LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124778.D
Acq On : 26 Jul 2021 22:39
Operator : JU/CG
Sample : M3151-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

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: BF124778.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	11	14	18	rBB	8865	10049	8.87%	1.263%
2	5.098	509	512	515	rBB	3991	3548	3.13%	0.446%
3	5.492	575	579	582	rBB	127521	108944	96.11%	13.693%
4	6.498	745	750	753	rBV	117942	104981	92.62%	13.195%
5	6.875	811	814	817	rBB	34990	25480	22.48%	3.202%
6	7.434	905	909	912	rBB	79776	68425	60.37%	8.600%
7	8.051	1012	1014	1019	rBB	6916	5693	5.02%	0.716%
8	8.157	1029	1032	1035	rBB	42214	31429	27.73%	3.950%
9	9.233	1211	1215	1218	rBV	140448	113350	100.00%	14.246%
10	9.910	1327	1330	1333	rBB	40649	30109	26.56%	3.784%
11	10.698	1461	1464	1467	rBB	71137	53102	46.85%	6.674%
12	11.398	1580	1583	1586	rBB	35075	26146	23.07%	3.286%
13	11.916	1669	1671	1673	rBB	4185	3002	2.65%	0.377%
14	12.986	1849	1853	1856	rBB	116824	103422	91.24%	12.999%
15	13.551	1947	1949	1951	rBB	2791	2022	1.78%	0.254%
16	13.880	2002	2005	2011	rBV2	7274	10845	9.57%	1.363%
17	14.039	2028	2032	2035	rVB	30432	25955	22.90%	3.262%
18	14.198	2055	2059	2061	rBB	6249	4730	4.17%	0.594%
19	14.498	2107	2110	2114	rBV	6231	5785	5.10%	0.727%
20	14.792	2155	2160	2161	rBV	4989	5521	4.87%	0.694%
21	14.810	2161	2163	2166	rVB	5747	5379	4.75%	0.676%
22	14.886	2173	2176	2179	rVB	2163	2514	2.22%	0.316%
23	15.151	2217	2221	2225	rBV	5792	6692	5.90%	0.841%
24	15.515	2276	2283	2289	rBV	18185	26791	23.64%	3.367%
25	15.968	2356	2360	2365	rBV2	2794	4340	3.83%	0.545%
26	16.068	2374	2377	2379	rBV2	1281	1815	1.60%	0.228%
27	16.092	2379	2381	2386	rVB2	1503	1735	1.53%	0.218%
28	16.486	2443	2448	2452	rVB2	1623	2430	2.14%	0.305%
29	16.851	2509	2510	2516	rVB2	1046	1406	1.24%	0.177%

