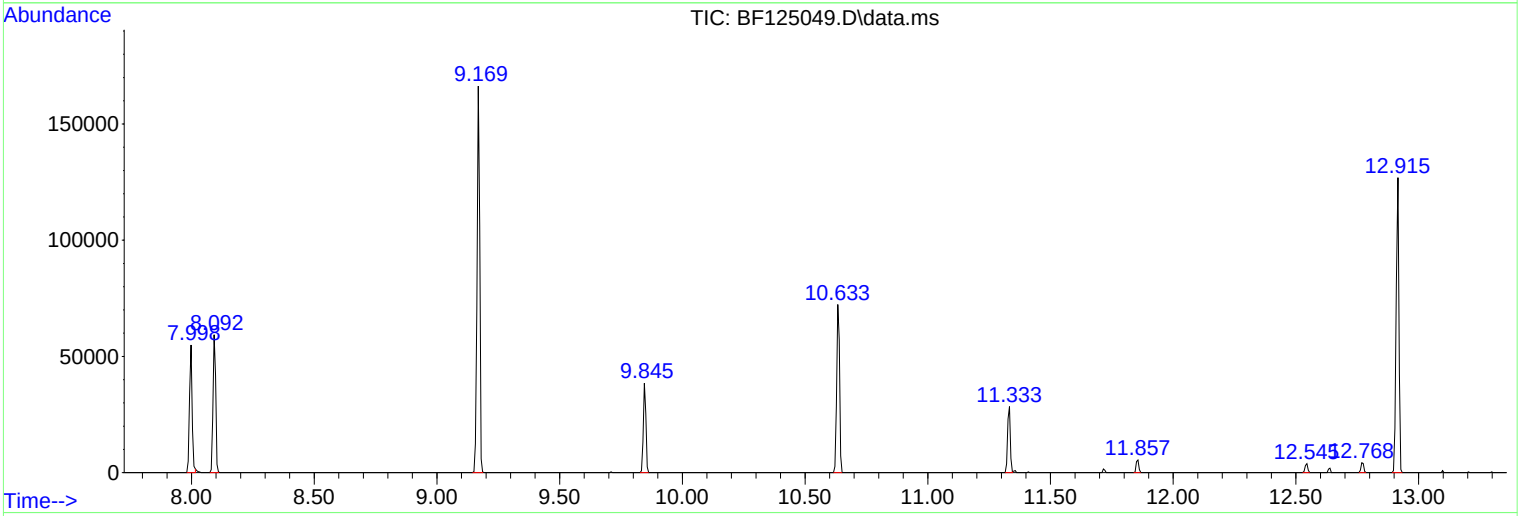
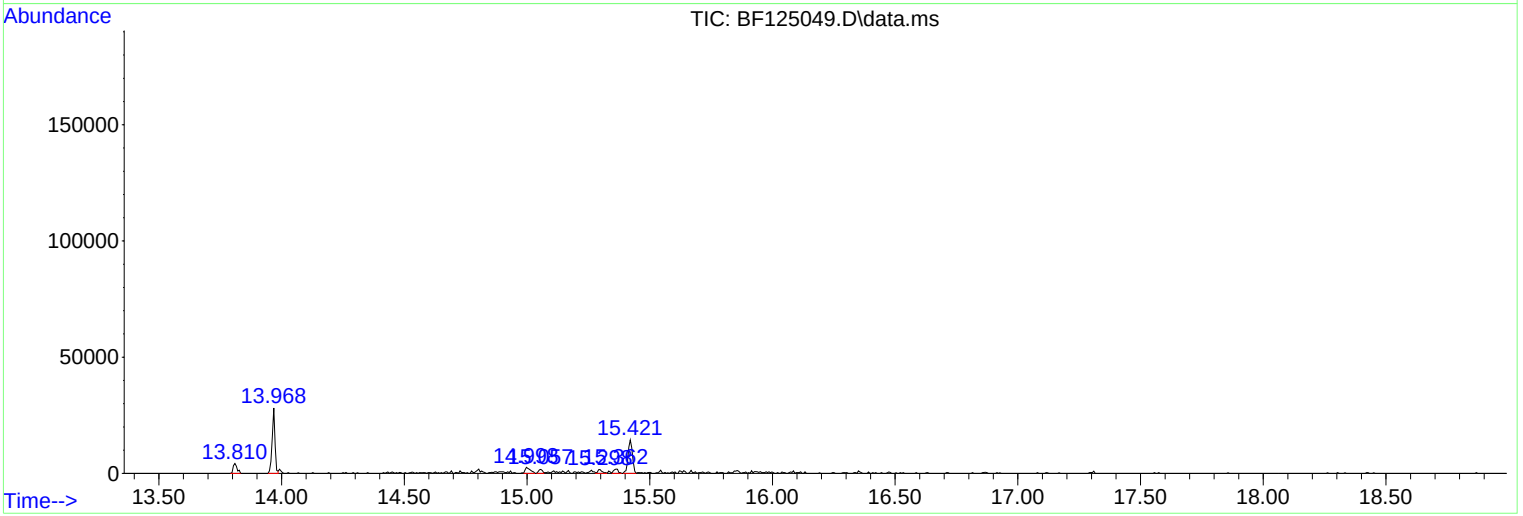
Instrument :
BNA_F
ClientSampleId :
FK-EF-01-022-ABCD

