LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124792.D
Acq On : 27 Jul 2021 13:47
Operator : JU/CG
Sample : M3175-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-03-025-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-BF072221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124792.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	7	11	14	rBB	8648	9928	5.59%	0.896%
2	5.093	507	511	514	rBB	2344	2919	1.64%	0.263%
3	5.487	574	578	581	rBV	116115	104328	58.72%	9.415%
4	6.498	745	750	753	rBV	115886	108803	61.24%	9.819%
5	6.869	811	813	816	rBB	33826	27465	15.46%	2.479%
6	7.434	905	909	912	rBB	90308	72191	40.63%	6.515%
7	8.057	1013	1015	1021	rBB	6898	8048	4.53%	0.726%
8	8.151	1028	1031	1035	rBB	45247	38455	21.65%	3.470%
9	9.228	1210	1214	1217	rBV	178847	145575	81.94%	13.137%
10	9.910	1327	1330	1333	rBB	59179	46291	26.06%	4.177%
11	10.698	1460	1464	1467	rBV	108457	85860	48.33%	7.748%
12	11.398	1580	1583	1586	rBB	65041	49914	28.10%	4.504%
13	11.916	1663	1671	1680	rVB	31304	42498	23.92%	3.835%
14	12.698	1795	1804	1815	rBV2	47868	71604	40.30%	6.462%
15	12.986	1848	1853	1856	rBV	208422	177660	100.00%	16.033%
16	13.592	1952	1956	1961	rBB2	2695	4022	2.26%	0.363%
17	13.910	2007	2010	2011	rBV	3861	4315	2.43%	0.389%
18	14.033	2028	2031	2035	rBB	42936	39623	22.30%	3.576%
19	14.227	2060	2064	2068	rBB2	4107	6042	3.40%	0.545%
20	14.763	2149	2155	2160	rBV	5361	8160	4.59%	0.736%
21	14.880	2173	2175	2179	rBB	3941	4129	2.32%	0.373%
22	15.333	2249	2252	2259	rBB2	3528	6296	3.54%	0.568%
23	15.510	2278	2282	2287	rBB	28545	33592	18.91%	3.031%
24	15.974	2357	2361	2370	rBB2	2009	5411	3.05%	0.488%
25	16.492	2447	2449	2458	rVB	1342	2289	1.29%	0.207%
26	16.751	2487	2493	2496	rBV2	1526	2699	1.52%	0.244%

Sum of corrected areas: 1108117

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
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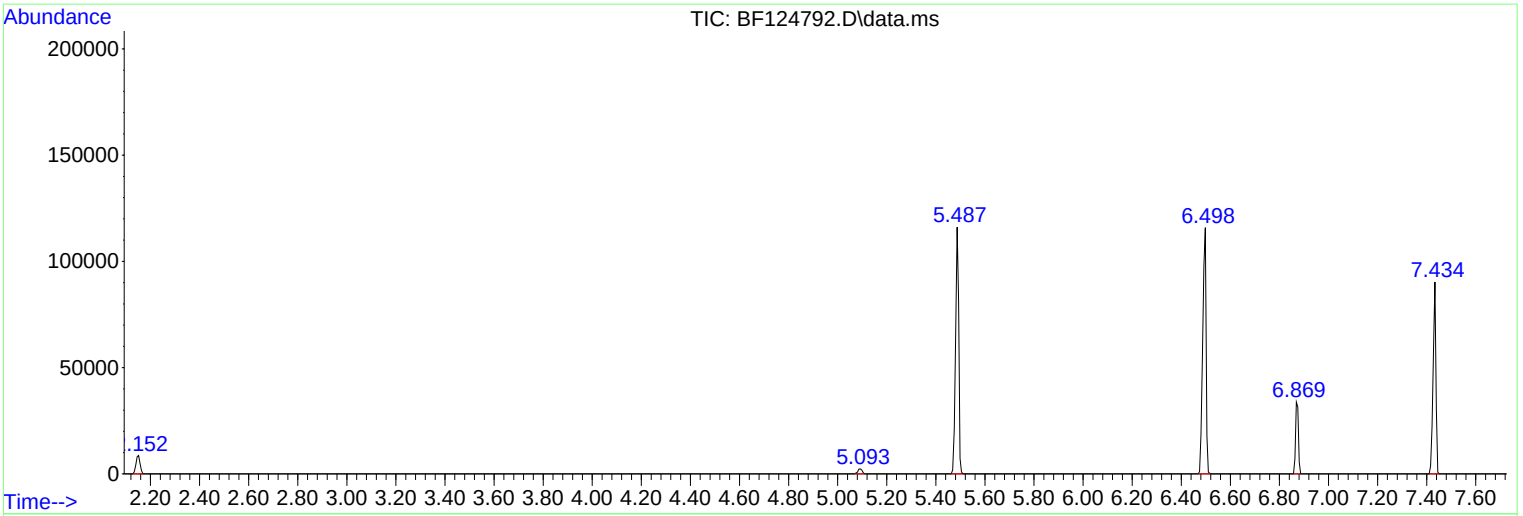
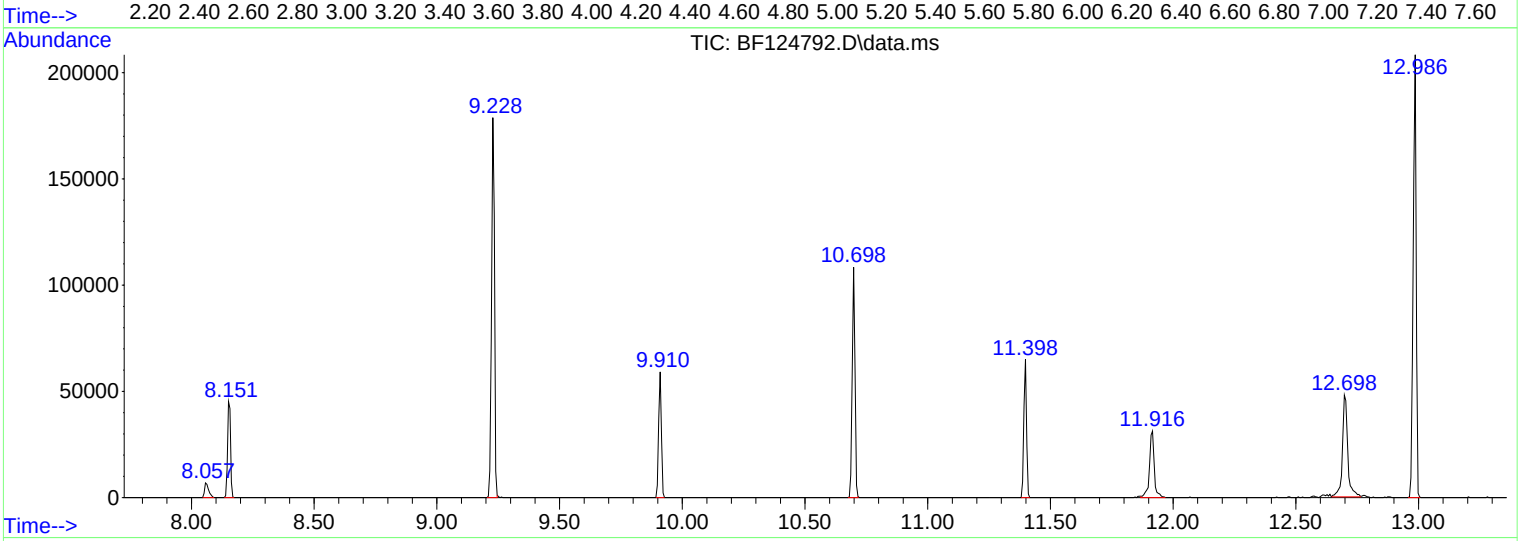
Misc :
ALS Vial : 9 Sample Multiplier: 1