Sum of corrected areas: 795640

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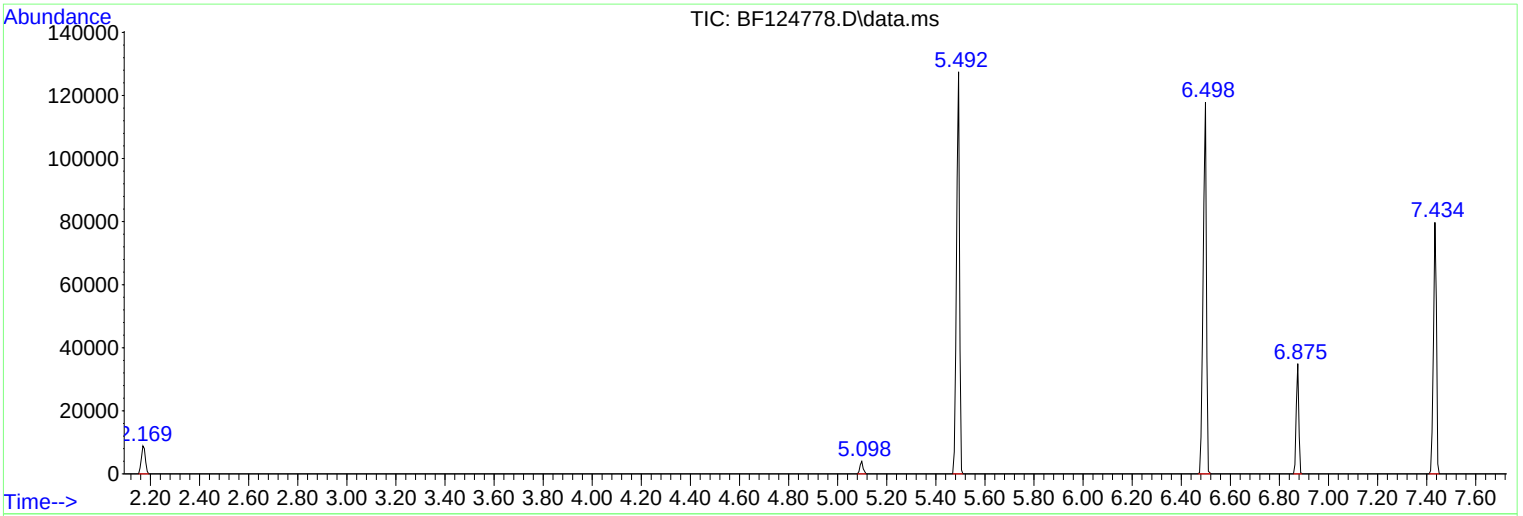
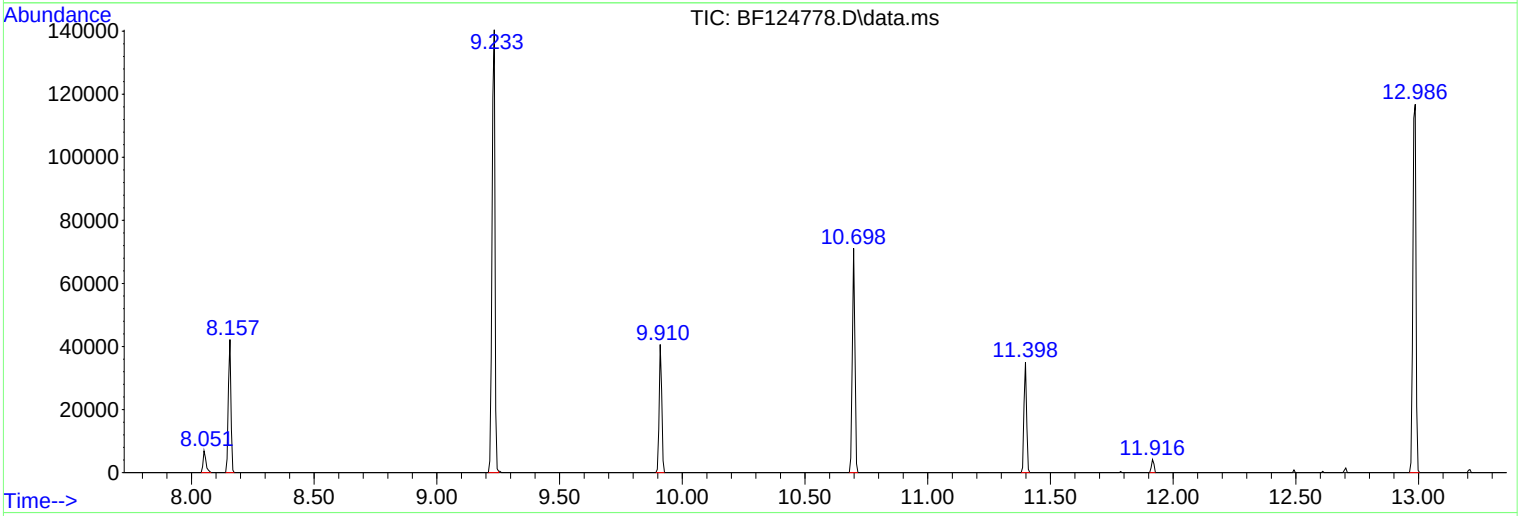
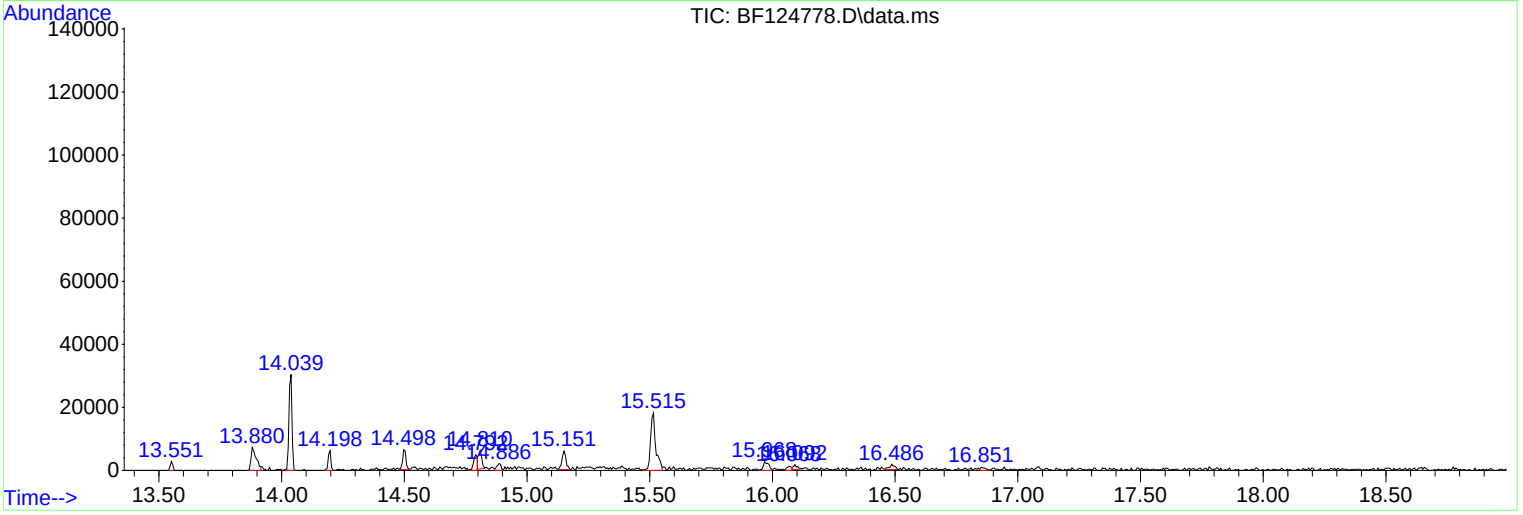
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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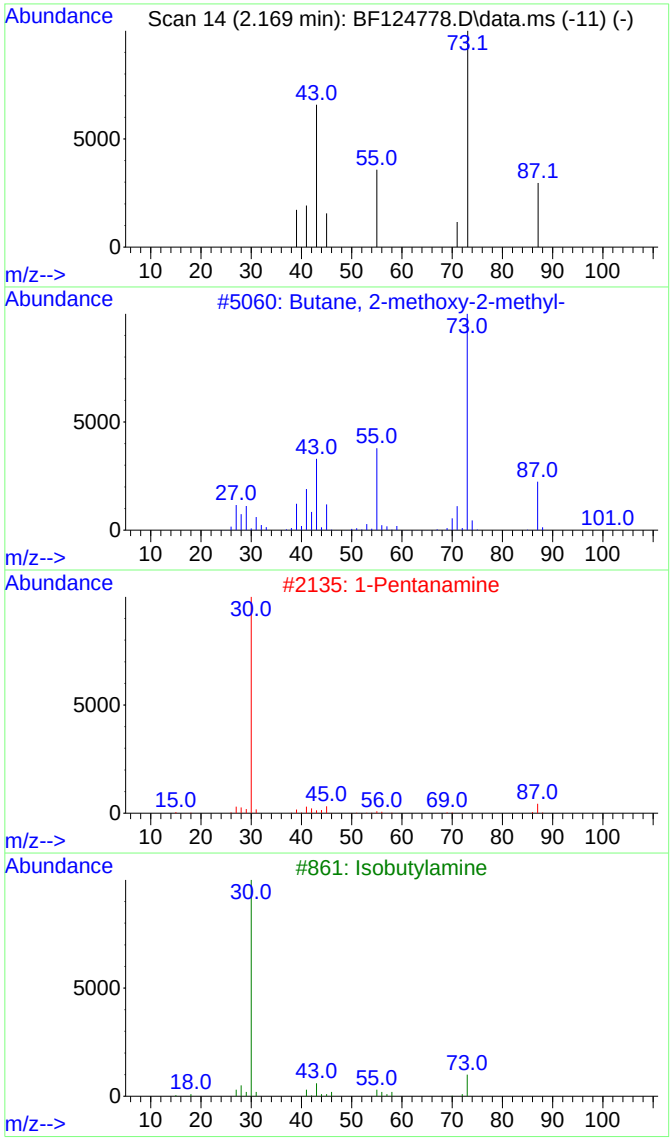
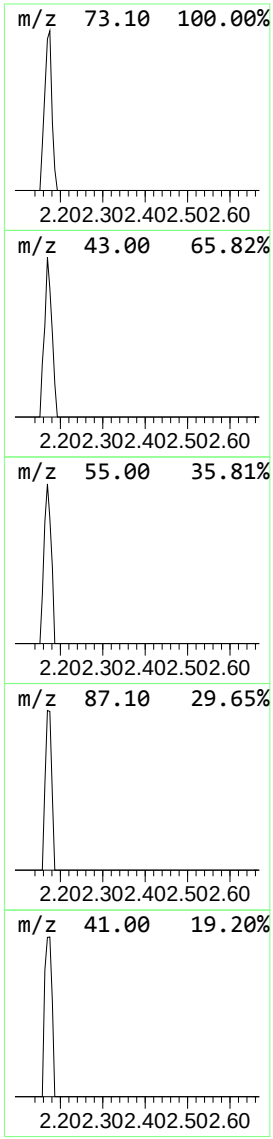
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	7.89 ng	10049	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	1-Pentanamine	87	C5H13N	000110-58-7	4
3	Isobutylamine	73	C4H11N	000078-81-9	4
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4
5	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4





