LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210539-COM-12

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: BF124830.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	11	rBB	6709	7432	5.29%	0.739%
2	5.087	507	510	514	rBB	1653	1934	1.38%	0.192%
3	5.487	574	578	581	rBV	126775	109964	78.33%	10.932%
4	6.498	745	750	752	rBV	114076	115593	82.34%	11.491%
5	6.869	811	813	816	rBB	39861	29094	20.73%	2.892%
6	7.433	905	909	911	rBB	90969	74194	52.85%	7.376%
7	8.051	1012	1014	1020	rBB	4816	5872	4.18%	0.584%
8	8.151	1028	1031	1034	rBV	51172	38683	27.56%	3.846%
9	9.227	1210	1214	1217	rBV	180704	134054	95.49%	13.327%
10	9.910	1327	1330	1333	rBB	58326	47322	33.71%	4.704%
11	10.698	1460	1464	1467	rBV	118910	98983	70.51%	9.840%
12	11.392	1579	1582	1586	rBB	61008	51411	36.62%	5.111%
13	11.916	1667	1671	1675	rBB	17255	15335	10.92%	1.524%
14	12.698	1800	1804	1808	rBB	12175	13046	9.29%	1.297%
15	12.874	1830	1834	1838	rBV	2317	3242	2.31%	0.322%
16	12.980	1848	1852	1855	rBV	172873	140380	100.00%	13.956%
17	13.663	1964	1968	1973	rBB	2873	4545	3.24%	0.452%
18	13.821	1993	1995	1999	rBB	1753	1750	1.25%	0.174%
19	13.862	1999	2002	2005	rBV	2225	2529	1.80%	0.251%
20	13.898	2005	2008	2015	rVB3	11178	14647	10.43%	1.456%
21	14.033	2028	2031	2034	rBB	51748	40356	28.75%	4.012%
22	14.268	2067	2071	2075	rBB	3484	5199	3.70%	0.517%
23	14.798	2155	2161	2164	rBB4	3786	6731	4.79%	0.669%
24	14.880	2173	2175	2177	rVB	3113	2677	1.91%	0.266%
25	15.357	2252	2256	2262	rBB2	2449	4048	2.88%	0.402%
26	15.509	2277	2282	2287	rBB	28082	34183	24.35%	3.398%
27	16.009	2363	2367	2372	rBB	1506	2706	1.93%	0.269%

