LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124749.D
Acq On : 24 Jul 2021 16:01
Operator : JU/CG
Sample : M3117-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NJ-CLEAN-5

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-BF072221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124749.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	4	7	11	rBB	12065	13978	9.60%	1.502%
2	5.093	508	511	514	rBB	2630	2786	1.91%	0.299%
3	5.481	573	577	580	rBB	124549	125379	86.09%	13.471%
4	6.492	744	749	752	rBB	127733	125009	85.84%	13.431%
5	6.869	810	813	816	rBB	45303	33298	22.86%	3.578%
6	7.434	905	909	912	rBB	101304	82826	56.87%	8.899%
7	8.051	1011	1014	1017	rBV	47130	37105	25.48%	3.987%
8	8.151	1028	1031	1034	rBB	61140	44315	30.43%	4.761%
9	9.228	1211	1214	1217	rBV	203618	145634	100.00%	15.647%
10	9.904	1327	1329	1332	rBB	50373	42957	29.50%	4.615%
11	10.692	1460	1463	1466	rBB	83944	65722	45.13%	7.061%
12	11.392	1579	1582	1585	rBV	42970	32010	21.98%	3.439%
13	11.910	1668	1670	1673	rBB	6975	5895	4.05%	0.633%
14	12.833	1825	1827	1829	rBB	4252	2647	1.82%	0.284%
15	12.980	1848	1852	1855	rBB	114980	94951	65.20%	10.202%
16	13.880	1999	2005	2012	rBV4	5878	10748	7.38%	1.155%
17	14.033	2027	2031	2033	rBV	29102	26261	18.03%	2.822%
18	15.068	2205	2207	2210	rBV2	2356	2415	1.66%	0.259%
19	15.145	2217	2220	2223	rBV	3535	4065	2.79%	0.437%
20	15.504	2277	2281	2284	rBV	18813	21240	14.58%	2.282%
21	15.527	2284	2285	2290	rVB2	3117	2986	2.05%	0.321%
22	15.968	2356	2360	2364	rVB2	3551	5155	3.54%	0.554%
23	16.480	2443	2447	2453	rVB2	2095	3361	2.31%	0.361%