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Instrument : BNA_F
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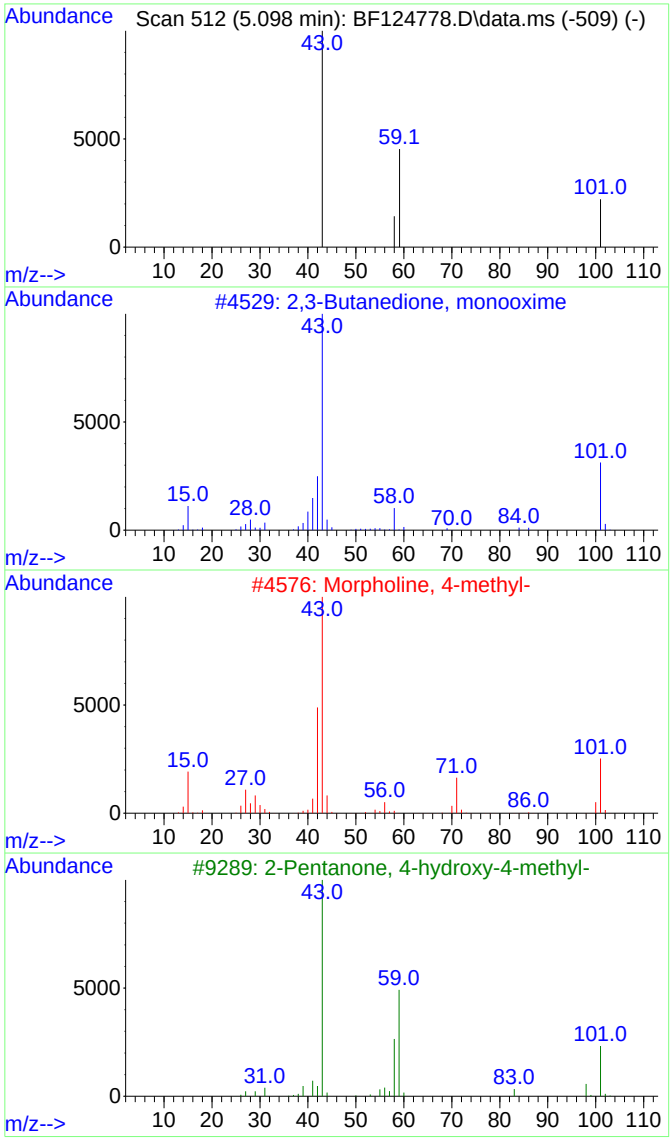
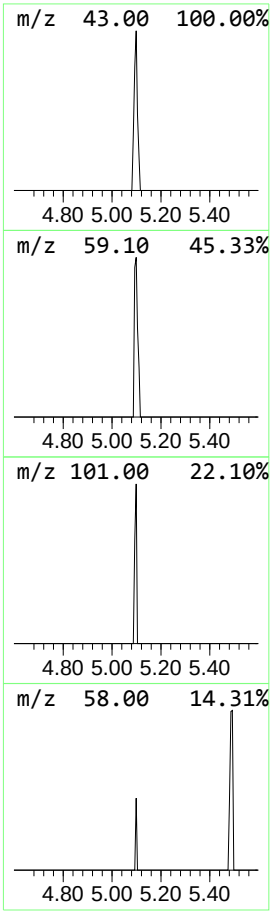
Peak Number 2 unknown5.098 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	2.78 ng	3548	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	5
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	4
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	4
4	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	3
5	Propylamine	59	C3H9N	000107-10-8	3





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Instrument : BNA_F
ClientSampleId : COMP-3

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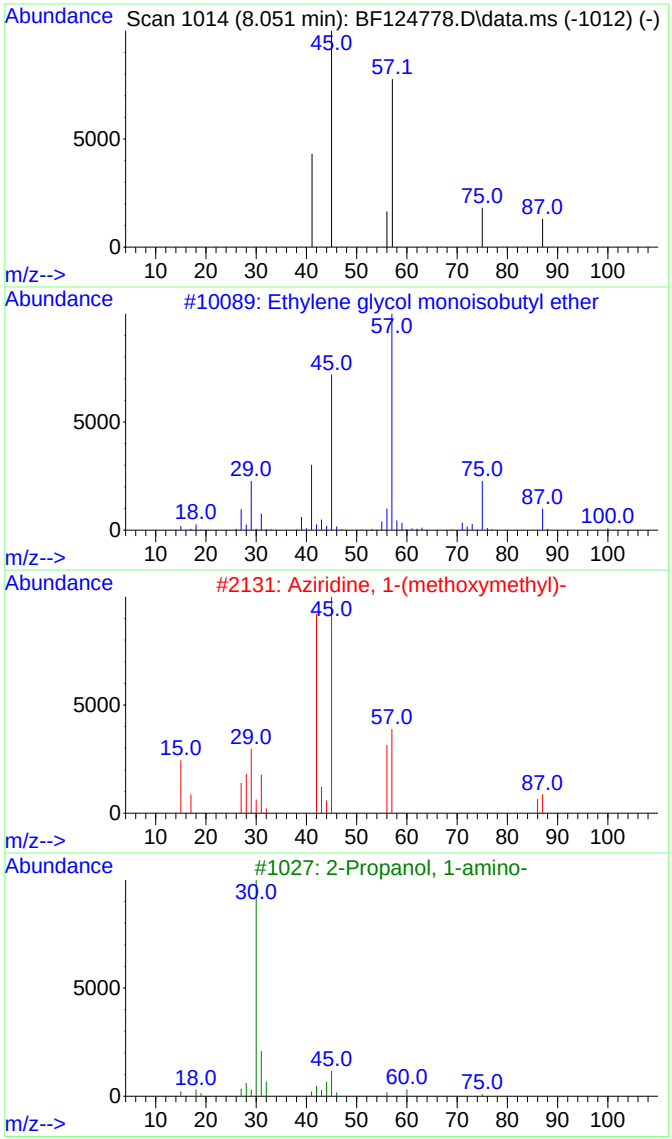
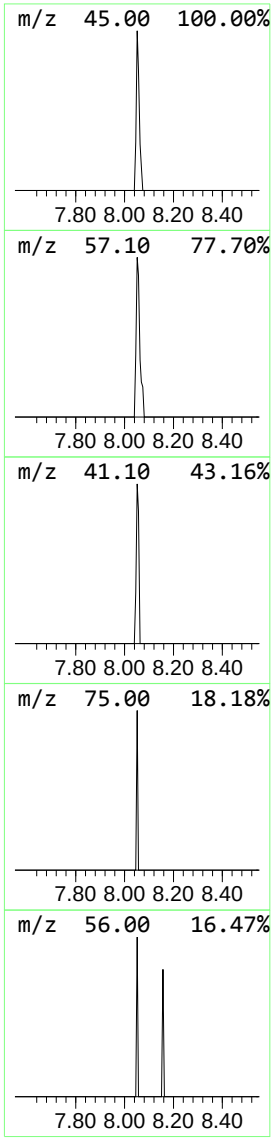
Peak Number 3 unknown8.051 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	3.62 ng	5693	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	4
2	Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	4
3	2-Propanol, 1-amino-	75	C3H9NO	000078-96-6	3
4	2-Propanol, 1-amino-, (R)-	75	C3H9NO	002799-16-8	3
5	2-Propanol, 1-amino-, (S)-	75	C3H9NO	002799-17-9	3