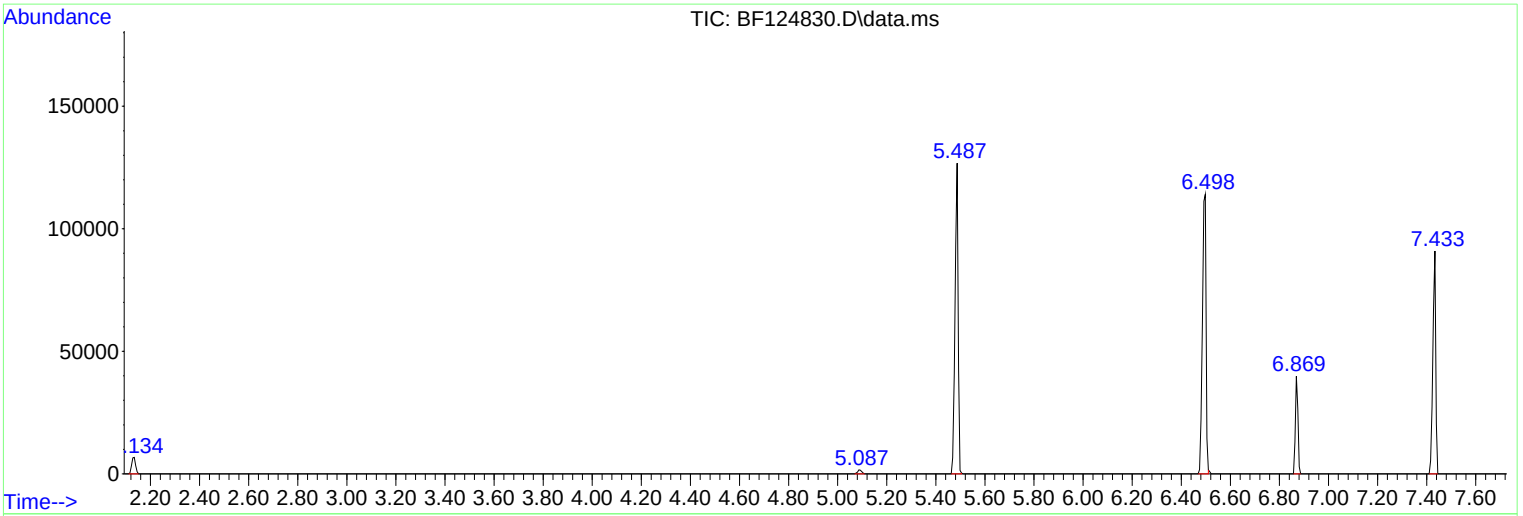
Sum of corrected areas: 1005910

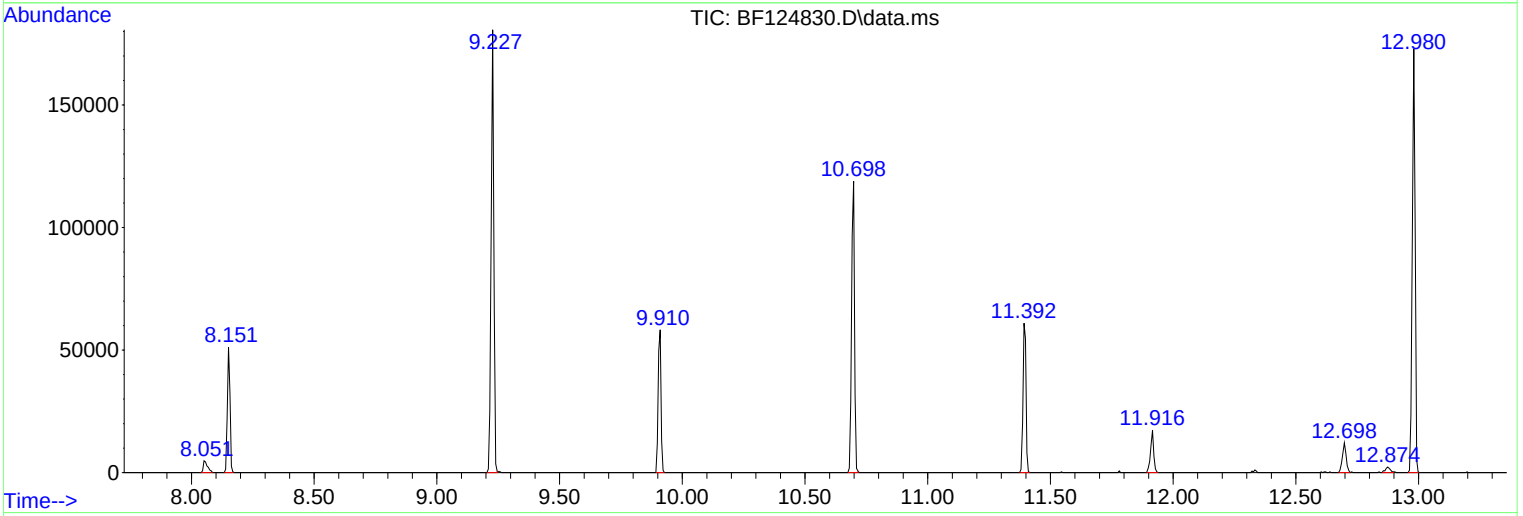
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

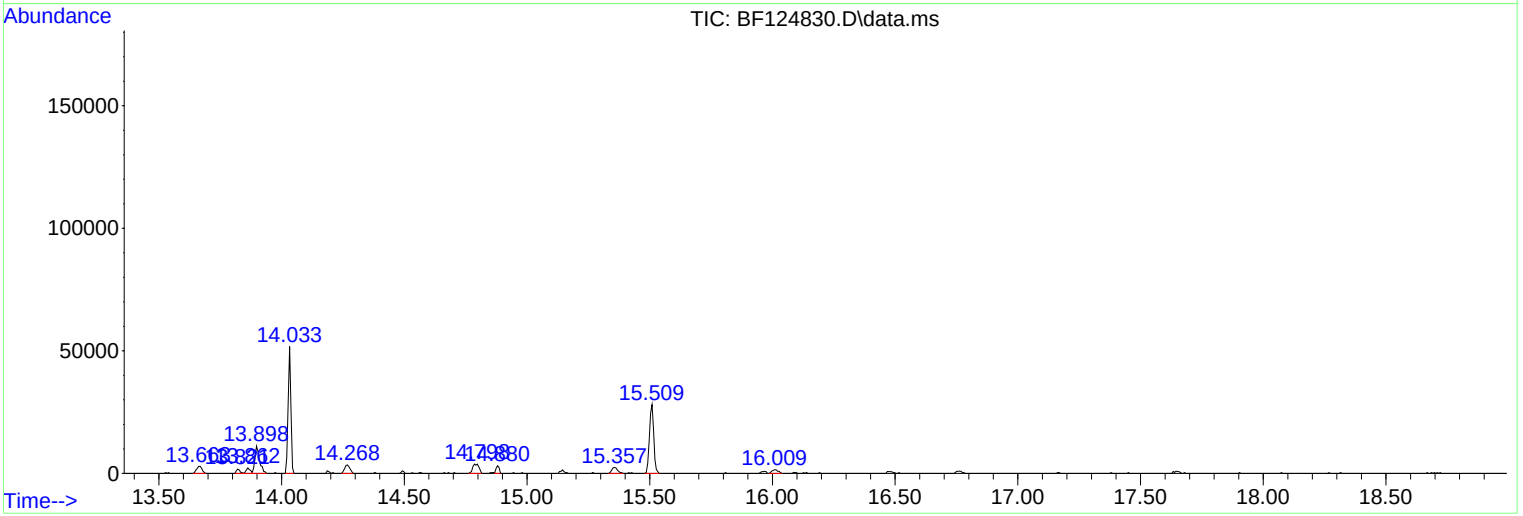
Instrument :
BNA_F
ClientSampleId :
20210539-COM-12

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210539-COM-12

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

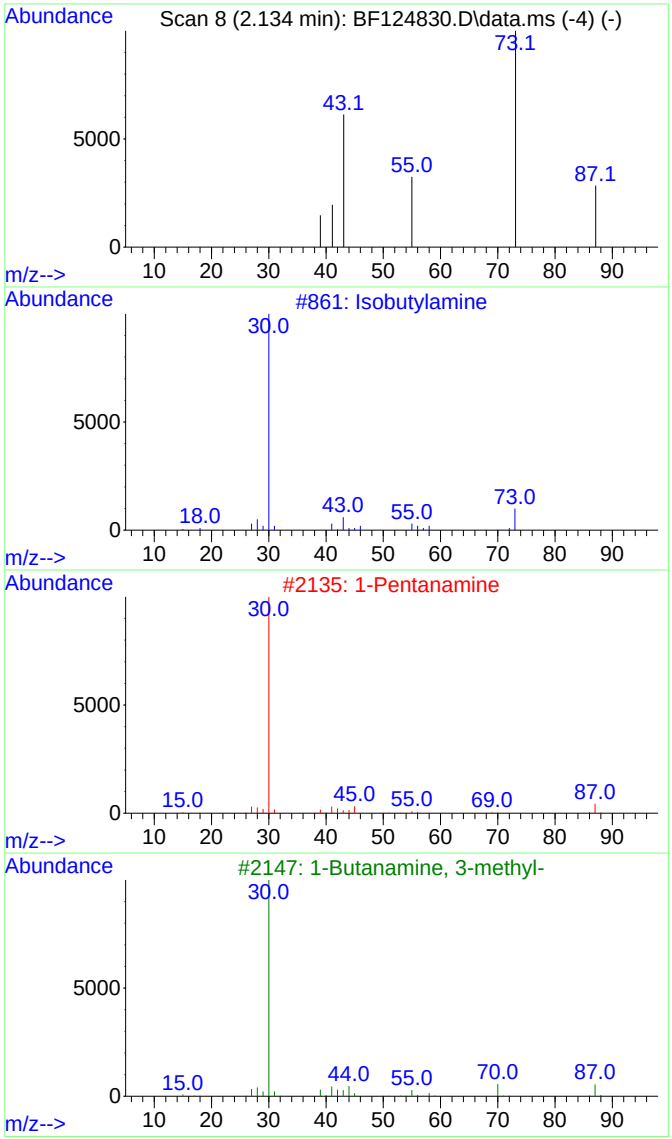
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