Sum of corrected areas: 930743

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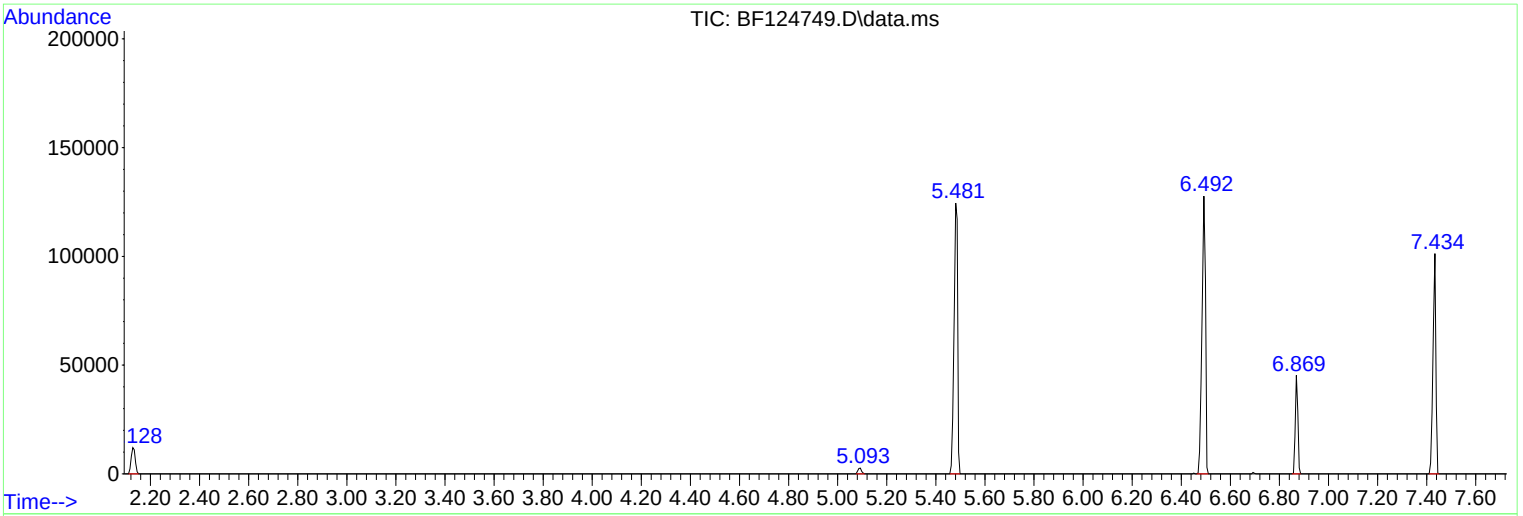
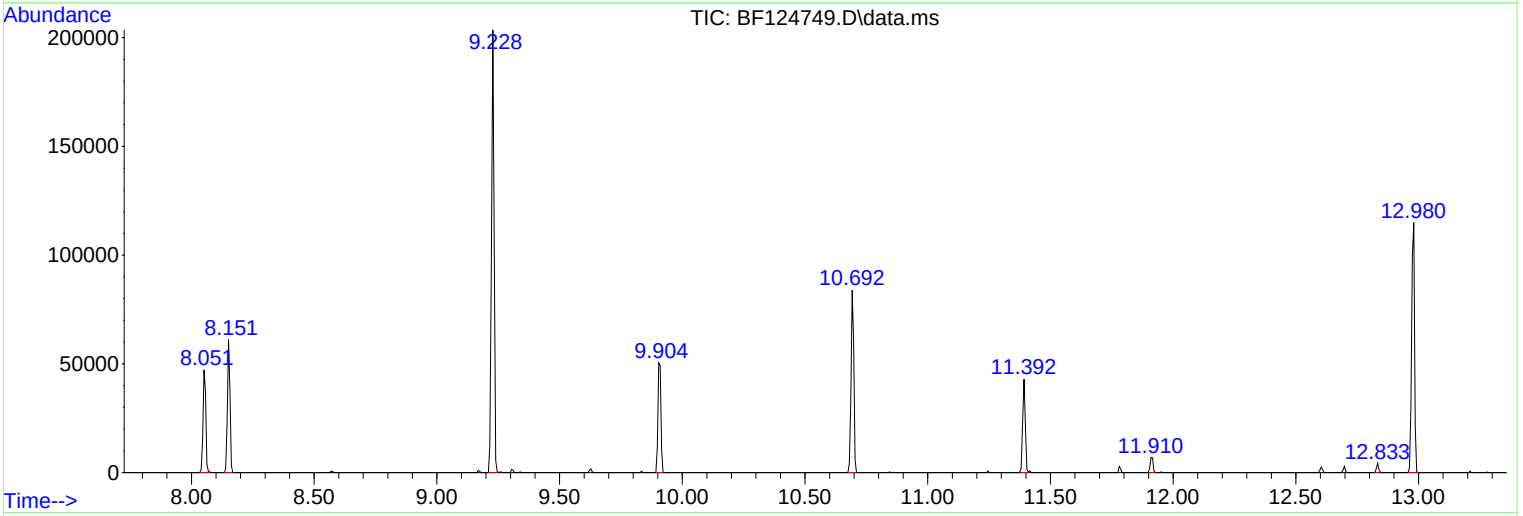
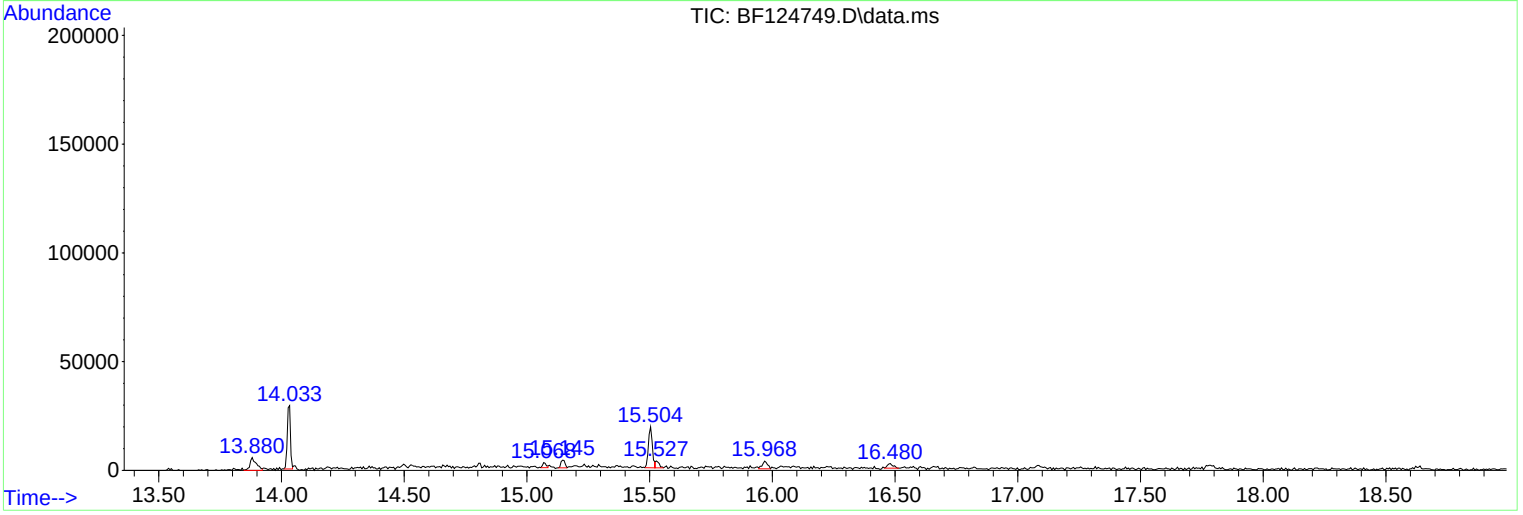
BNA_F
ClientSampleId :
NJ-CLEAN-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.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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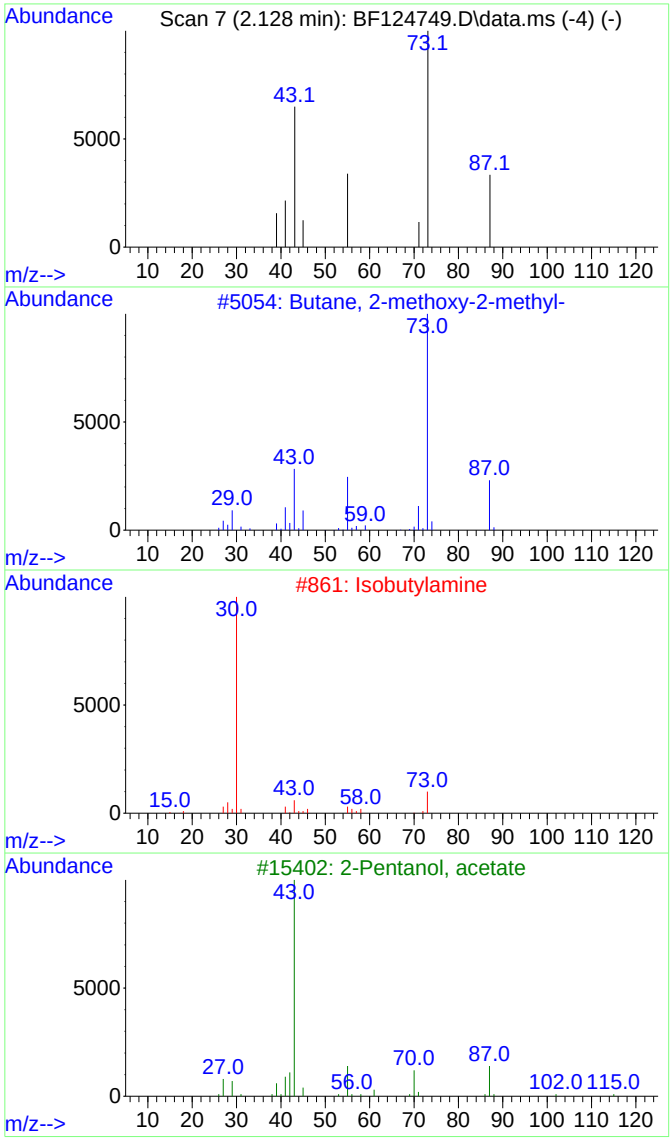
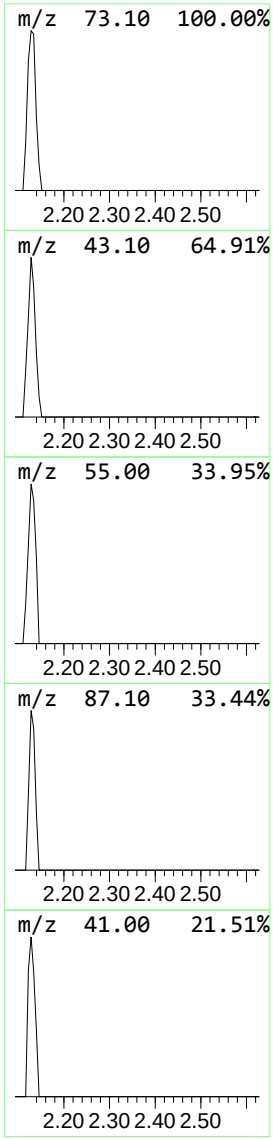
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	8.40 ng	13978	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
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