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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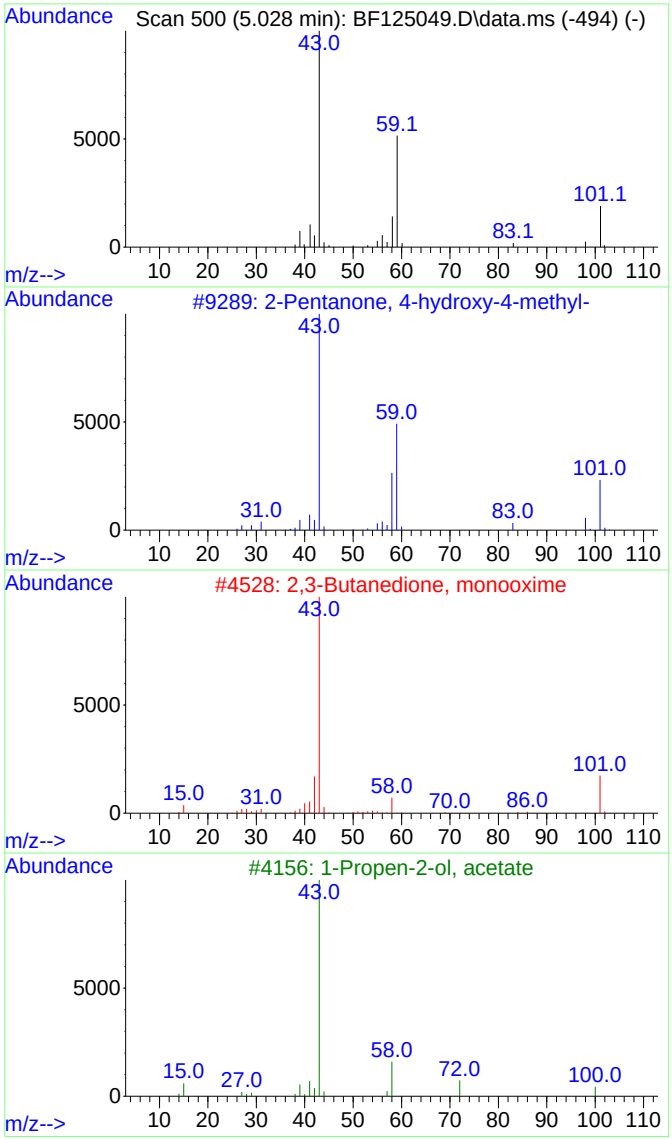
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