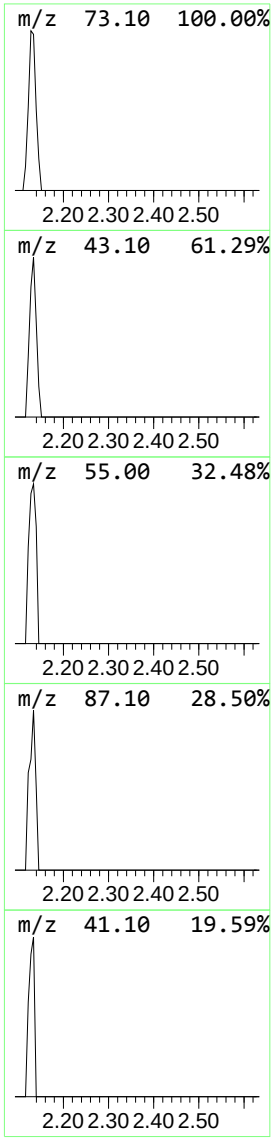
****

Peak Number 1 unknown2.134 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	5.11 ng	7432	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutylamine	73	C4H11N	000078-81-9	4
2	1-Pentanamine	87	C5H13N	000110-58-7	3
3	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	3
4	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	2
5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210539-COM-12

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

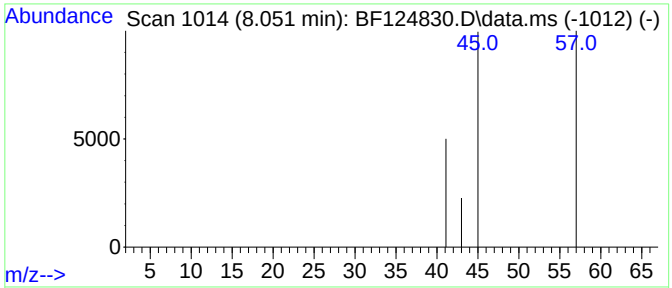
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

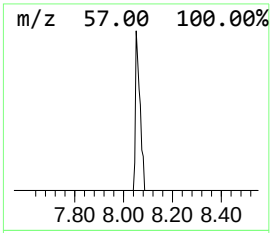
****

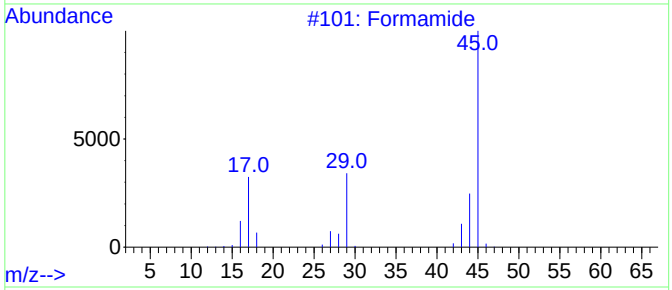
Peak Number 2 unknown8.051 Concentration Rank 6

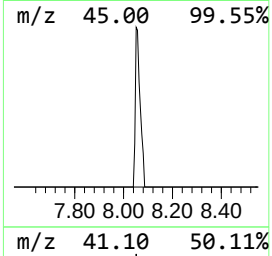
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	3.04 ng	5872	Naphthalene-d8	8.151

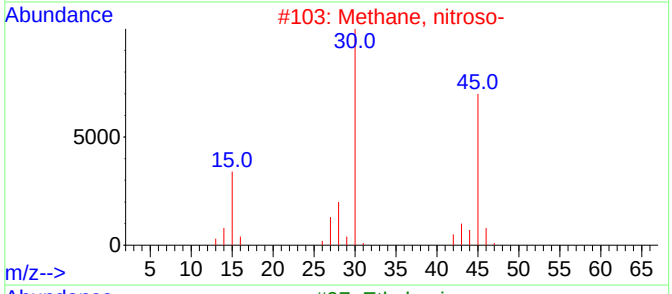
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formamide	45	CH3NO	000075-12-7	2
2	Methane, nitroso-	45	CH3NO	000865-40-7	2
3	Ethylamine	45	C2H7N	000075-04-7	1
4	Methane, isocyanato-	57	C2H3NO	000624-83-9	1
5	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	1