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Sample : M3117-05
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ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NJ-CLEAN-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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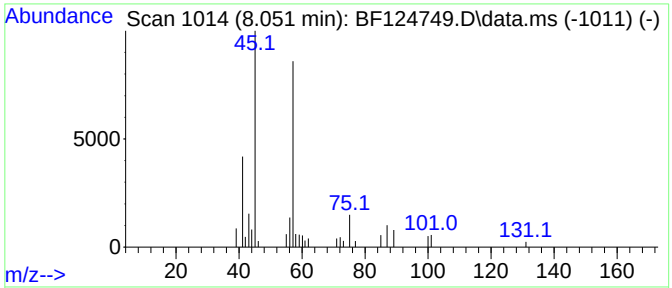
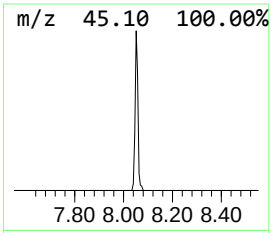
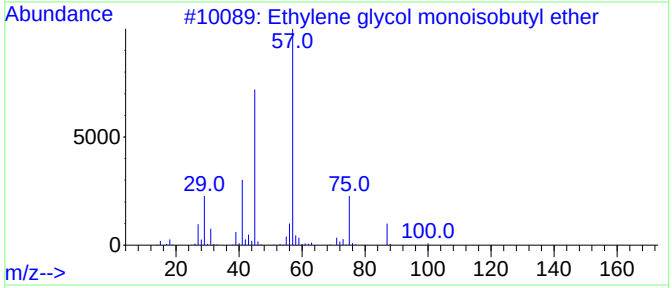
****
Peak Number 2 Ethylene glycol monoisobuty... Concentration Rank 1