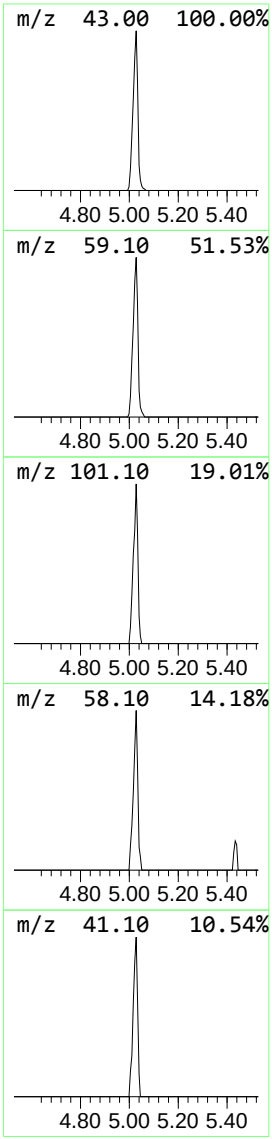
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	70.14 ng	125952	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

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
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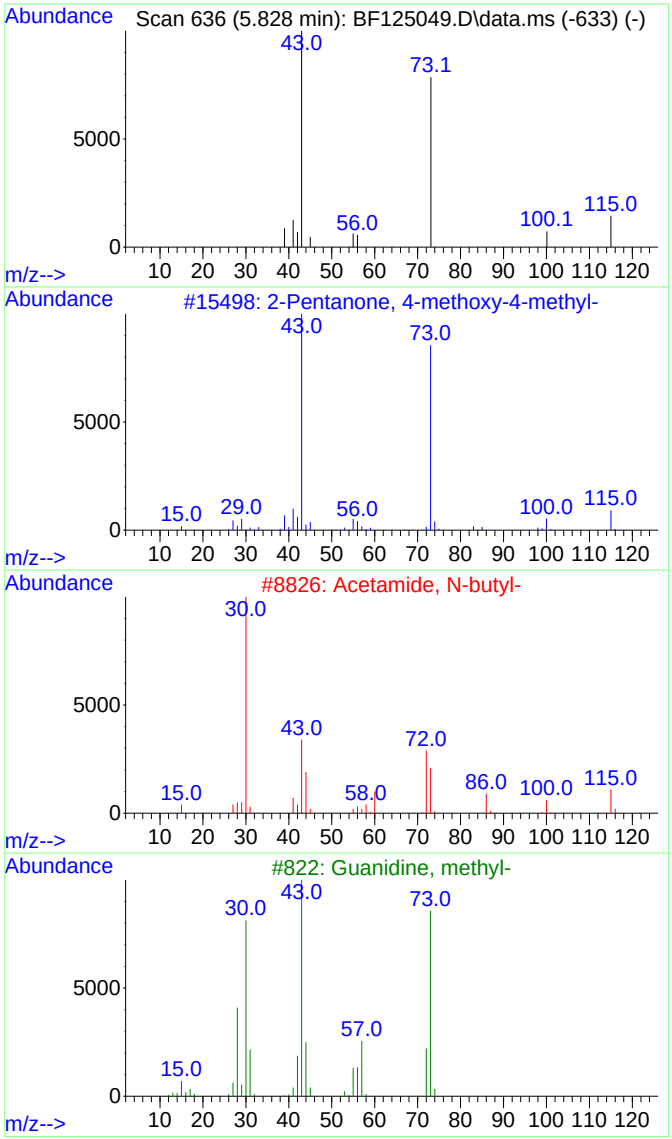
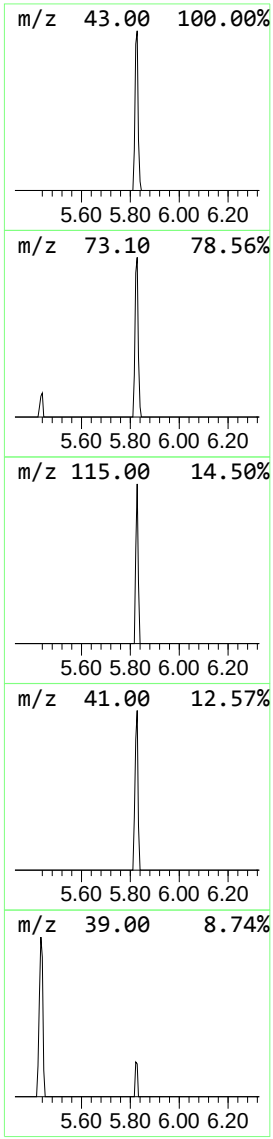
****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	10.30 ng	18504	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	5
3	Guanidine, methyl-	73	C2H7N3	000471-29-4	5
4	N-Ethylformamide	73	C3H7NO	000627-45-2	5
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	5