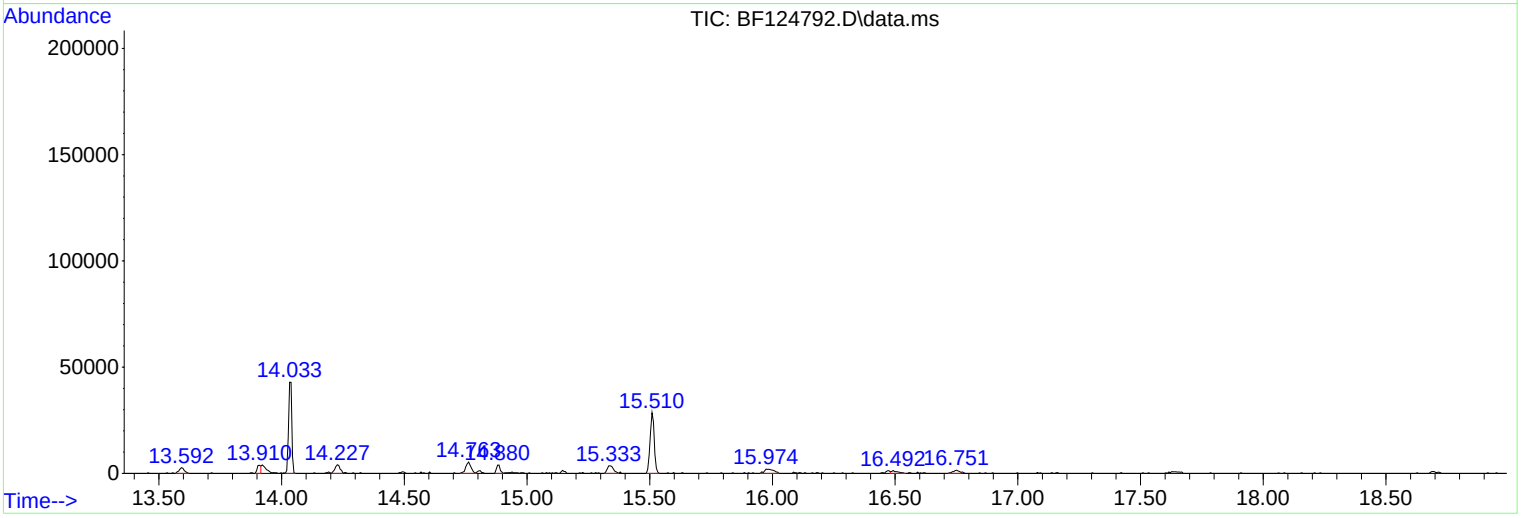
Instrument :
BNA_F
ClientSampleId :
FK-BPM-03-025-ABCD

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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BNA_F
ClientSampleId :
FK-BPM-03-025-ABCD

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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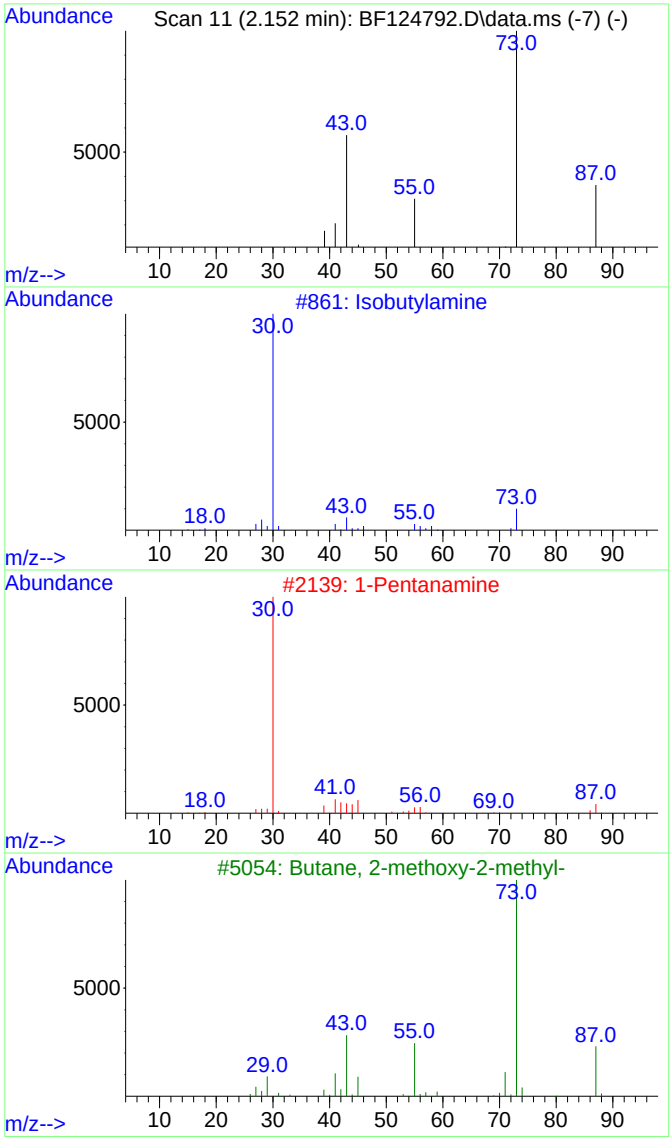
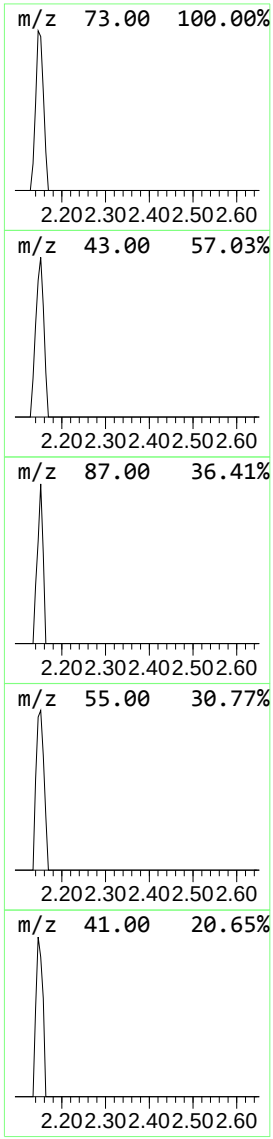
Peak Number 1 unknown2.152 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	7.23 ng	9928	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutylamine	73	C4H11N	000078-81-9	7
2	1-Pentanamine	87	C5H13N	000110-58-7	4
3	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	4
4	2-Pentanol, acetate	130	C7H14O2	000626-38-0	4
5	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124792.D
Acq On : 27 Jul 2021 13:47
Operator : JU/CG
Sample : M3175-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-03-025-ABCD