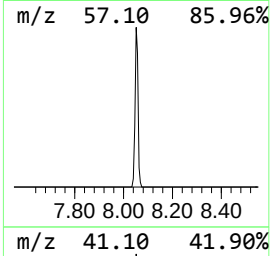
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	16.75 ng	37105	Naphthalene-d8	8.151

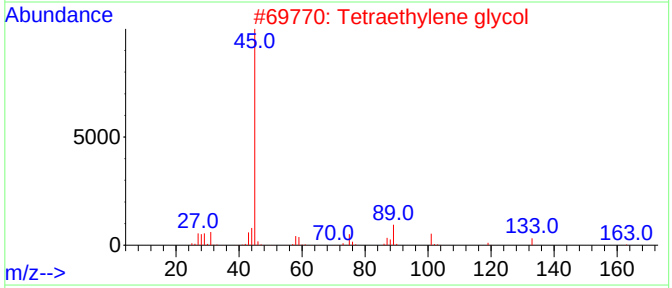
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
2	Tetraethylene glycol	194	C8H18O5	000112-60-7	53
3	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	53
4	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50
5	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50

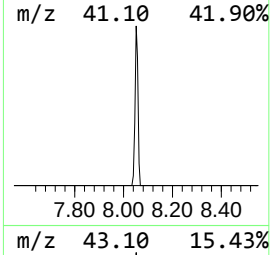


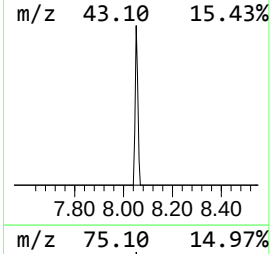


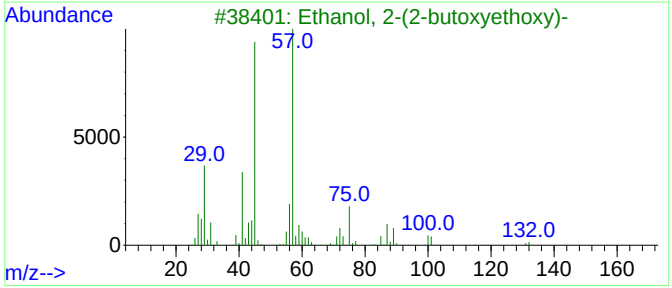


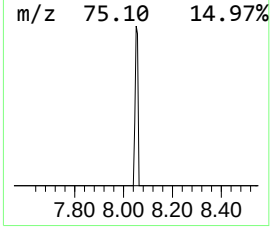












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Sample : M3117-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