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Misc :
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Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

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

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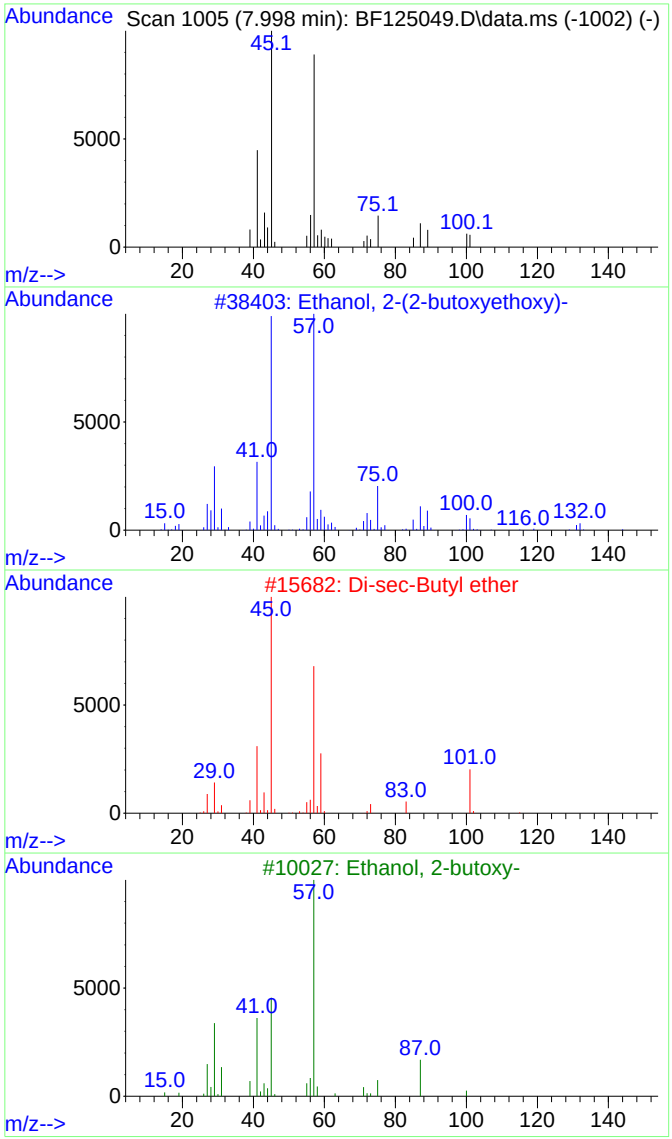
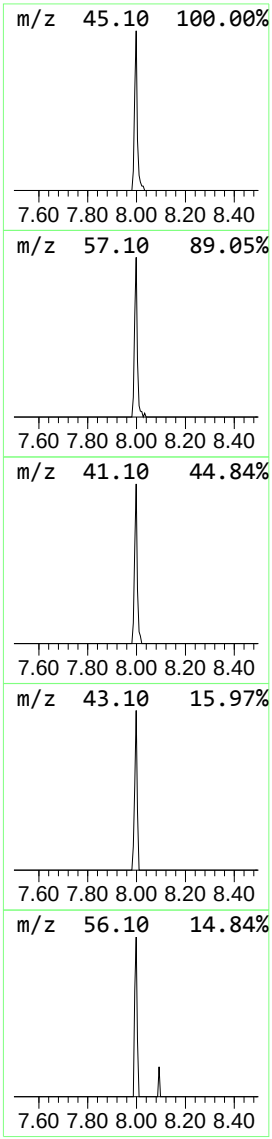
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.998	18.05 ng	41289	Naphthalene-d8	8.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	53
4	1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	42