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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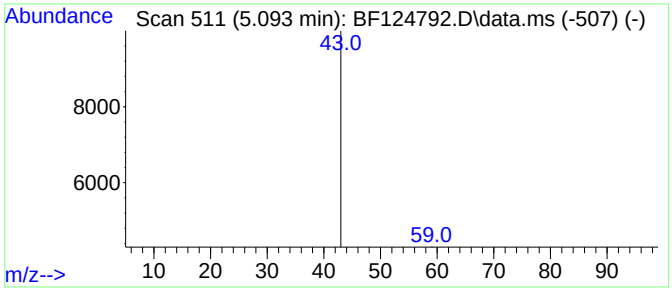
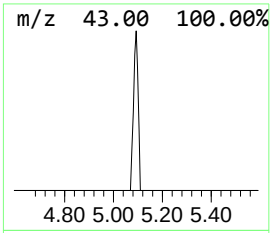
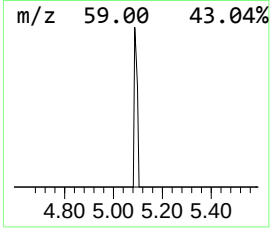
Peak Number 2 unknown5.093 Concentration Rank 11

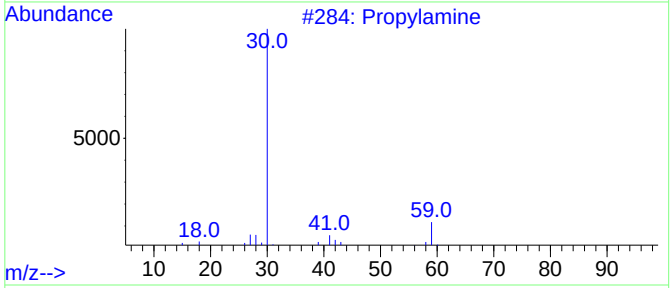
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.13 ng	2919	1,4-Dichlorobenzene-d4	6.875

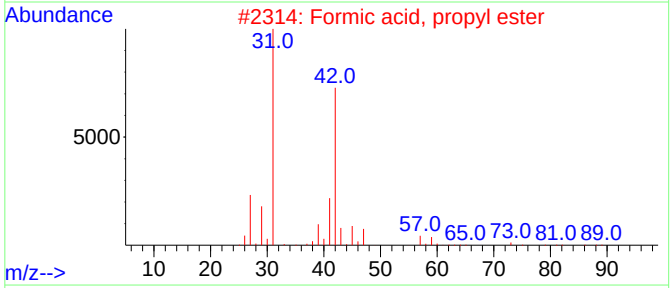
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylamine	59	C3H9N	000107-10-8	1
2	Formic acid, propyl ester	88	C4H8O2	000110-74-7	1
3	Oxirane, (ethoxymethyl)-	102	C5H10O2	004016-11-9	1
4	tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	1
5	Guanidine carbonate	180	C3H12N6O3	000593-85-1	1

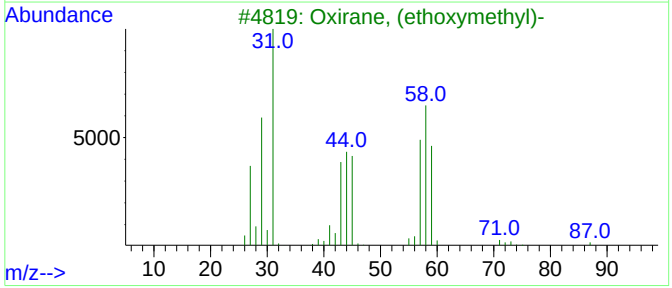












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Sample : M3175-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-03-025-ABCD

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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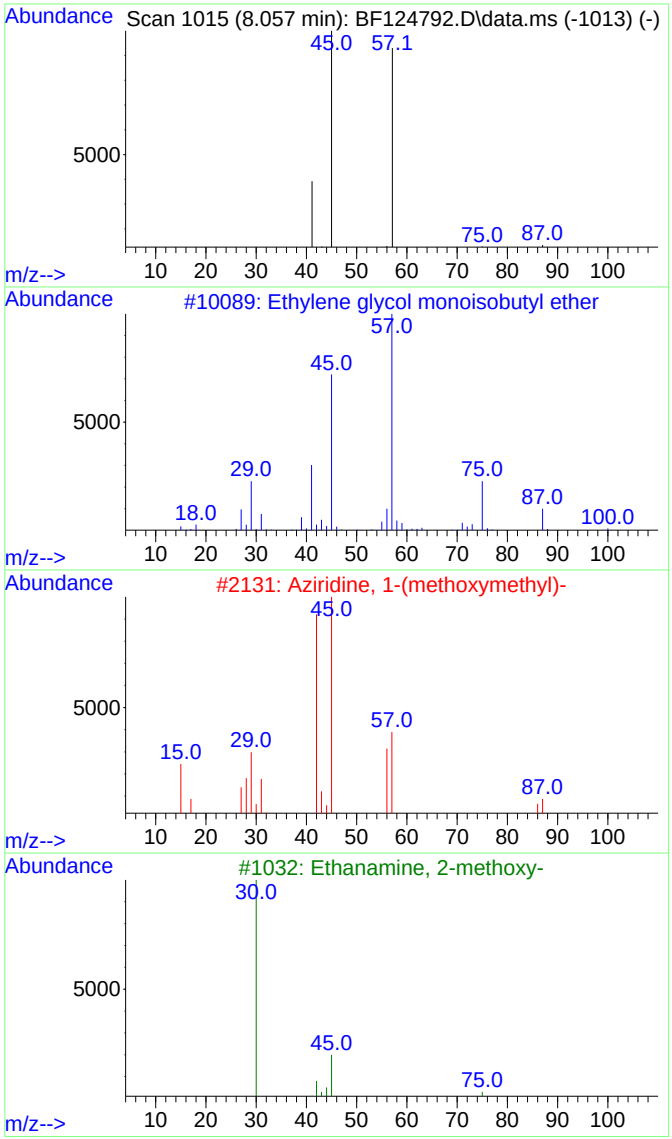
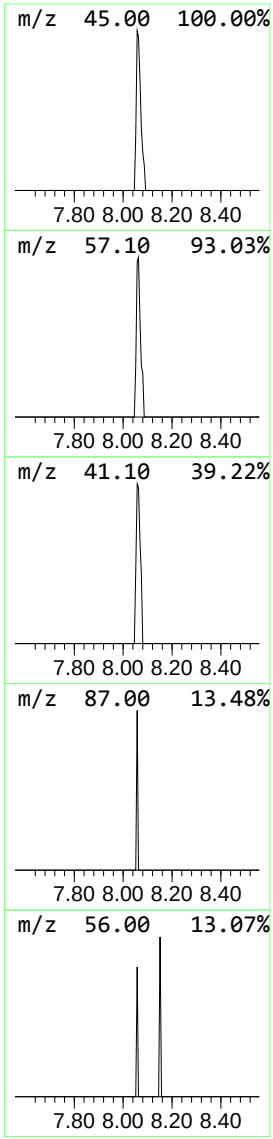
Peak Number 3 unknown8.057 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.057	4.19 ng	8048	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	9
2	Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	5
3	Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	4
5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	4