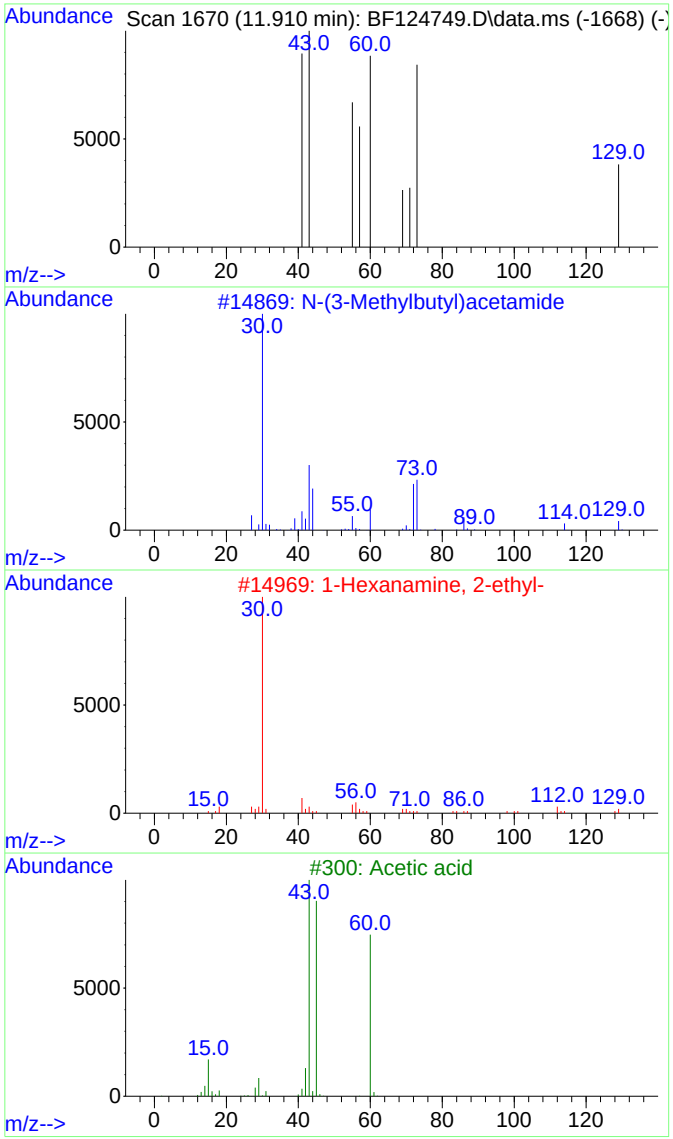
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

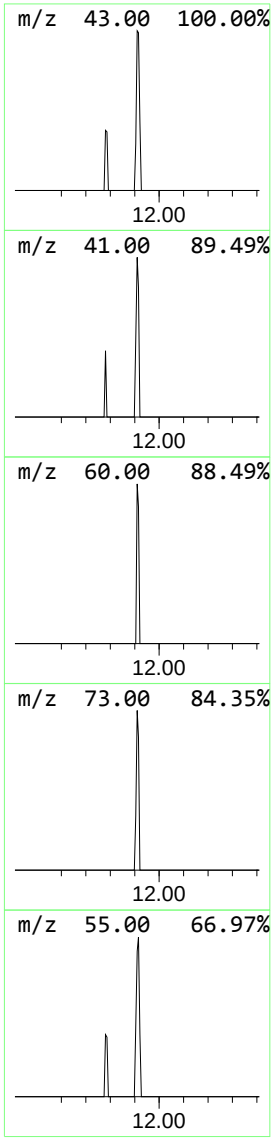
****

Peak Number 3 unknown11.910 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.68 ng	5895	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	9
2	1-Hexanamine, 2-ethyl-	129	C8H19N	000104-75-6	5
3	Acetic acid	60	C2H4O2	000064-19-7	4
4	3-Pentane isothiocyanate	129	C6H11NS	201224-89-7	4
5	N-Pentylacetamide	129	C7H15NO	002524-60-9	4