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

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
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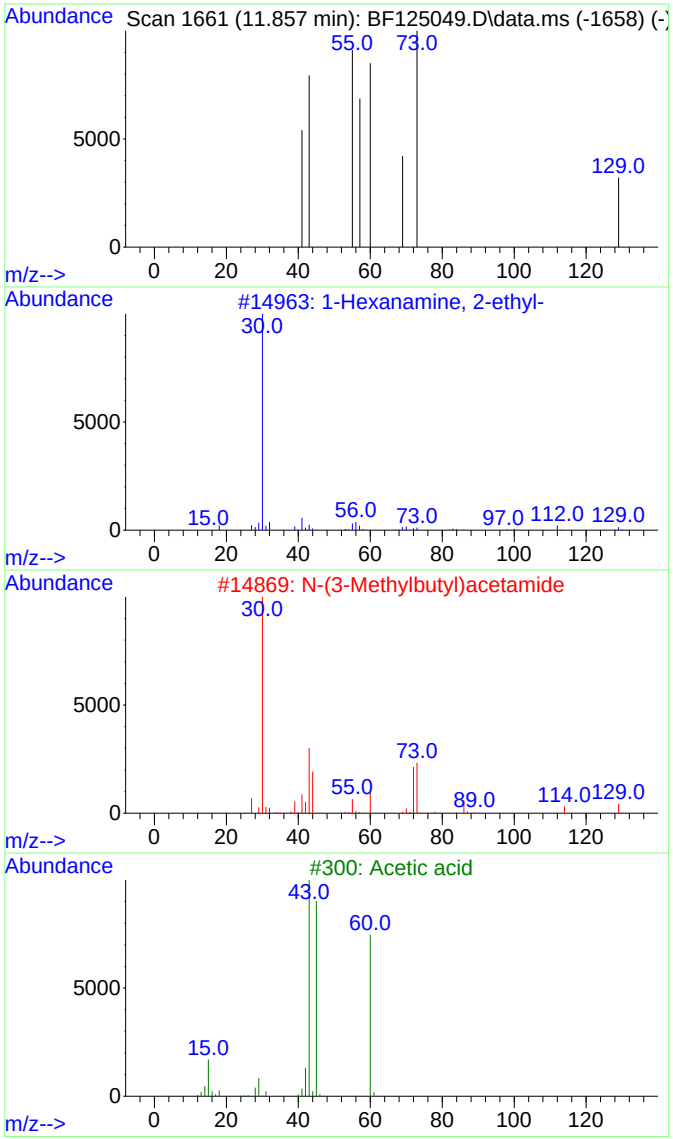
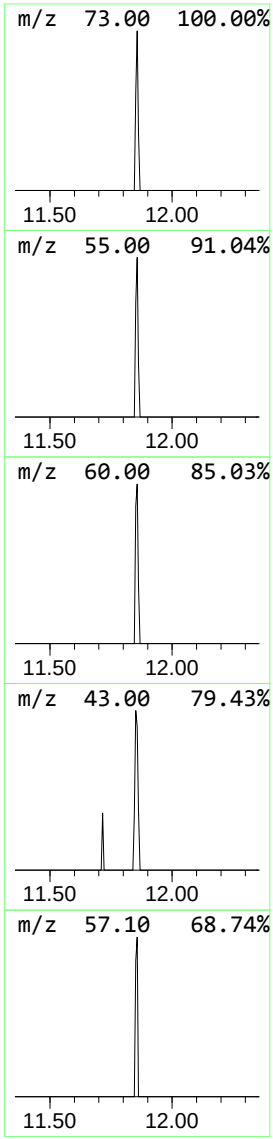
****

Peak Number 4 unknown11.857 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	3.80 ng	4159	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanamine, 2-ethyl-	129	C8H19N	000104-75-6	5
2	N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	5
3	Acetic acid	60	C2H4O2	000064-19-7	4
4	(S)-3-Aminotetrahydrofuran, Ac d...	129	C6H11NO2	1000496-60-7	4
5	Nonanoic acid	158	C9H18O2	000112-05-0	4





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Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