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Acq On : 27 Jul 2021 13:47
Operator : JU/CG
Sample : M3175-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-03-025-ABCD

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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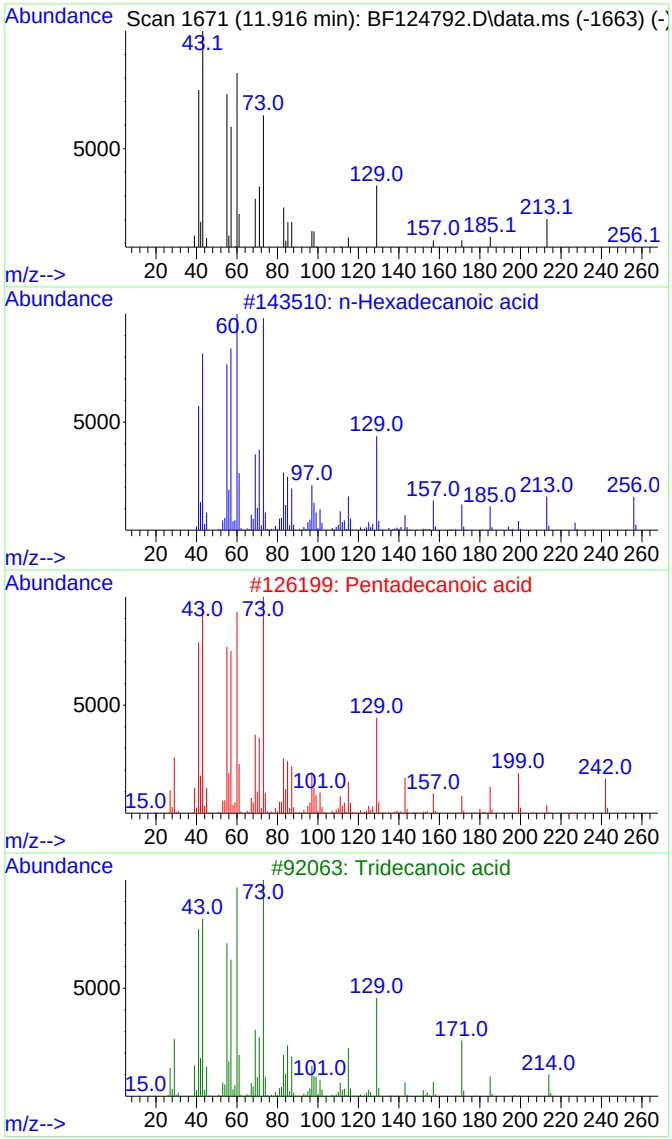
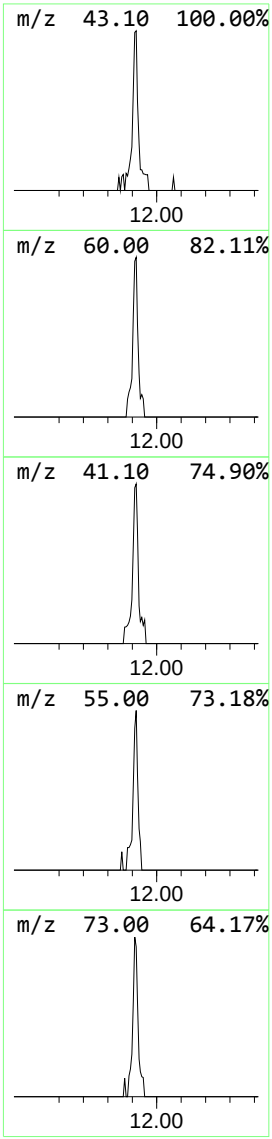
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	17.03 ng	42498	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
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Operator : JU/CG
Sample : M3175-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-03-025-ABCD

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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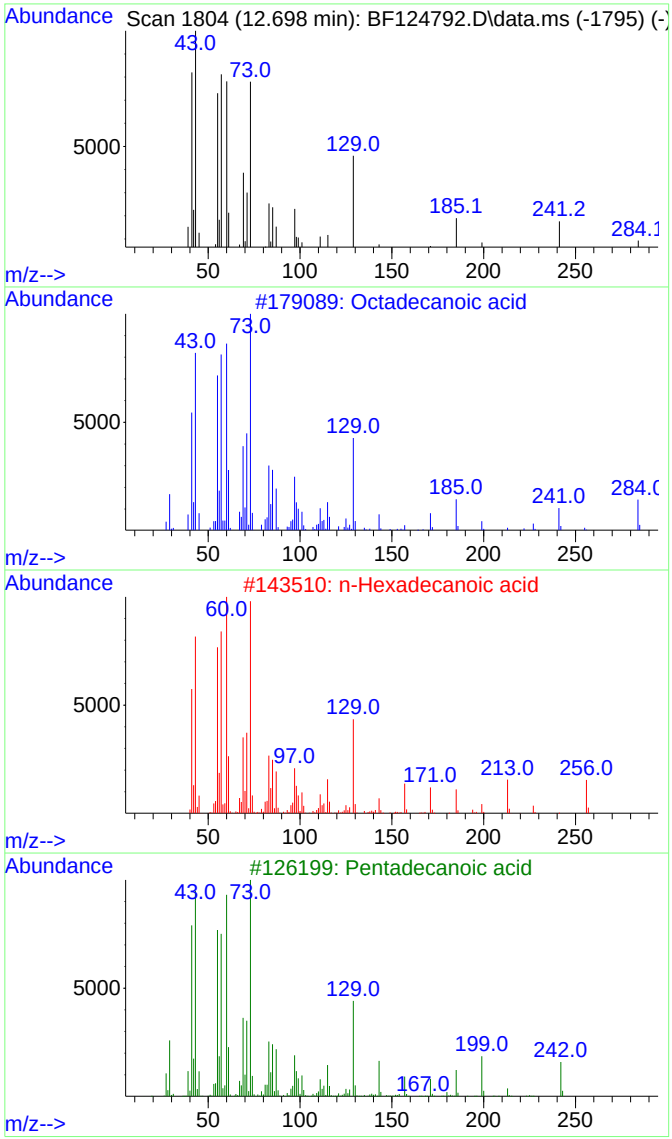
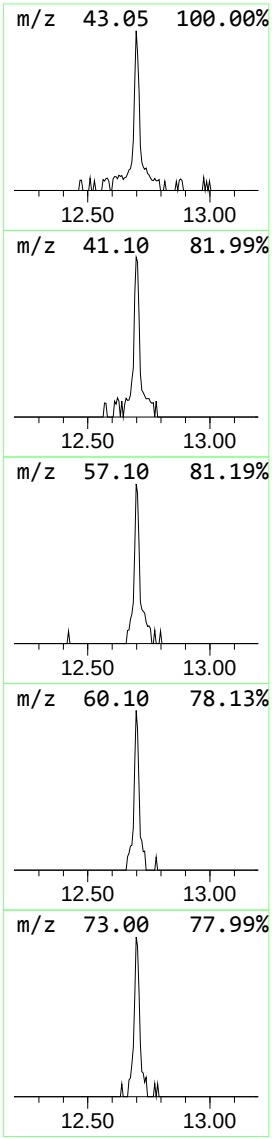
Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	28.69 ng	71604	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