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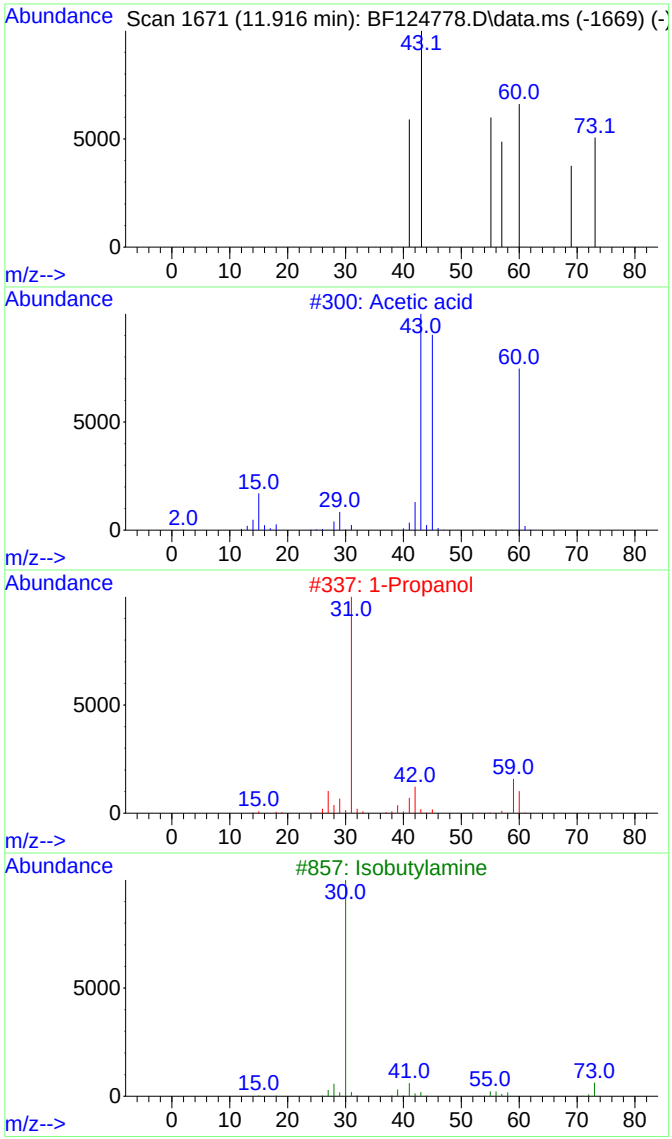
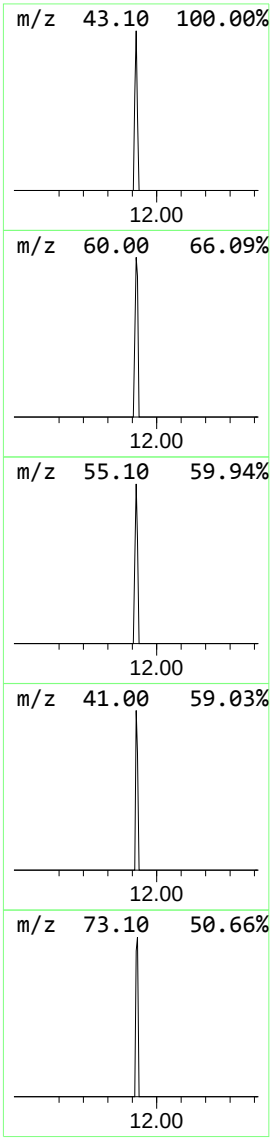
Peak Number 4 unknown11.916 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.30 ng	3002	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	4
2	1-Propanol	60	C3H8O	000071-23-8	3
3	Isobutylamine	73	C4H11N	000078-81-9	3
4	Carbonyl sulfide	60	COS	000463-58-1	2
5	Urea	60	CH4N2O	000057-13-6	2