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

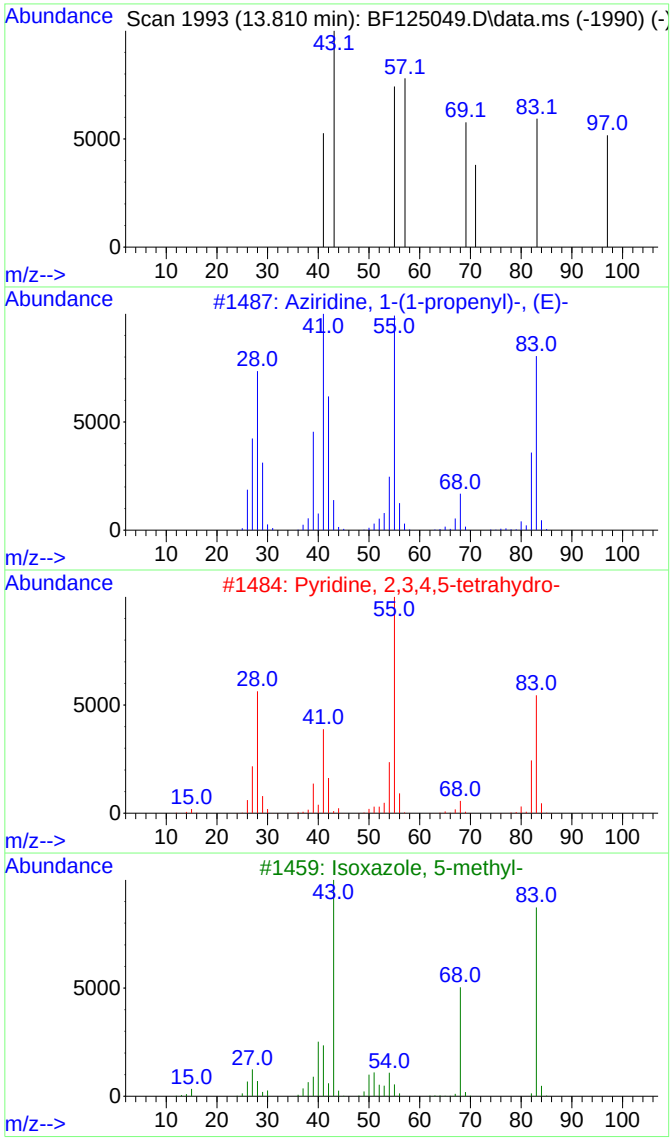
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

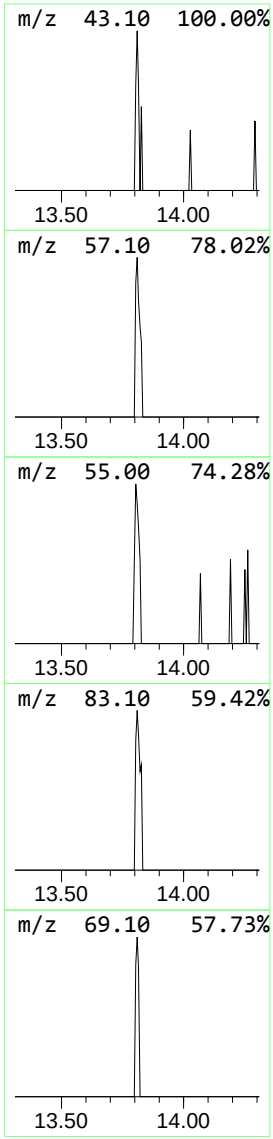
****

Peak Number 5 unknown13.810 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	4.20 ng	4764	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7
2	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	4
3	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	4
4	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	4
5	Cyclohexane, nitro-	129	C6H11NO2	001122-60-7	2