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TIC Library : C:\Database\NIST20.L
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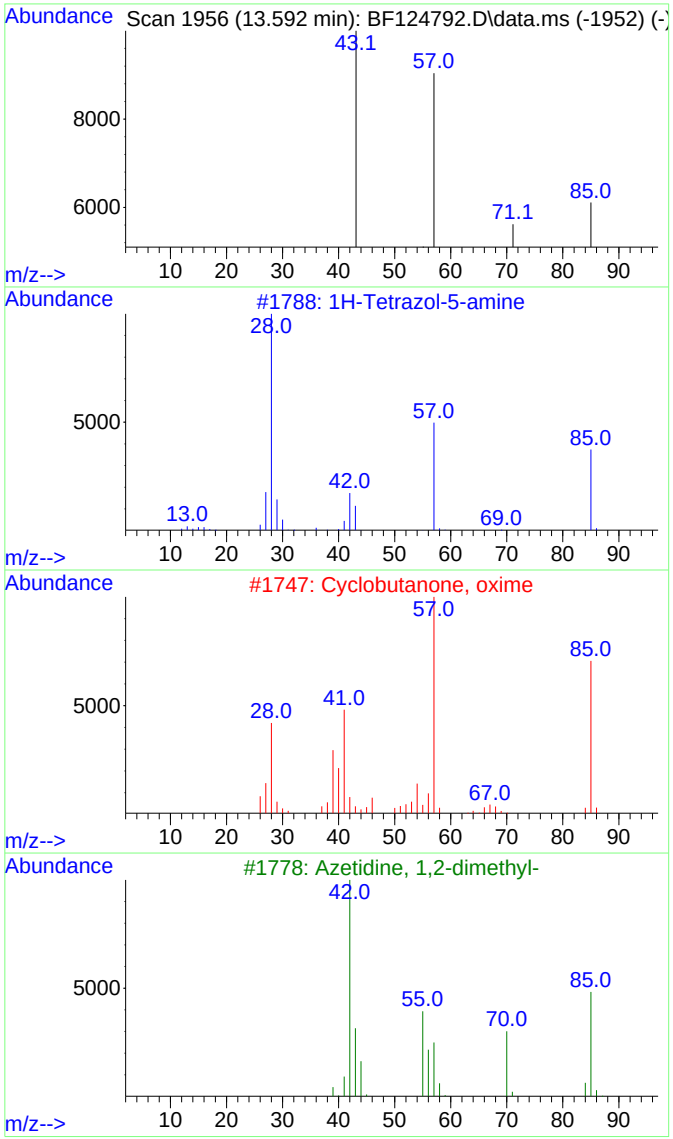
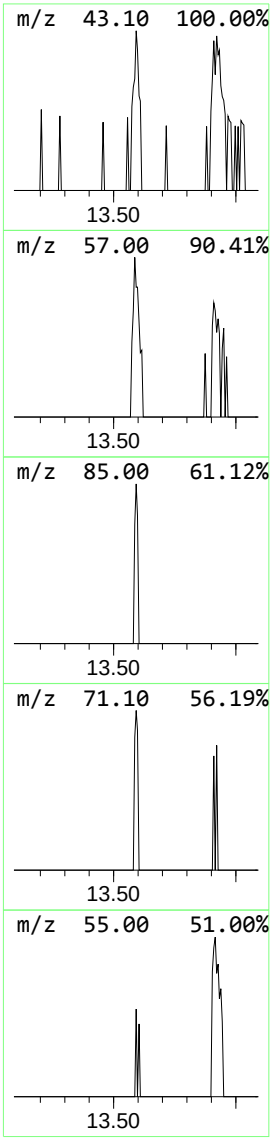
Peak Number 6 unknown13.592 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.592	2.03 ng	4022	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	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





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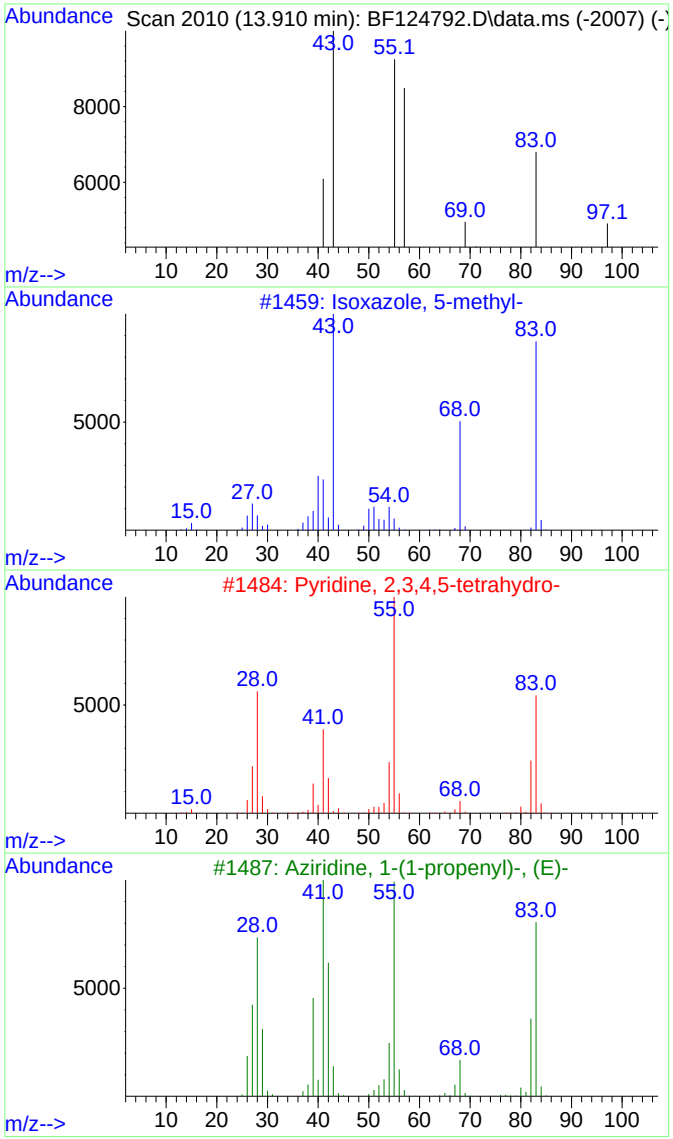
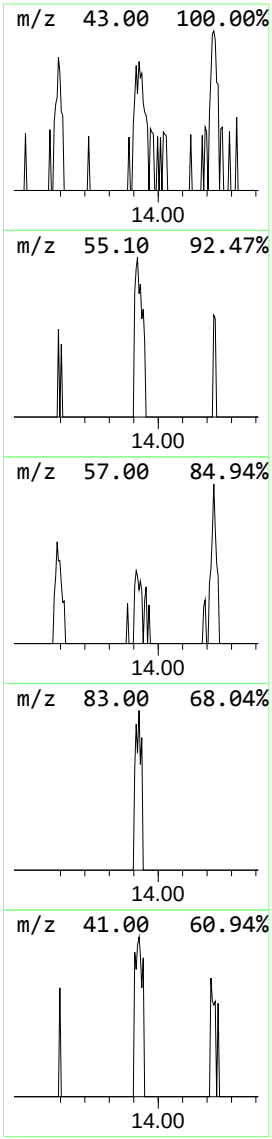
Peak Number 7 unknown13.910 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	2.18 ng	4315	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	4
2	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	4
3	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	4
4	Oxalic acid, cyclobutyl octyl ester	256	C14H24O4	1000309-69-9	2
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	2