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Sample : M3151-03
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ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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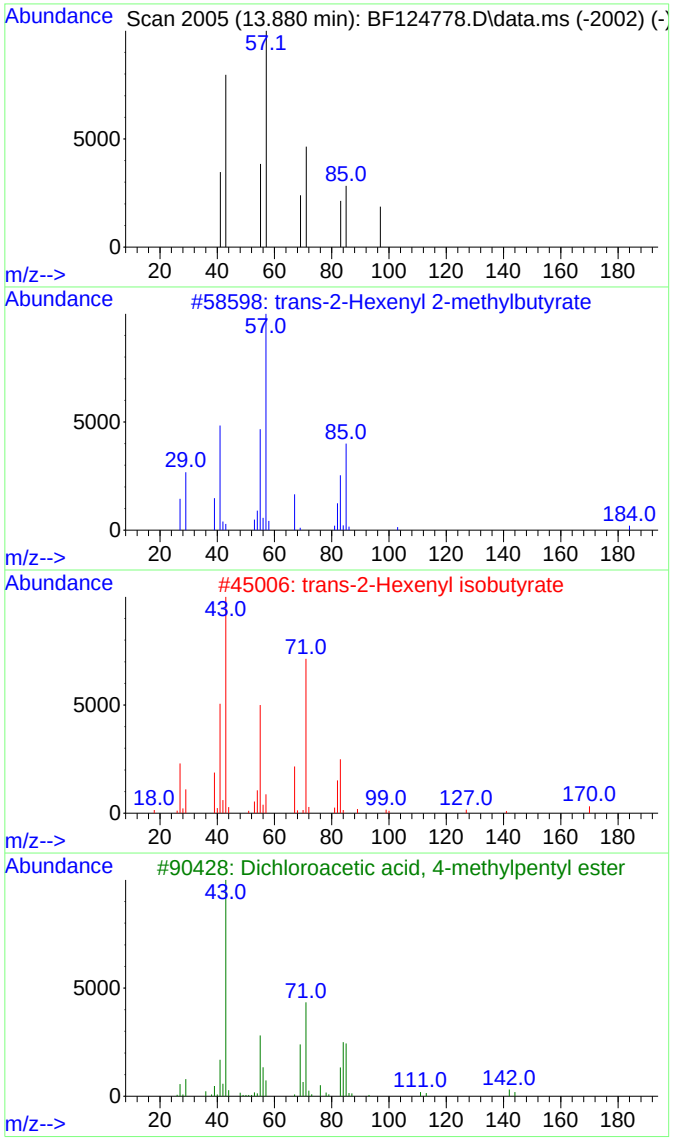
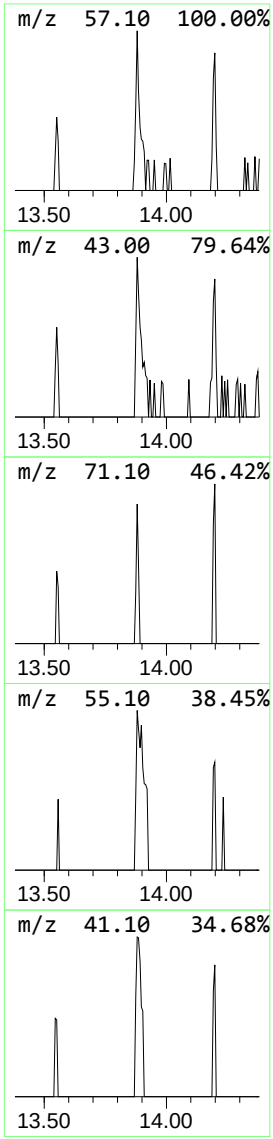
Peak Number 5 unknown13.880 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	8.36 ng	10845	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	25
2	trans-2-Hexenyl isobutyrate	170	C10H18O2	1000429-31-4	9
3	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	9
4	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
5	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5





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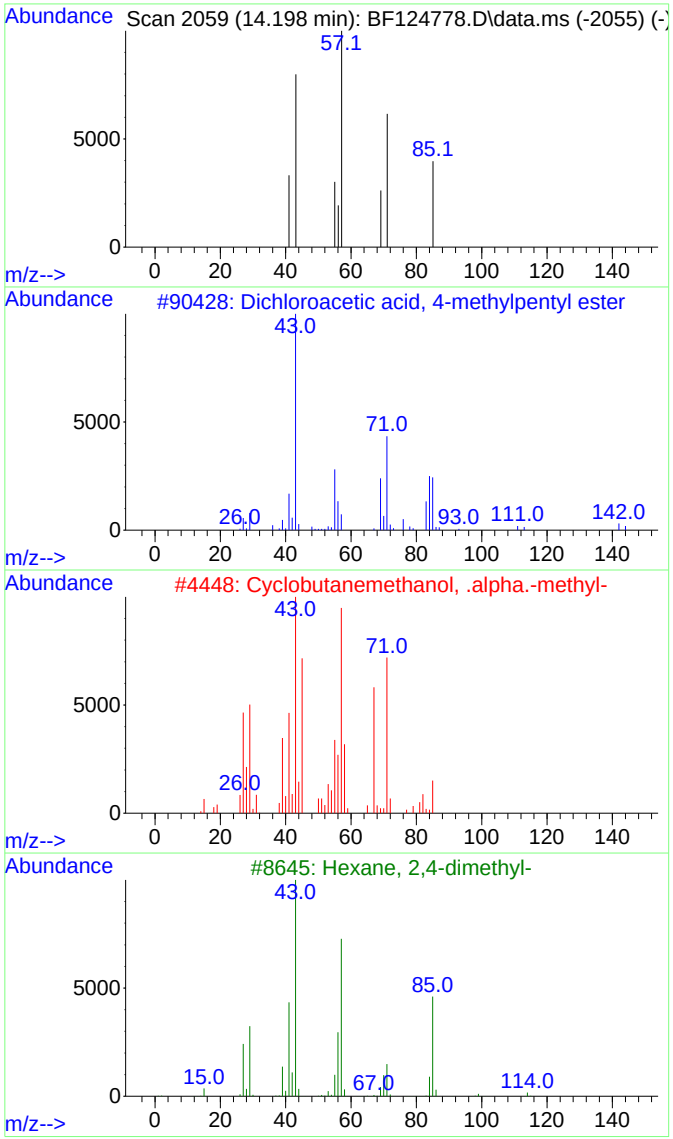
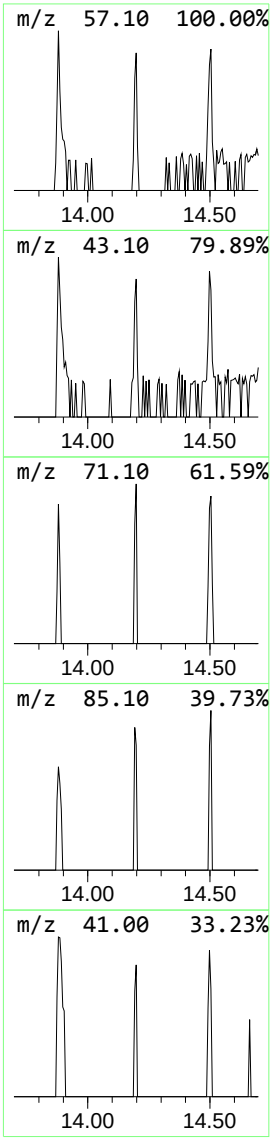
Peak Number 6 unknown14.198 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	3.64 ng	4730	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	9
2	Cyclobutanemethanol, .alpha.-met...	100	C6H12O	007515-29-9	9
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	9
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
5	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5