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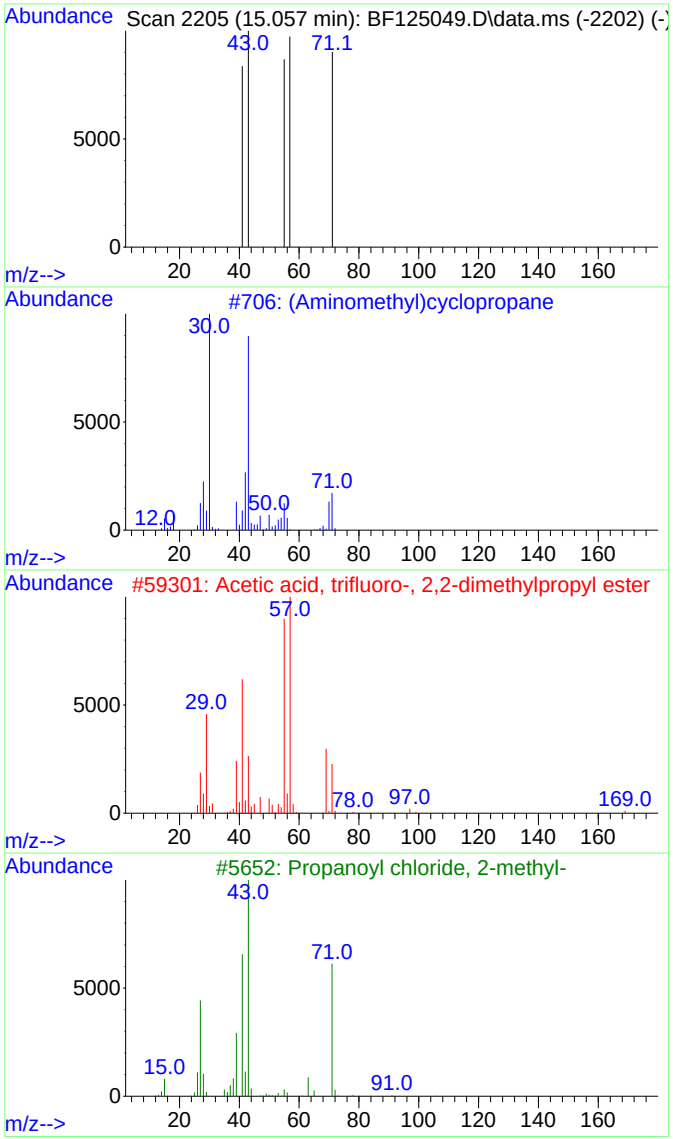
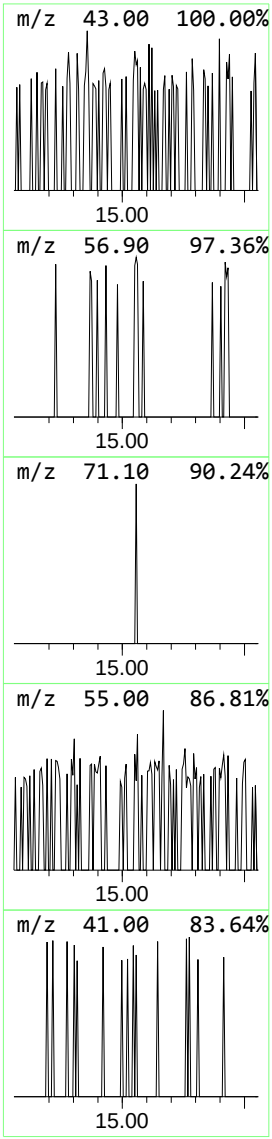
Peak Number 6 unknown15.057 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.057	2.22 ng	1954	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
2	Acetic acid, trifluoro-, 2,2-dim...	184	C7H11F3O2	007556-79-8	2
3	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	2
4	Oxalic acid, butyl propyl ester	188	C9H16O4	1000309-25-6	2
5	2-Propenamide	71	C3H5NO	000079-06-1	2





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Sample : M3295-01
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BNA_F
ClientSampleId :
FK-EF-01-022-ABCD

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

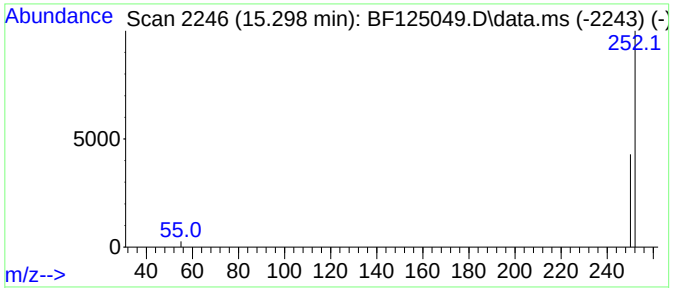
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