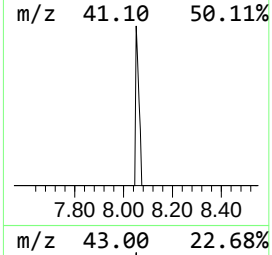


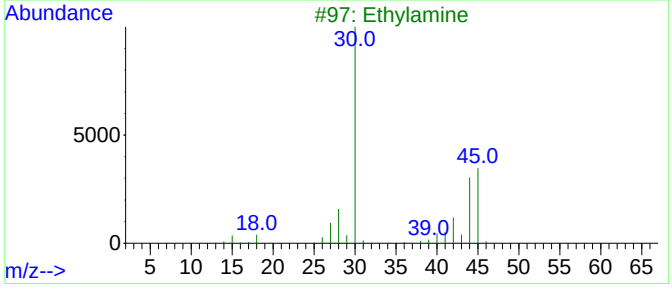


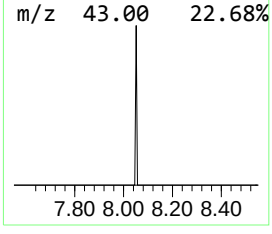












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210539-COM-12

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

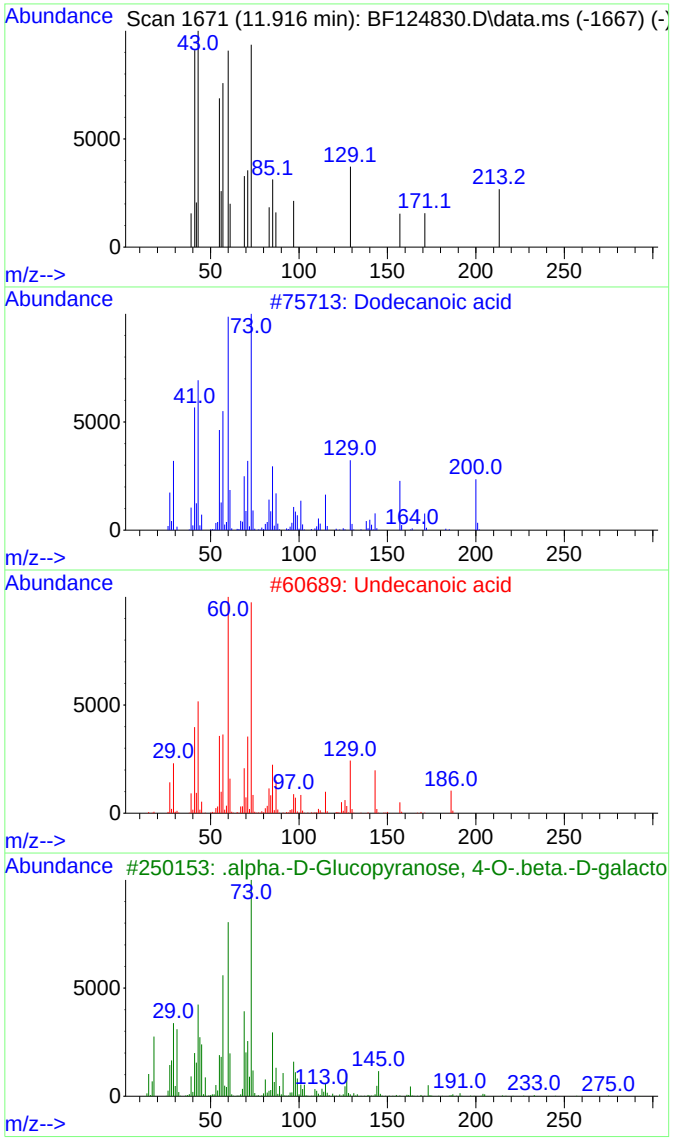
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

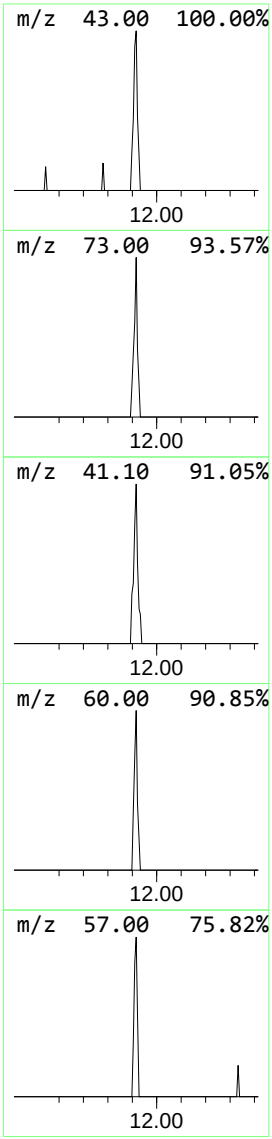
****

Peak Number 3 Dodecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	5.97 ng	15335	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	64
2	Undecanoic acid	186	C11H22O2	000112-37-8	59
3	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	53
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	Butanoic acid, 3-methyl-, 1-meth...	144	C8H16O2	032665-23-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210539-COM-12