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BNA_F
ClientSampleId :
FK-BPM-03-025-ABCD

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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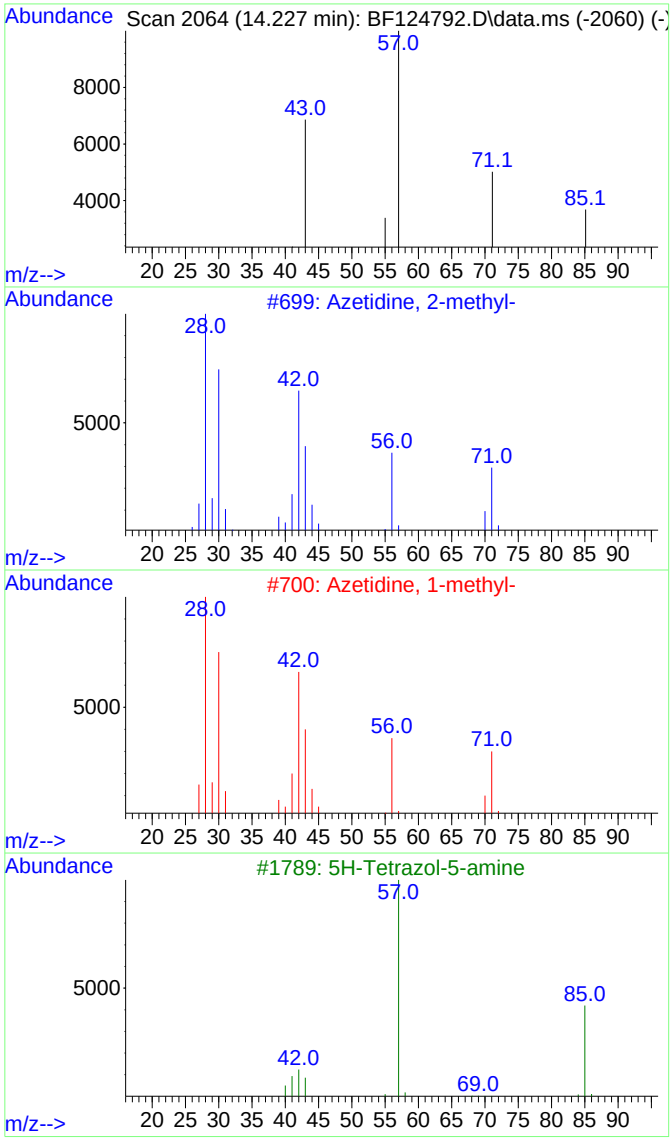
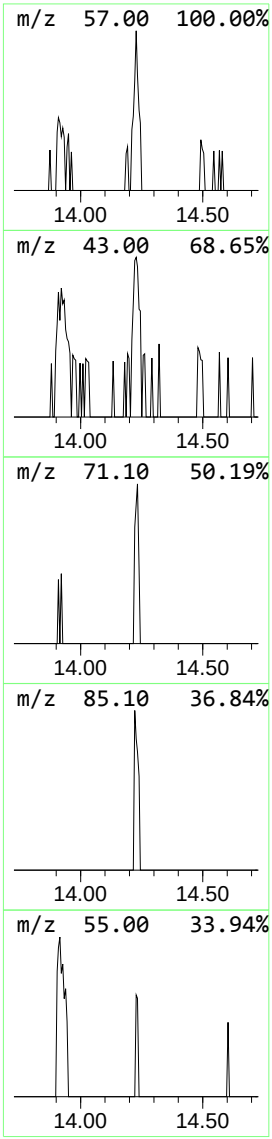
Peak Number 8 unknown14.227 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.227	3.05 ng	6042	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
2	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
3	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4	2-Propenamide	71	C3H5NO	000079-06-1	4
5	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124792.D
Acq On : 27 Jul 2021 13:47
Operator : JU/CG
Sample : M3175-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-BPM-03-025-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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TIC Library : C:\Database\NIST20.L
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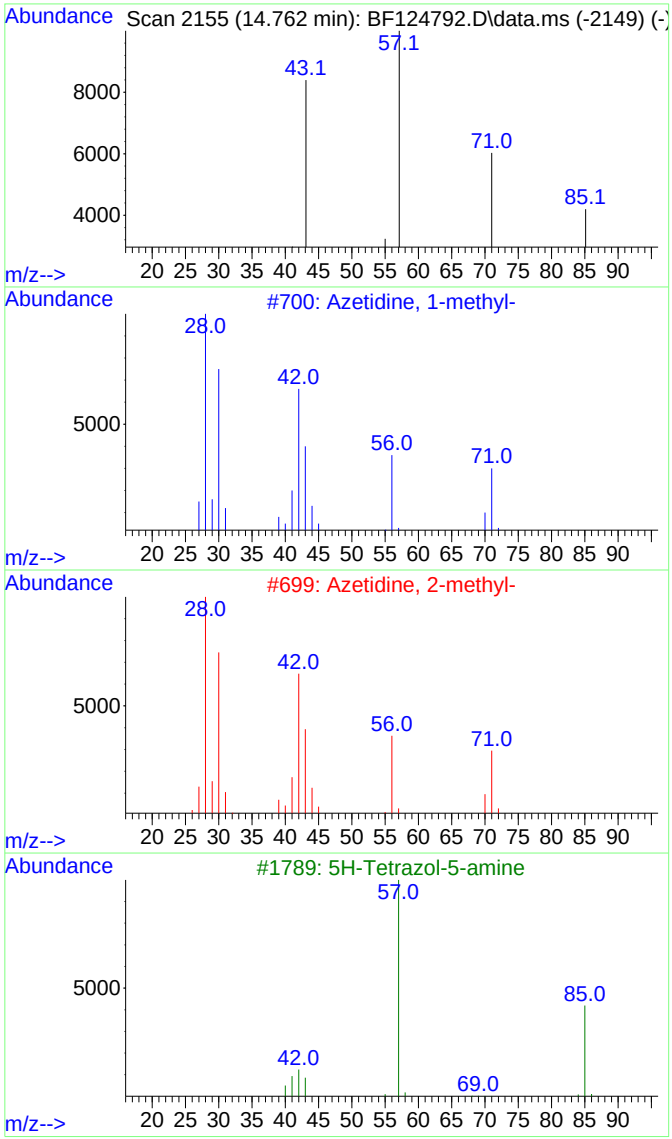
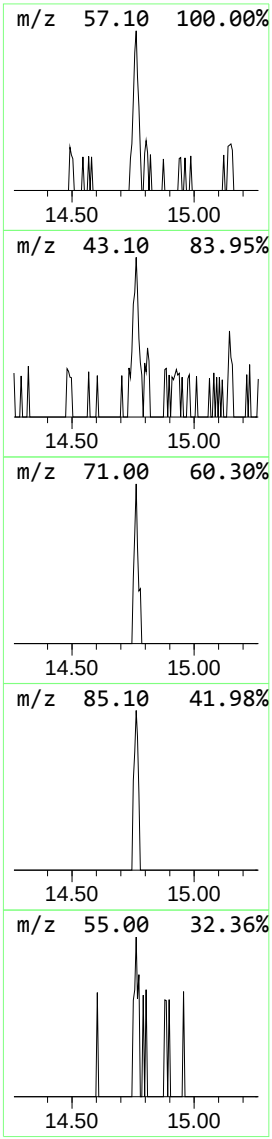
Peak Number 9 unknown14.762 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.762	4.12 ng	8160	Chrysene-d12	14.039