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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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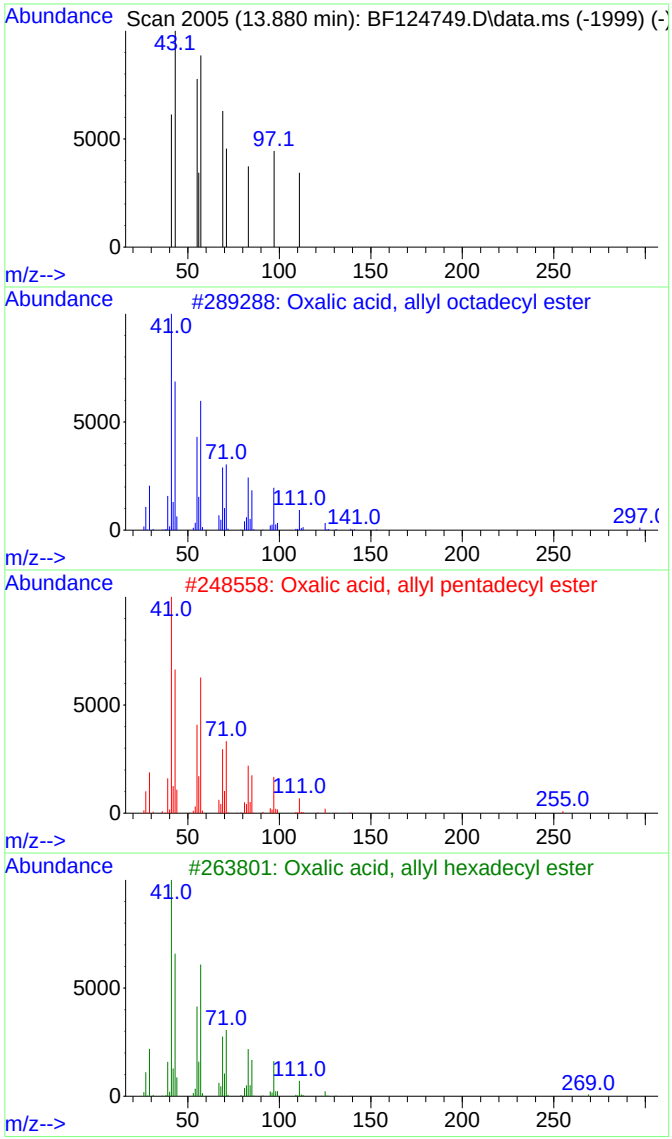
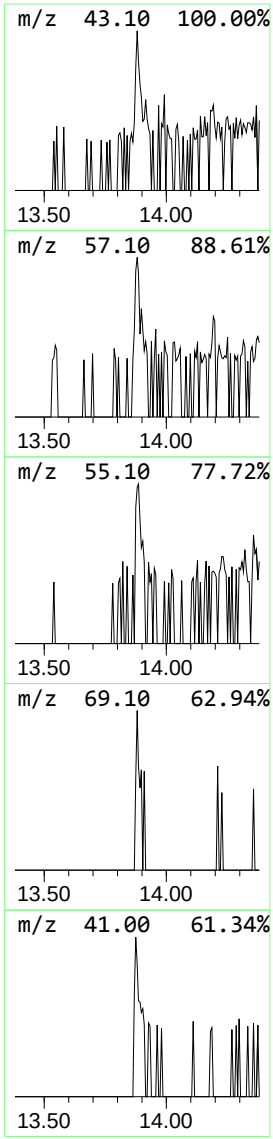
****
Peak Number 4 Oxalic acid, allyl octadecy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	8.19 ng	10748	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	56
2	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	39
3	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	39
4	2-Hexenal, (E)-	98	C6H10O	006728-26-3	9
5	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	9





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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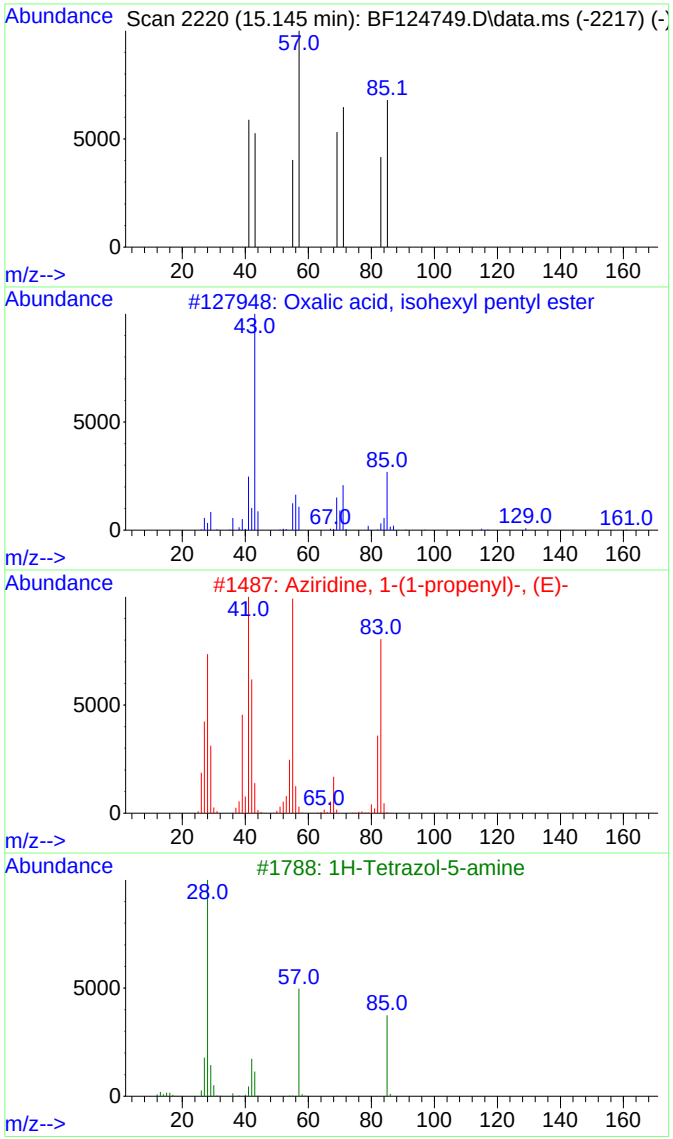
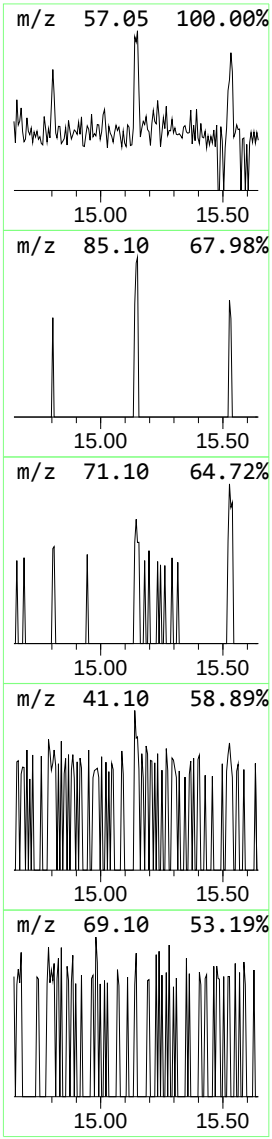
****