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

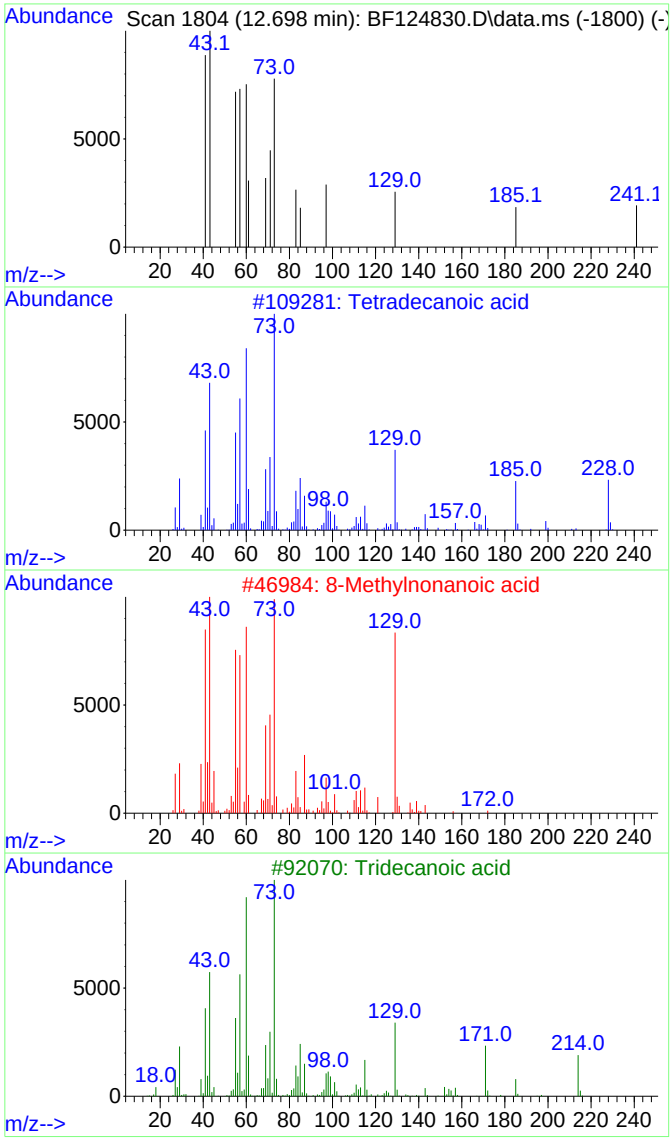
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

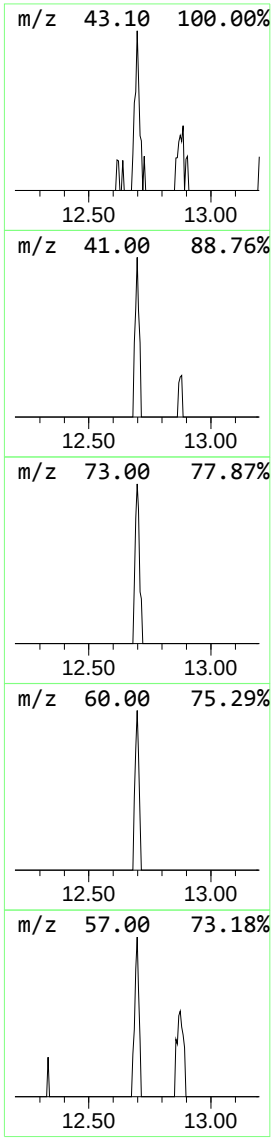
****

Peak Number 4 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	5.08 ng	13046	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
2	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53
3	Tridecanoic acid	214	C13H26O2	000638-53-9	40
4	Decanoic acid, 2,3-dihydroxyprop...	246	C13H26O4	002277-23-8	38
5	Lactose	342	C12H22O11	000063-42-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210539-COM-12

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

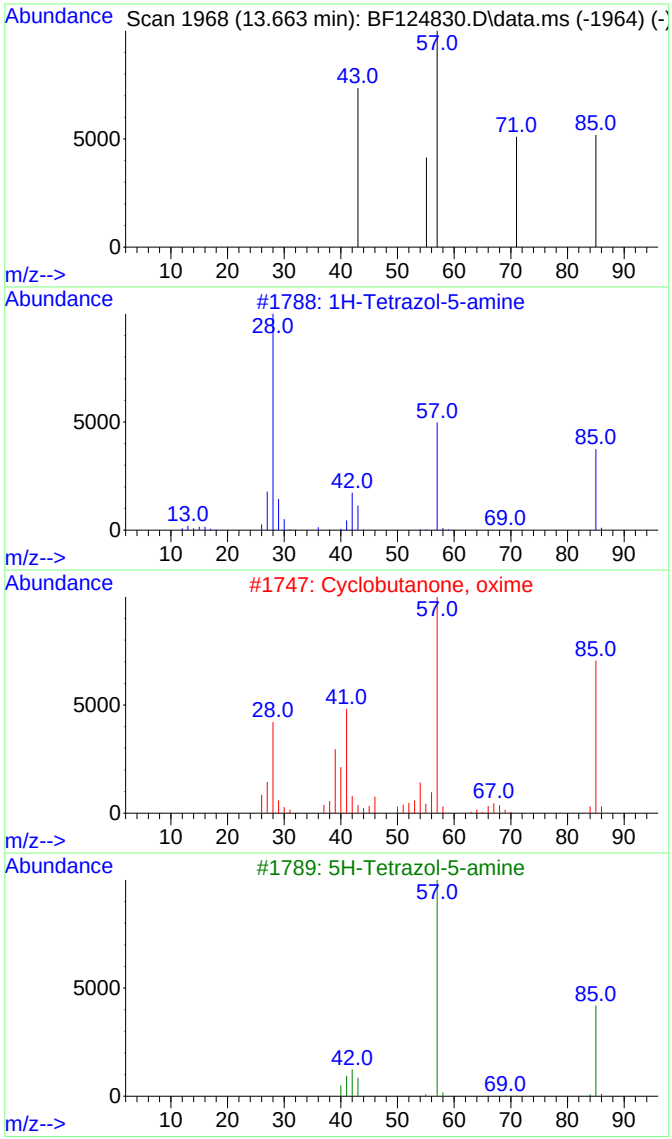
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

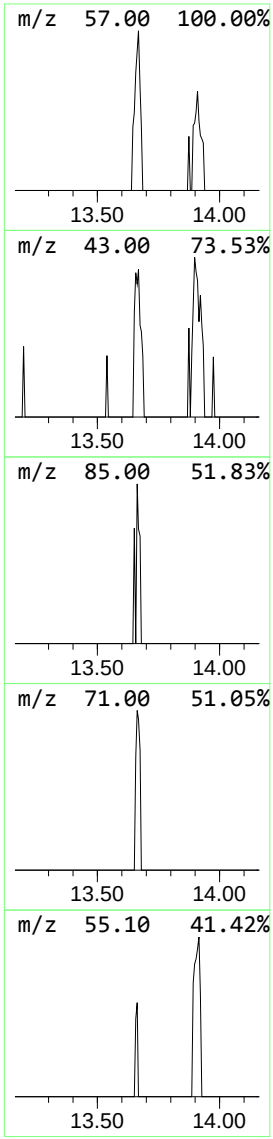
****

Peak Number 5 unknown13.663 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.663	2.25 ng	4545	Chrysene-d12	14.033