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	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4	2-Propenamide	71	C3H5NO	000079-06-1	4
5	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4





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Data File : BF124792.D
Acq On : 27 Jul 2021 13:47
Operator : JU/CG
Sample : M3175-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-BPM-03-025-ABCD

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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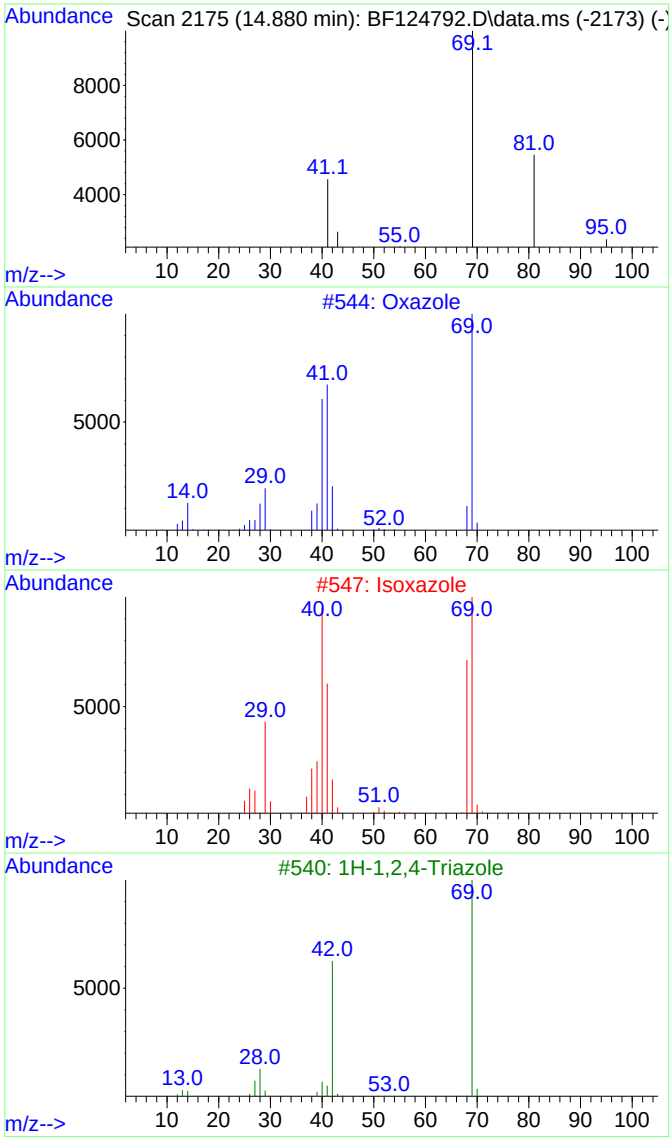
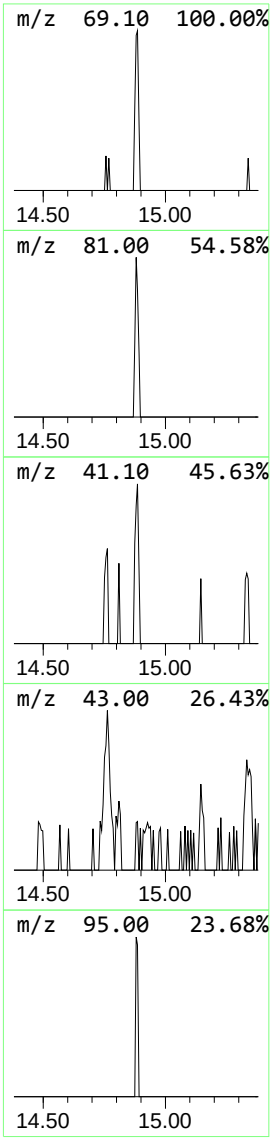
Peak Number 10 unknown14.880 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	2.46 ng	4129	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazole	69	C3H3NO	000288-42-6	4
2	Isoxazole	69	C3H3NO	000288-14-2	4
3	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	2
4	1H-1,2,3-Triazole	69	C2H3N3	000288-36-8	2
5	2-Propynenitrile, 3-fluoro-	69	C3FN	032038-83-8	2





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Data File : BF124792.D
Acq On : 27 Jul 2021 13:47
Operator : JU/CG
Sample : M3175-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-BPM-03-025-ABCD