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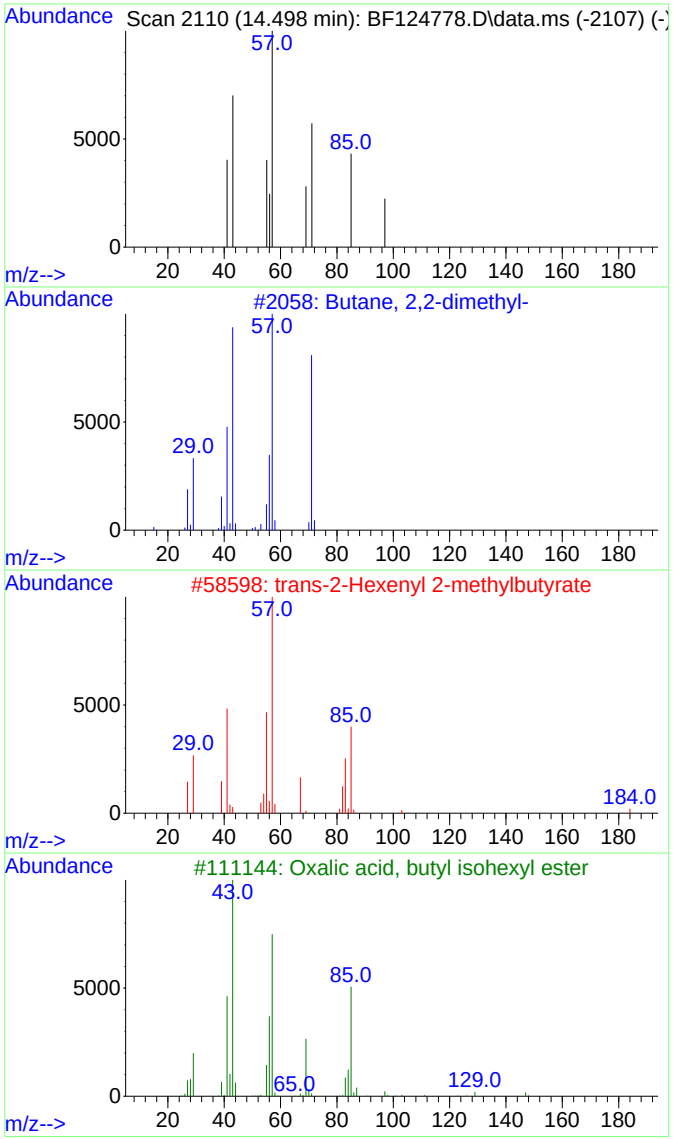
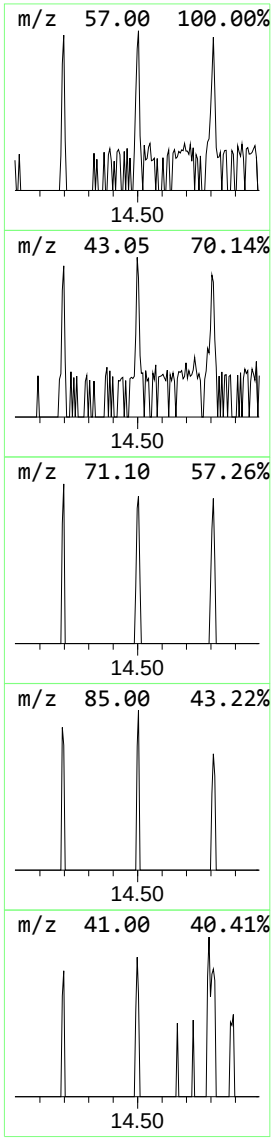
Peak Number 7 unknown14.498 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	4.46 ng	5785	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	25
2	trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
3	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	9
4	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	9
5	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5





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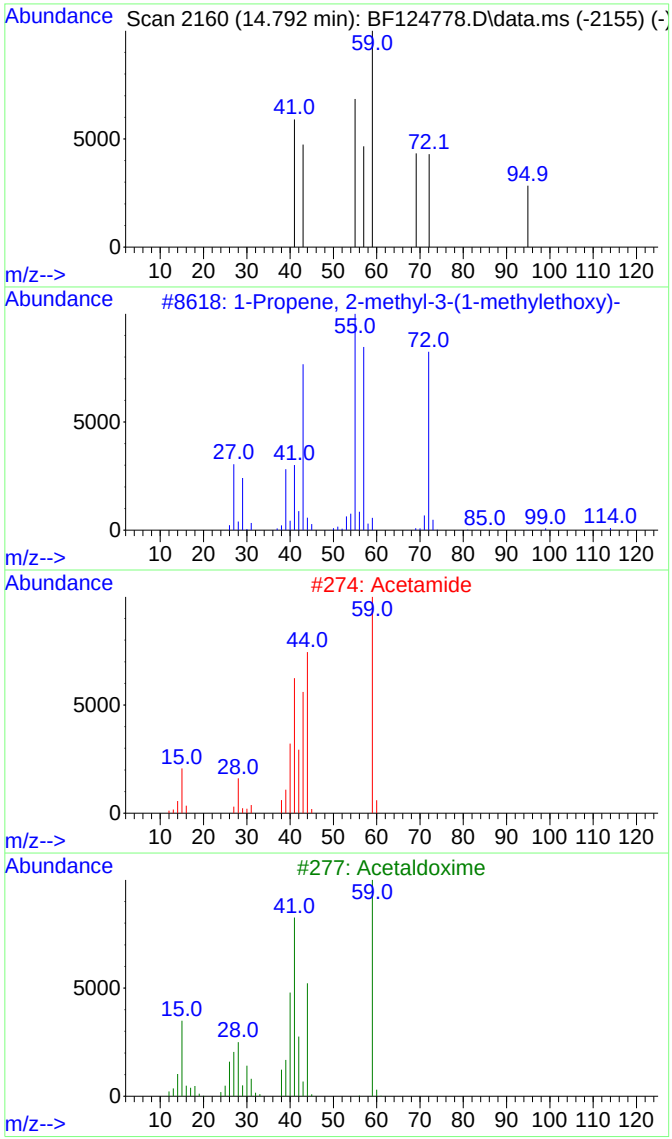
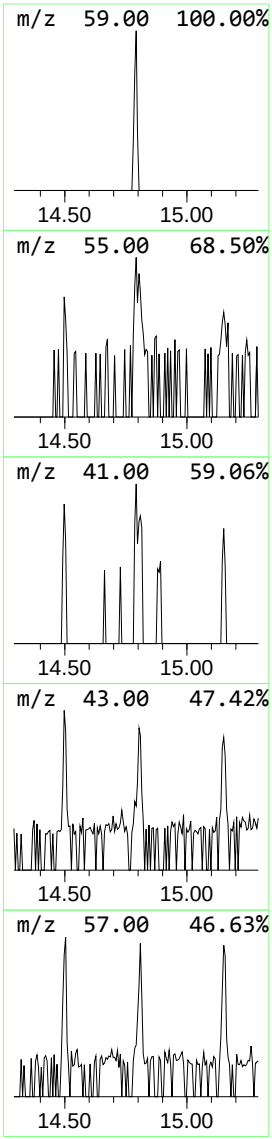
Peak Number 8 unknown14.792 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	4.12 ng	5521	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-3-(1-methyle...	114	C7H14O	044744-50-5	9
2	Acetamide	59	C2H5NO	000060-35-5	7
3	Acetaldoxime	59	C2H5NO	000107-29-9	4
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	4
5	Isobutylene epoxide	72	C4H8O	000558-30-5	4