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	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4	2-Propenamide	71	C3H5NO	000079-06-1	4
5	Azetidine, 1,2-dimethyl-	85	C5H11N	051764-32-0	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210539-COM-12

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

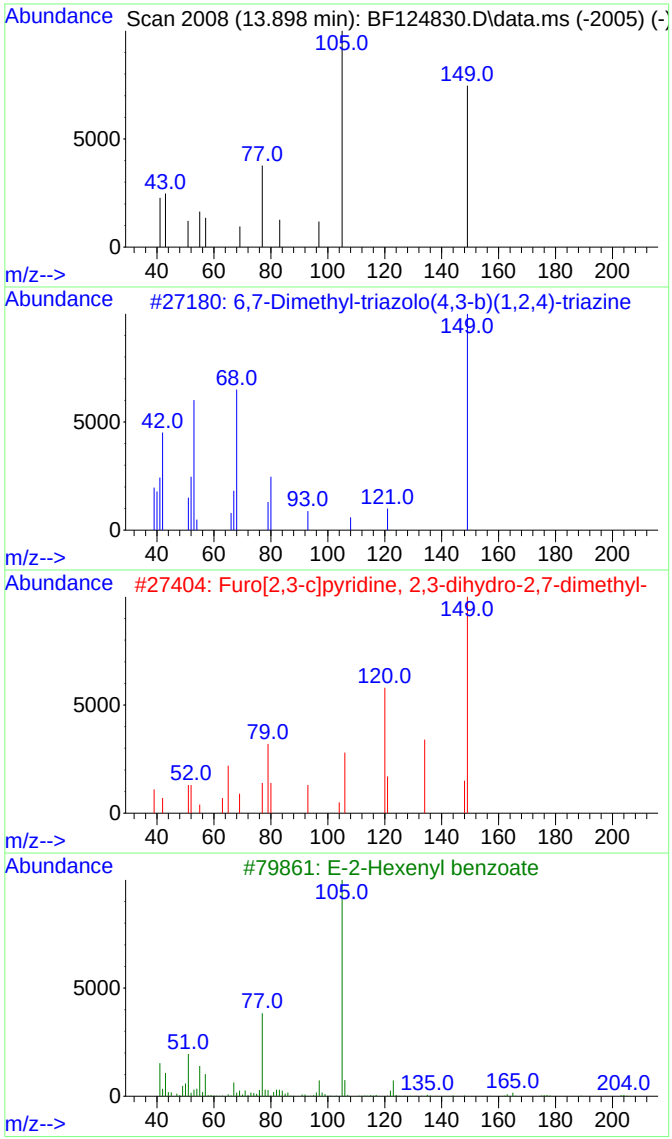
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

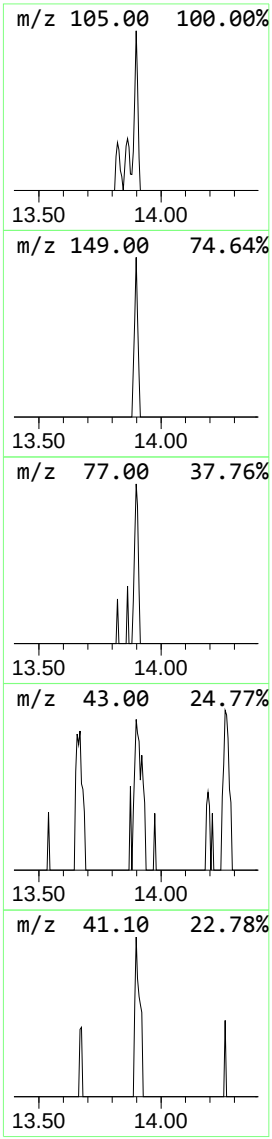
****

Peak Number 6 unknown13.898 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	7.26 ng	14647	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,7-Dimethyl-triazolo(4,3-b)(1,2...	149	C6H7N5	061139-73-9	7
2	Furo[2,3-c]pyridine, 2,3-dihydro...	149	C9H11NO	069022-82-8	7
3	E-2-Hexenyl benzoate	204	C13H16O2	076841-70-8	4
4	Valeric acid, 2-cyano-2-hydroxy-...	289	C16H19NO4	019788-61-5	4
5	N-Methylbenzamide, N-heptafluoro...	331	C12H8F7NO2	1000446-97-2	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210539-COM-12