Peak Number 5 unknown15.145 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	3.83 ng	4065	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	9
2	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	5
3	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
4	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
5	2-Propenamide	71	C3H5NO	000079-06-1	4





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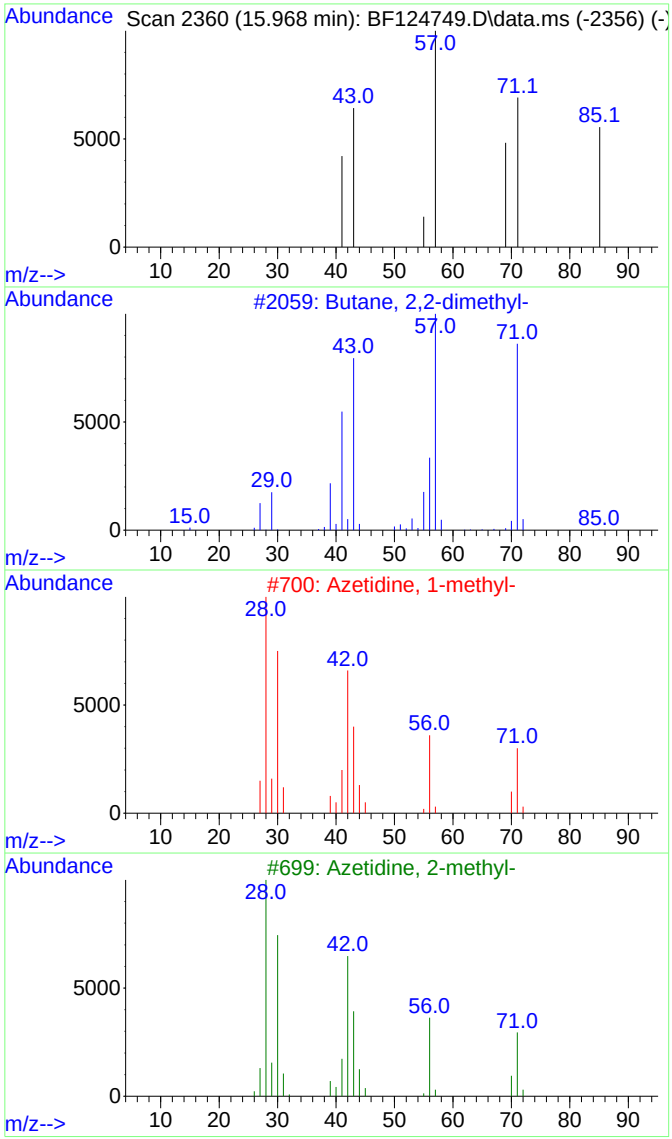
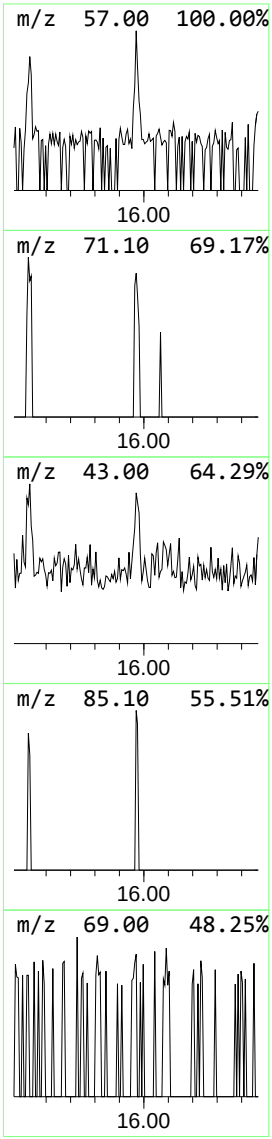
****