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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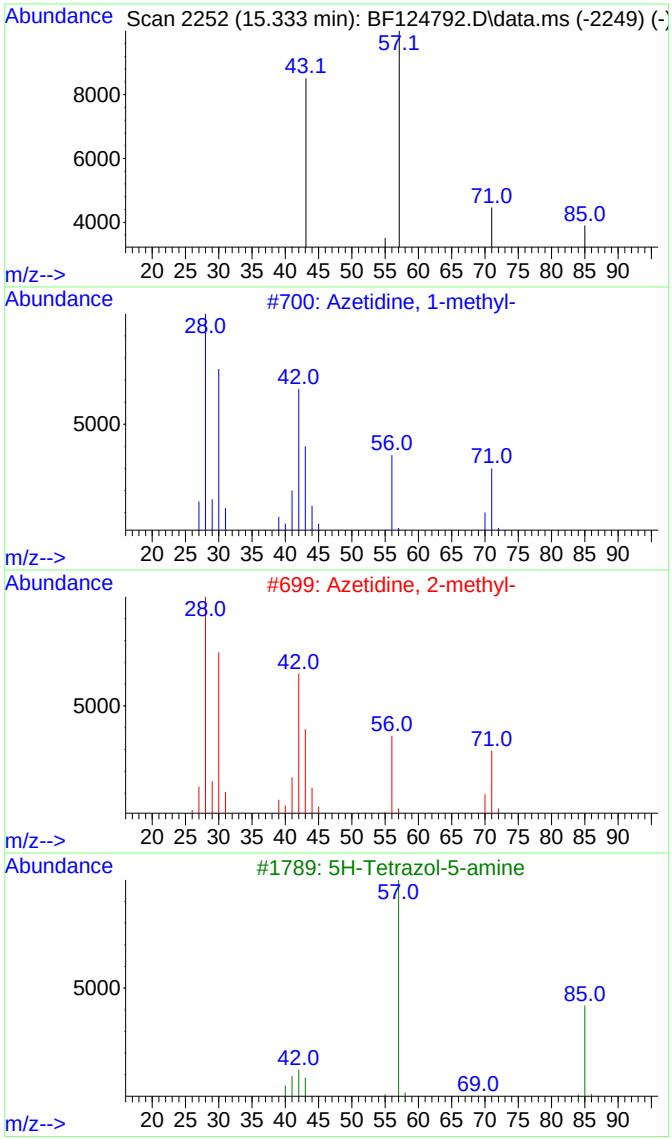
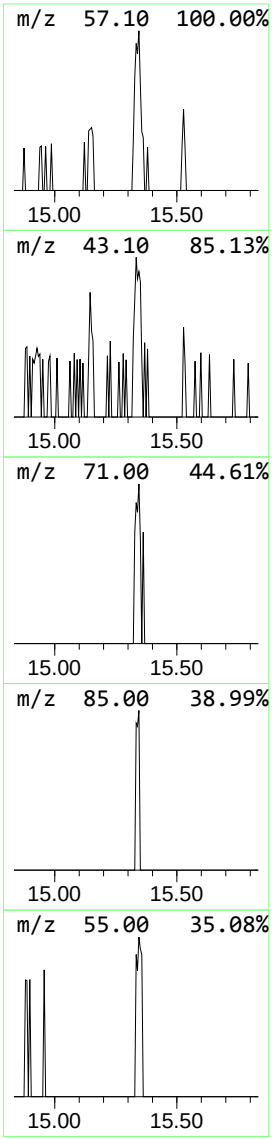
Peak Number 11 unknown15.333 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	3.75 ng	6296	Perylene-d12	15.509

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	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124792.D
Acq On : 27 Jul 2021 13:47
Operator : JU/CG
Sample : M3175-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-BPM-03-025-ABCD

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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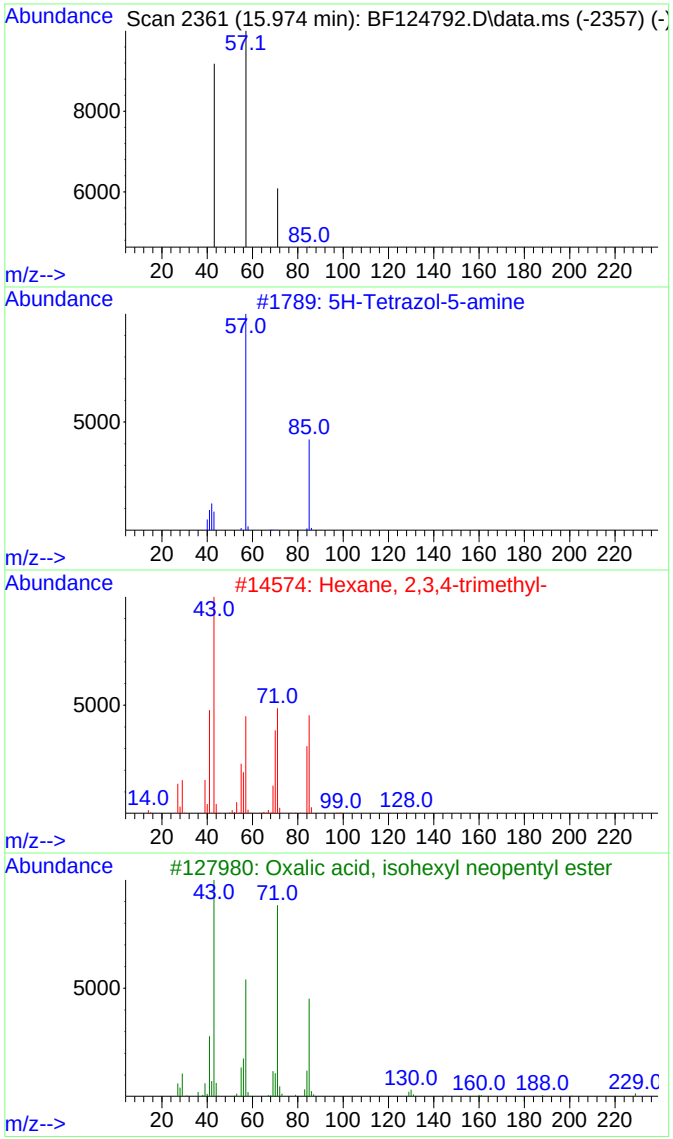
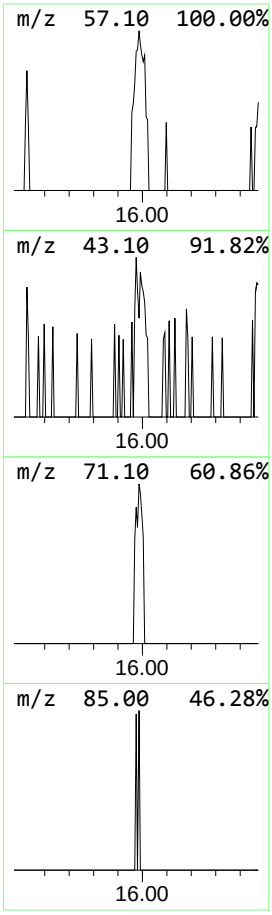
Peak Number 12 unknown15.974 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	3.22 ng	5411	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	4
3	Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	4
4	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3
5	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124792.D
Acq On : 27 Jul 2021 13:47
Operator : JU/CG
Sample : M3175-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-03-025-ABCD

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
unknown2.152	2.152	7.2	ng	9928	1	6.875	27465	20.0
unknown5.093	5.093	2.1	ng	2919	1	6.875	27465	20.0
unknown8.057	8.057	4.2	ng	8048	2	8.151	38455	20.0
n-Hexadecanoic ...	11.916	17.0	ng	42498	4	11.398	49914	20.0
Octadecanoic acid	12.698	28.7	ng	71604	4	11.398	49914	20.0
unknown13.592	13.592	2.0	ng	4022	5	14.039	39623	20.0
unknown13.910	13.910	2.2	ng	4315	5	14.039	39623	20.0
unknown14.227	14.227	3.0	ng	6042	5	14.039	39623	20.0
unknown14.762	14.762	4.1	ng	8160	5	14.039	39623	20.0
unknown14.880	14.880	2.5	ng	4129	6	15.509	33592	20.0
unknown15.333	15.333	3.8	ng	6296	6	15.509	33592	20.0
unknown15.974	15.974	3.2	ng	5411	6	15.509	33592	20.0