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

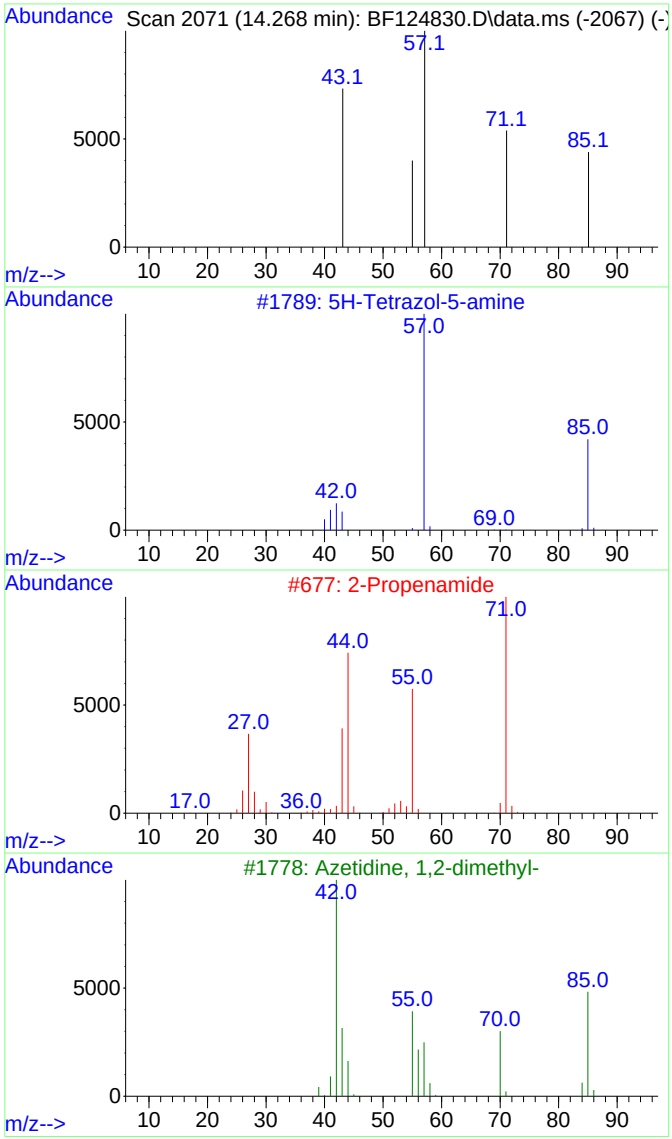
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

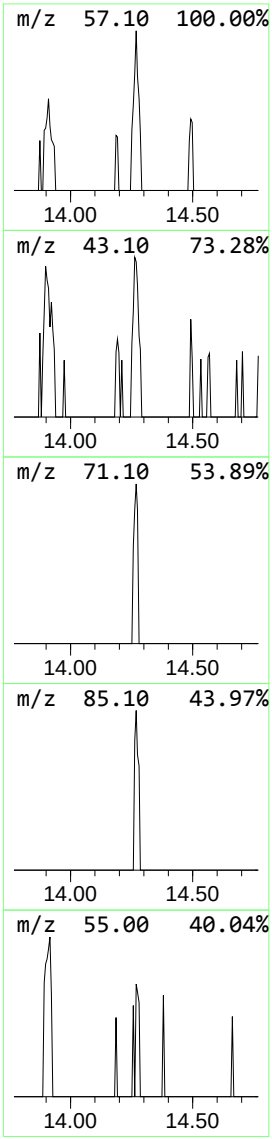
****

Peak Number 7 unknown14.268 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	2.58 ng	5199	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
2	2-Propenamide	71	C3H5NO	000079-06-1	4
3	Azetidine, 1,2-dimethyl-	85	C5H11N	051764-32-0	4
4	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4
5	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210539-COM-12

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

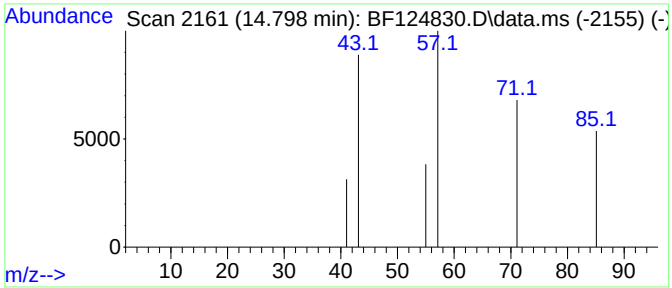
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

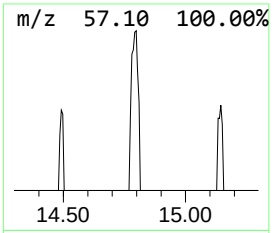
****

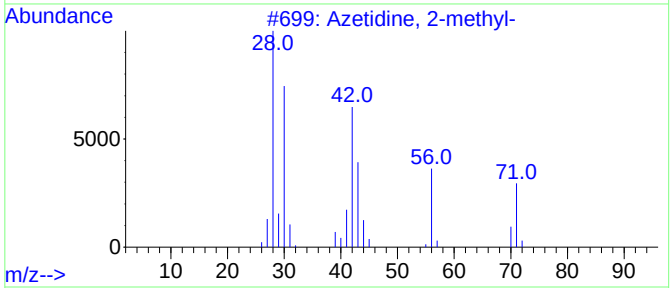
Peak Number 8 unknown14.798 Concentration Rank 5

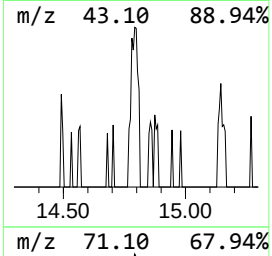
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.798	3.94 ng	6731	Perylene-d12	15.509

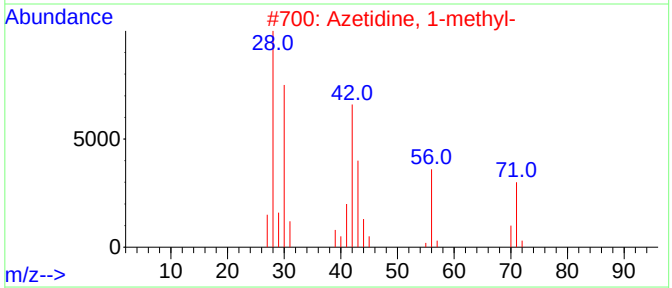
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
2	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
3	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
4	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
5	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4