Peak Number 6 unknown15.968 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	4.85 ng	5155	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	25
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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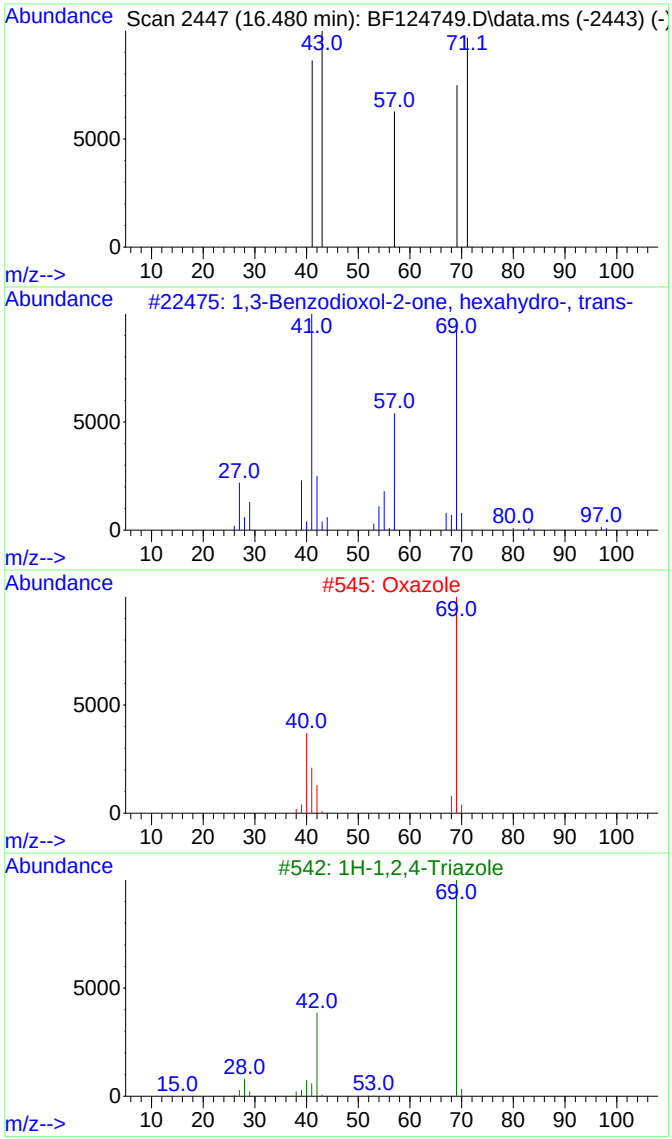
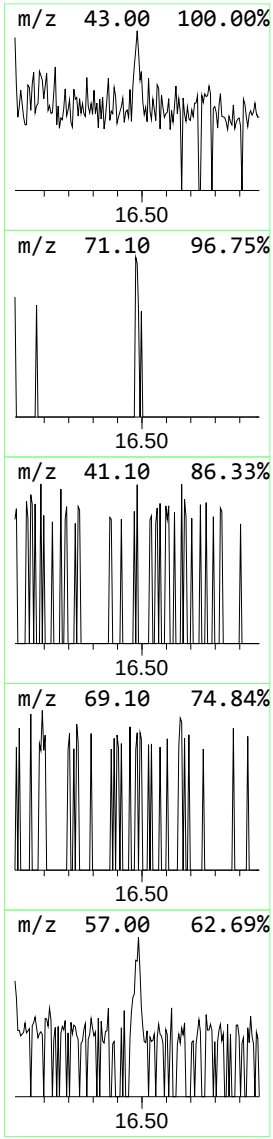
Peak Number 7 unknown16.480 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.480	3.16 ng	3361	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzodioxol-2-one, hexahydro...	142	C7H10O3	020192-66-9	2
2	Oxazole	69	C3H3NO	000288-42-6	2
3	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	2
4	2-Propynenitrile, 3-fluoro-	69	C3FN	032038-83-8	2
5	Isoxazole	69	C3H3NO	000288-14-2	2





Tentatively Identified Compound (LSC) summary

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Data File : BF124749.D
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Misc :
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Instrument : BNA_F
ClientSampleId : NJ-CLEAN-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.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
Butane, 2-metho...	2.128	8.4	ng	13978	1	6.869	33298	20.0
Ethylene glycol...	8.051	16.8	ng	37105	2	8.151	44315	20.0
unknown11.910	11.910	3.7	ng	5895	4	11.392	32010	20.0
Oxalic acid, al...	13.880	8.2	ng	10748	5	14.033	26261	20.0
unknown15.145	15.145	3.8	ng	4065	6	15.504	21240	20.0
unknown15.968	15.968	4.8	ng	5155	6	15.504	21240	20.0
unknown16.480	16.480	3.2	ng	3361	6	15.504	21240	20.0