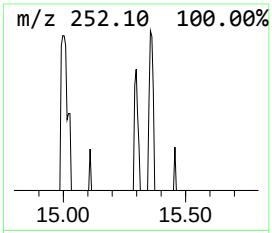
****

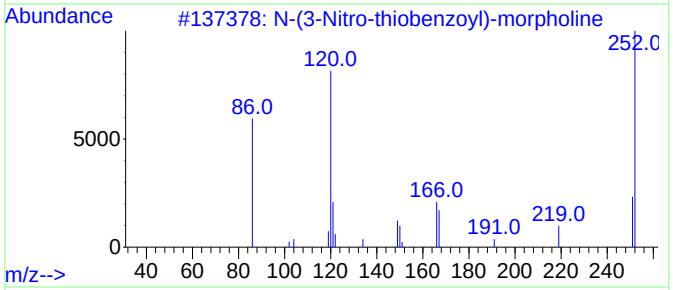
Peak Number 7 unknown15.298 Concentration Rank 6

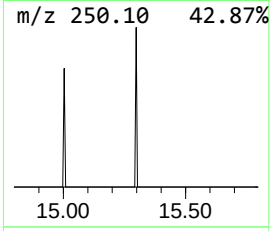
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	2.38 ng	2089	Perylene-d12	15.421

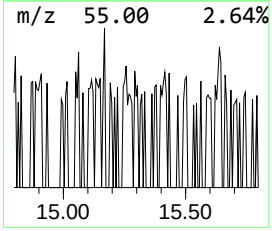
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(3-Nitro-thiobenzoyl)-morpholine	252	C11H12N2O3S	050903-05-4	3
2	1-Phenyl-3,5,7-trimethyl-6H-pyra...	252	C15H16N4	063536-14-1	3
3	2,6-Dimethoxy-9-methyl-anthracene	252	C17H16O2	110038-59-0	3
4	1,2,4-Triazole, 3-heptafluoropro...	252	C5H3F7N4	025979-02-6	2
5	4-[4-(4-Amino-1,2,5-oxadiazol-3-...	250	C7H6N8O3	1000436-51-4	2

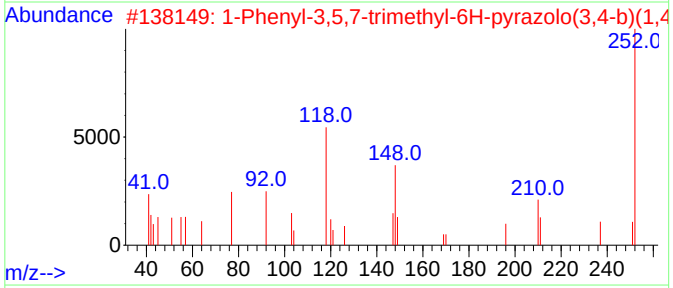


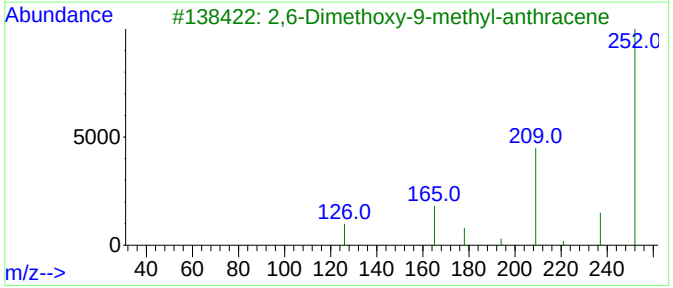












Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

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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
2-Pentanone, 4-...	5.028	70.1	ng	125952	1	6.810	35915	20.0
2-Pentanone, 4-...	5.828	10.3	ng	18504	1	6.810	35915	20.0
Ethanol, 2-(2-b...	7.998	18.1	ng	41289	2	8.092	45741	20.0
unknown11.857	11.857	3.8	ng	4159	4	11.333	21861	20.0
unknown13.810	13.810	4.2	ng	4764	5	13.968	22665	20.0
unknown15.057	15.057	2.2	ng	1954	6	15.421	17580	20.0
unknown15.298	15.298	2.4	ng	2089	6	15.421	17580	20.0