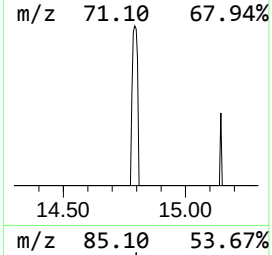


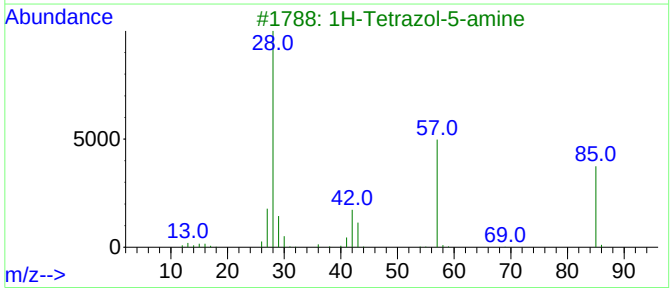


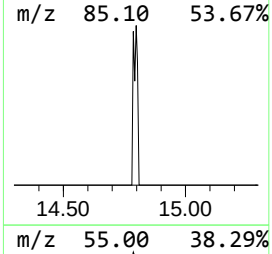


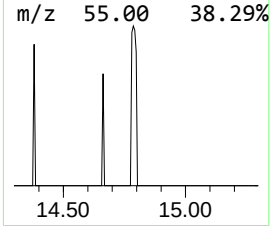












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210539-COM-12

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

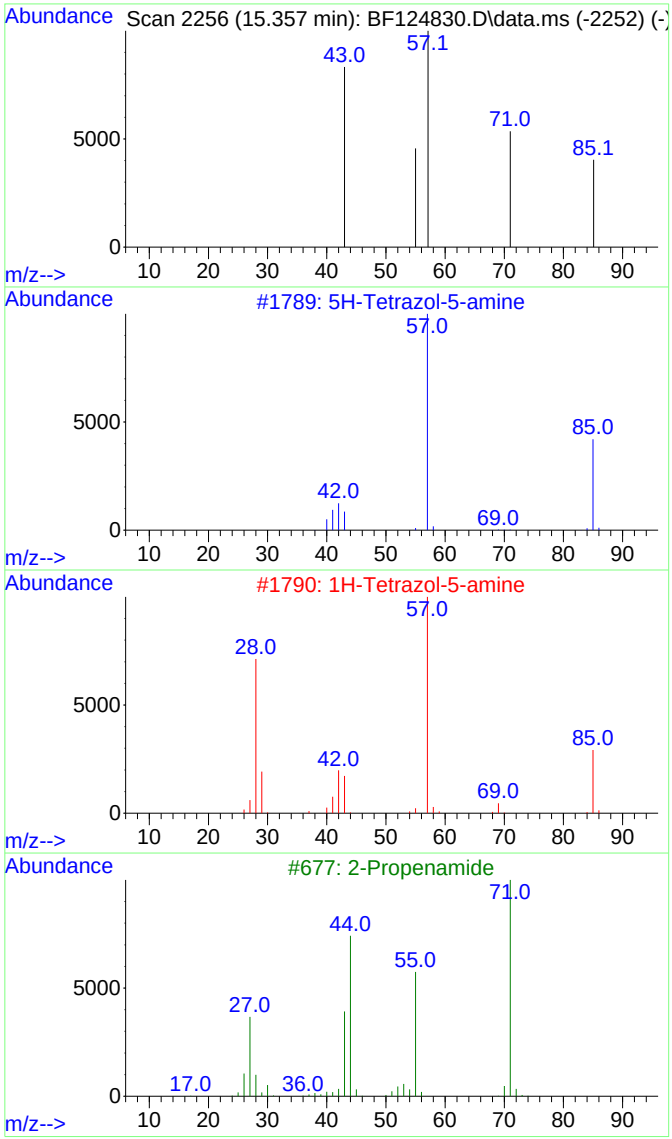
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

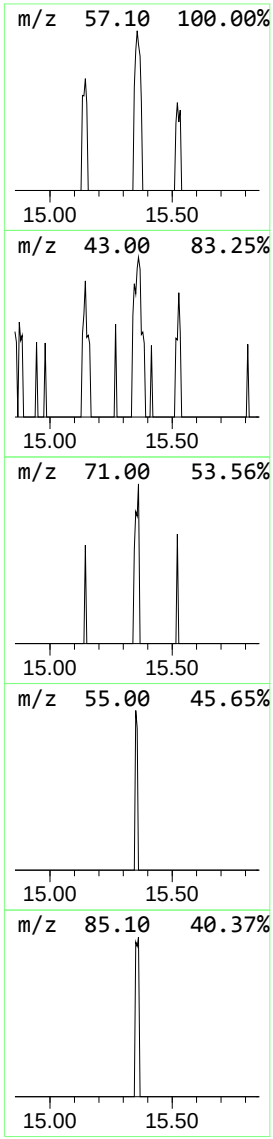
****

Peak Number 9 unknown15.357 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.357	2.37 ng	4048	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	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
3	2-Propenamide	71	C3H5NO	000079-06-1	4
4	Azetidine, 1,2-dimethyl-	85	C5H11N	051764-32-0	4
5	Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124830.D
Acq On : 28 Jul 2021 16:34
Operator : JU/CG
Sample : M3159-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210539-COM-12

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
unknown2.134	2.134	5.1	ng	7432	1	6.869	29094	20.0
unknown8.051	8.051	3.0	ng	5872	2	8.151	38683	20.0
Dodecanoic acid	11.916	6.0	ng	15335	4	11.392	51411	20.0
Tetradecanoic acid	12.698	5.1	ng	13046	4	11.392	51411	20.0
unknown13.663	13.663	2.3	ng	4545	5	14.033	40356	20.0
unknown13.898	13.898	7.3	ng	14647	5	14.033	40356	20.0
unknown14.268	14.268	2.6	ng	5199	5	14.033	40356	20.0
unknown14.798	14.798	3.9	ng	6731	6	15.509	34183	20.0
unknown15.357	15.357	2.4	ng	4048	6	15.509	34183	20.0