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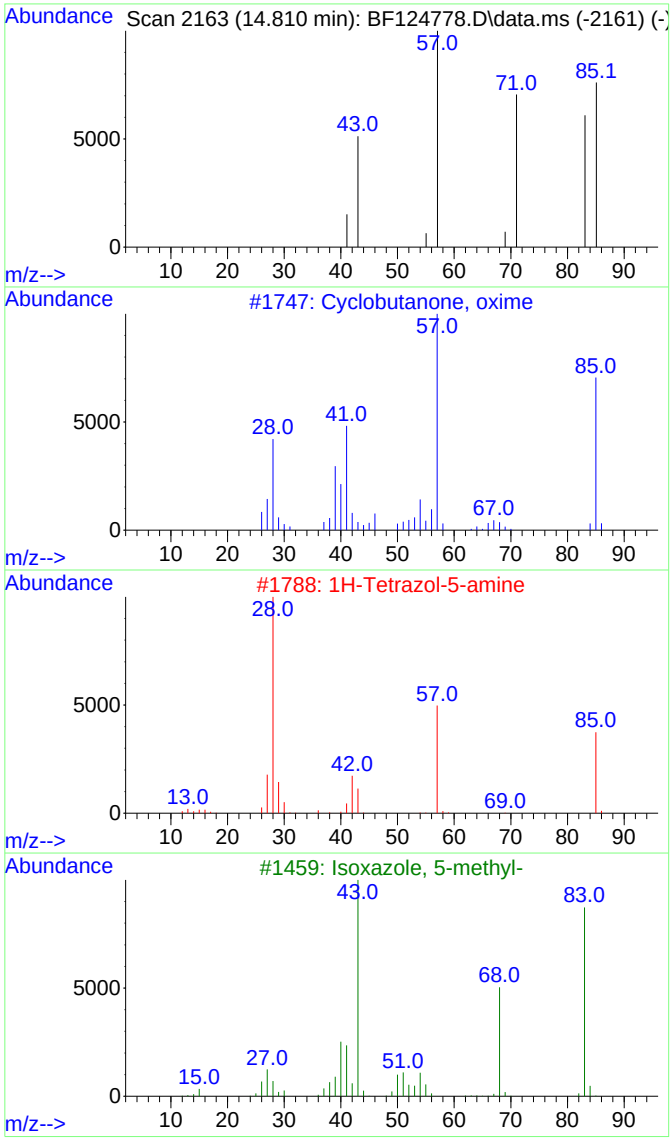
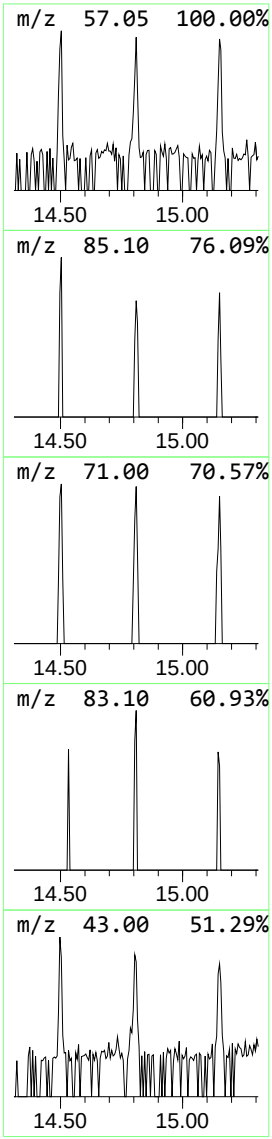
Peak Number 9 unknown14.810 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	4.02 ng	5379	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	7
2	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
3	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	4
4	Cyclopropanemethanol, .alpha.-bu...	128	C8H16O	004379-16-2	4
5	Oxirane, 2-methyl-3-propyl-, cis-	100	C6H12O	006124-90-9	4





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Acq On : 26 Jul 2021 22:39
Operator : JU/CG
Sample : M3151-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

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

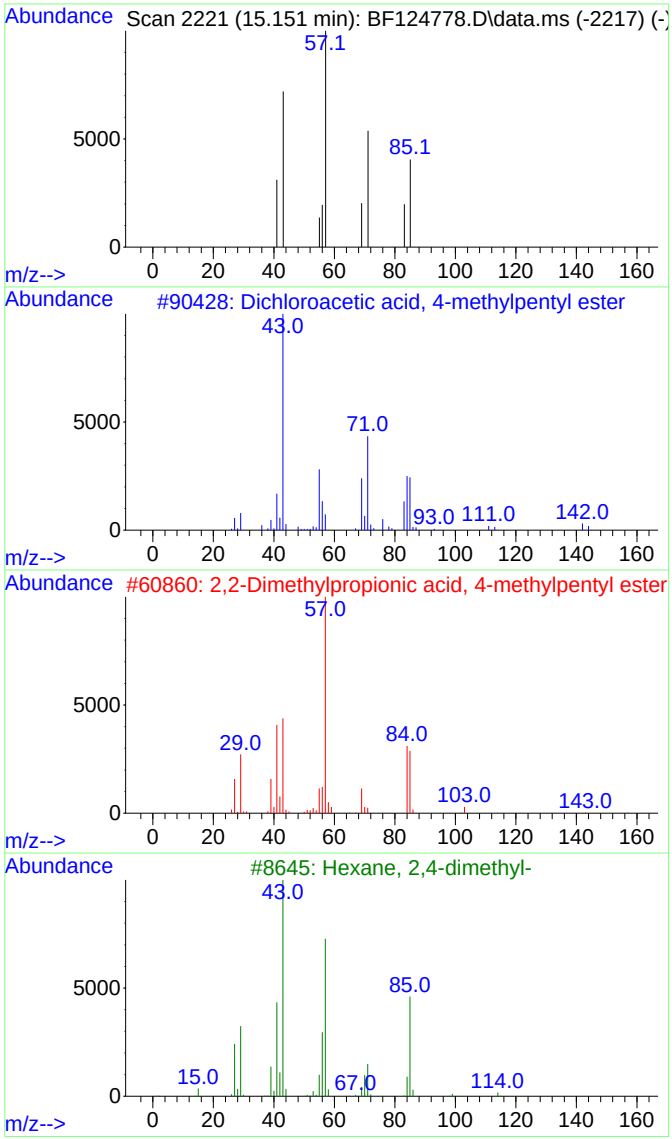
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

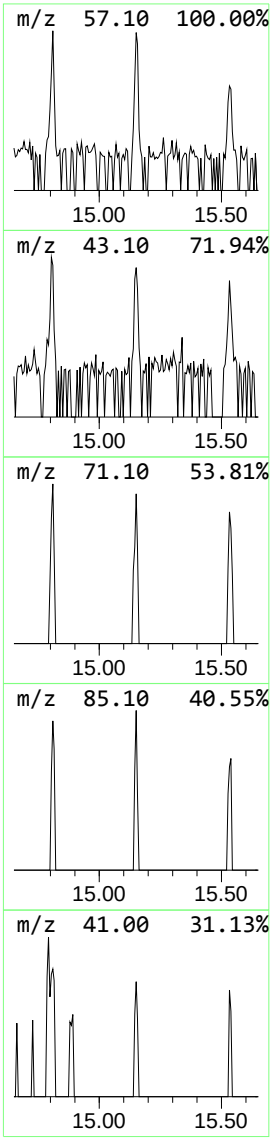
****

Peak Number 10 unknown15.151 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	5.00 ng	6692	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	9
2	2,2-Dimethylpropionic acid, 4-me...	186	C11H22O2	150588-62-8	9
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	9
4	Oxalic acid, isohexyl propyl ester	216	C11H20O4	1000309-32-6	9
5	Cyclobutanemethanol, .alpha.-met...	100	C6H12O	007515-29-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124778.D
Acq On : 26 Jul 2021 22:39
Operator : JU/CG
Sample : M3151-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-3

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

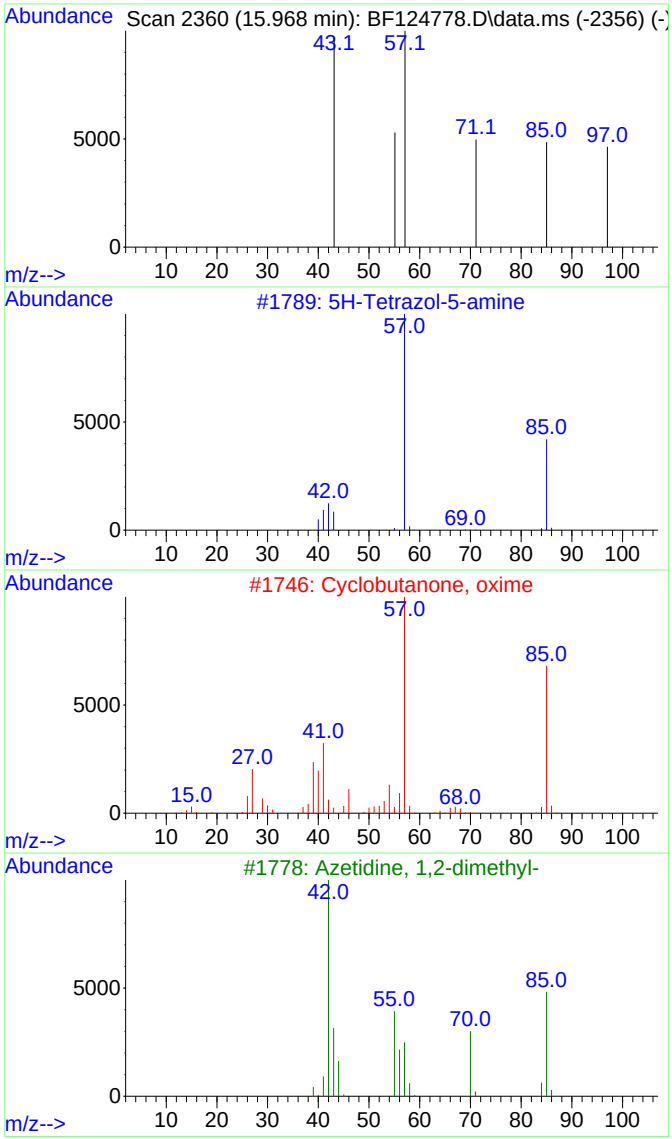
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

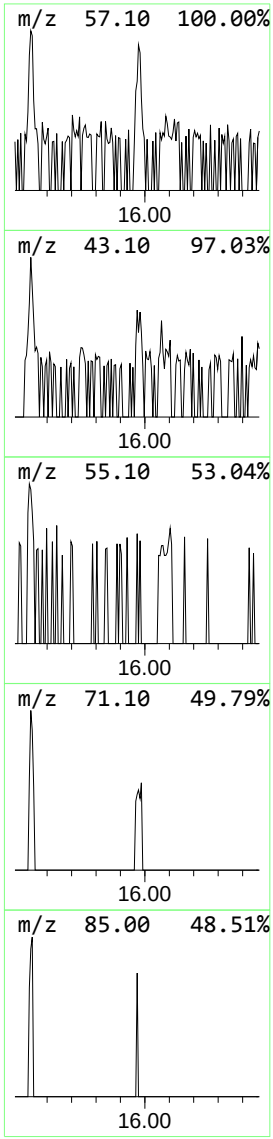
****

Peak Number 11 unknown15.968 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	3.24 ng	4340	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
2	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
3	Azetidine, 1,2-dimethyl-	85	C5H11N	051764-32-0	4
4	Oxirane, 2-methyl-3-propyl-, cis-	100	C6H12O	006124-90-9	4
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124778.D
Acq On : 26 Jul 2021 22:39
Operator : JU/CG
Sample : M3151-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

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...	2.169	7.9	ng	10049	1	6.875	25480	20.0
unknown5.098	5.098	2.8	ng	3548	1	6.875	25480	20.0
unknown8.051	8.051	3.6	ng	5693	2	8.157	31429	20.0
unknown11.916	11.916	2.3	ng	3002	4	11.398	26146	20.0
unknown13.880	13.880	8.4	ng	10845	5	14.039	25955	20.0
unknown14.198	14.198	3.6	ng	4730	5	14.039	25955	20.0
unknown14.498	14.498	4.5	ng	5785	5	14.039	25955	20.0
unknown14.792	14.792	4.1	ng	5521	6	15.515	26791	20.0
unknown14.810	14.810	4.0	ng	5379	6	15.515	26791	20.0
unknown15.151	15.151	5.0	ng	6692	6	15.515	26791	20.0
unknown15.968	15.968	3.2	ng	4340	6	15.515	26791	20.0