LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
Data File : BF124850.D
Acq On : 29 Jul 2021 14:30
Operator : JU/CG
Sample : M3206-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210581-COM-4

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: BF124850.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	6	9	12	rBB	3535	3770	1.42%	0.273%
2	5.492	574	579	582	rBV	142361	132859	49.99%	9.629%
3	6.498	746	750	753	rBV	136367	146708	55.20%	10.633%
4	6.869	810	813	816	rBB	38239	29509	11.10%	2.139%
5	7.434	905	909	912	rBB	105353	93531	35.19%	6.779%
6	8.057	1012	1015	1022	rBB	23163	22129	8.33%	1.604%
7	8.157	1028	1032	1035	rBB	47775	39781	14.97%	2.883%
8	9.233	1210	1215	1218	rBV	212094	193893	72.95%	14.053%
9	9.910	1327	1330	1333	rBV	67673	50617	19.04%	3.669%
10	10.704	1461	1465	1468	rBV	181051	149985	56.43%	10.870%
11	11.398	1580	1583	1586	rBV	77014	56206	21.15%	4.074%
12	11.921	1667	1672	1675	rBV	32584	27875	10.49%	2.020%
13	12.621	1787	1791	1793	rBV	2768	3620	1.36%	0.262%
14	12.645	1793	1795	1801	rVV2	3554	6163	2.32%	0.447%
15	12.704	1801	1805	1809	rVB	14019	11846	4.46%	0.859%
16	12.986	1849	1853	1856	rBV	268031	265794	100.00%	19.264%
17	13.639	1956	1964	1969	rBB	5276	10000	3.76%	0.725%
18	13.898	1999	2008	2014	rBV3	9727	19956	7.51%	1.446%
19	14.039	2029	2032	2035	rVB	61492	51254	19.28%	3.715%
20	14.327	2073	2081	2086	rBV3	5525	11272	4.24%	0.817%
21	14.904	2175	2179	2186	rVB2	4227	6668	2.51%	0.483%
22	15.515	2279	2283	2288	rBV	36019	42201	15.88%	3.059%
23	16.315	2415	2419	2427	rVB3	1703	4135	1.56%	0.300%

Sum of corrected areas: 1379772

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
Data File : BF124850.D
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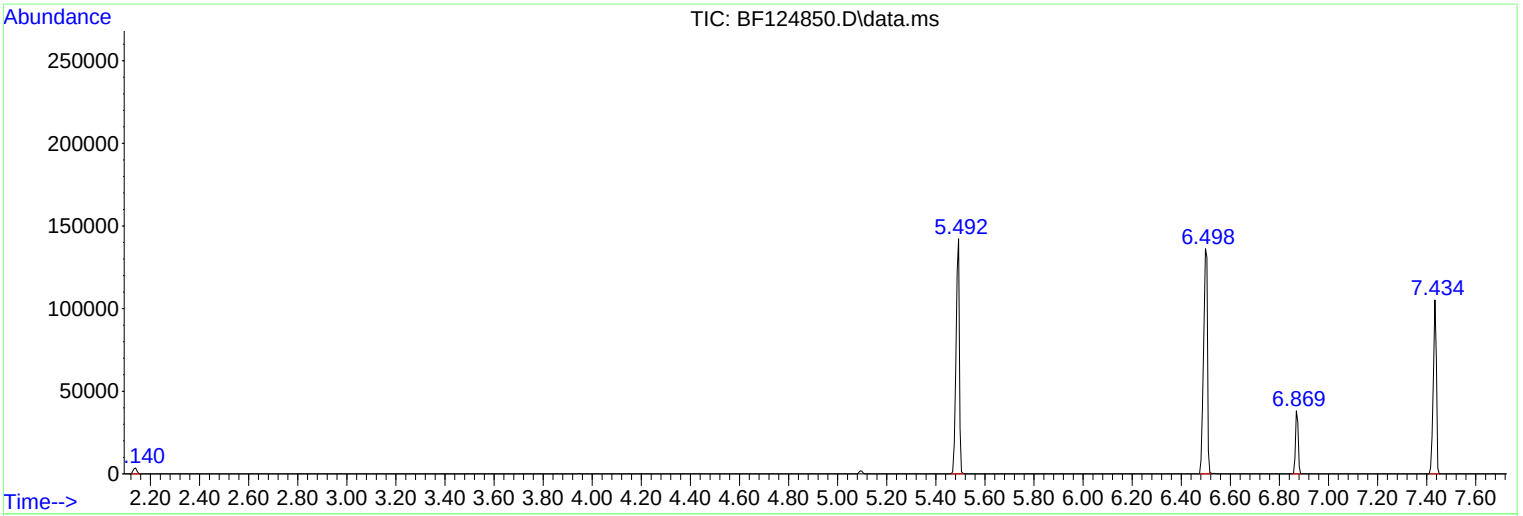
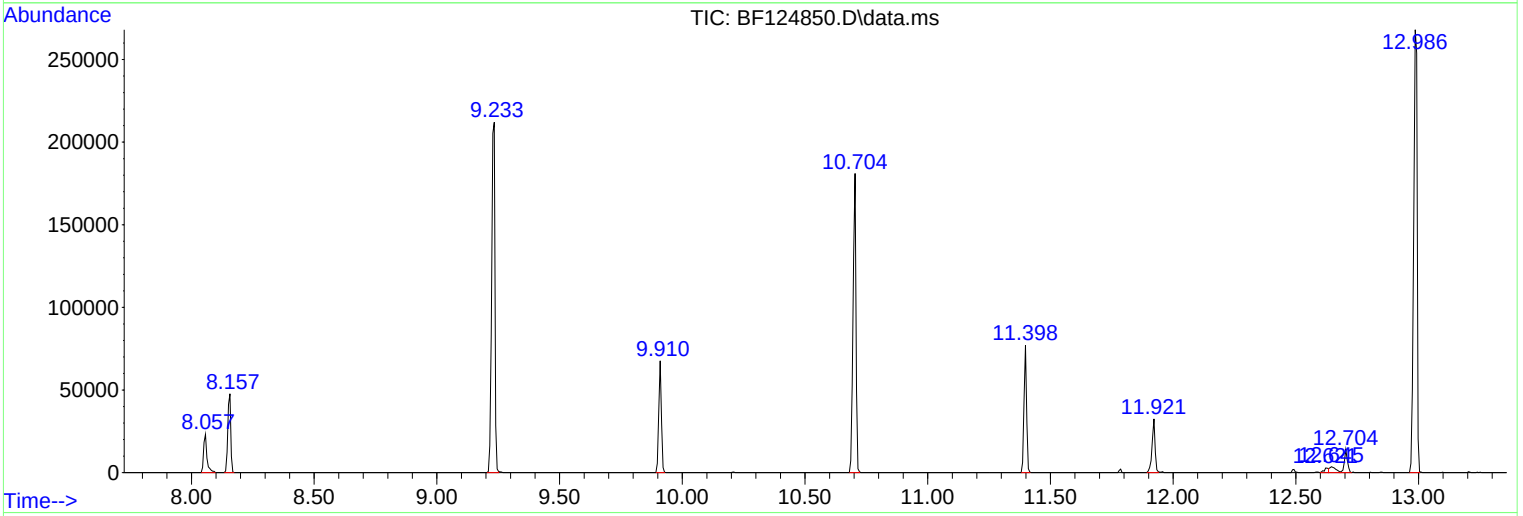
Sample : M3206-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

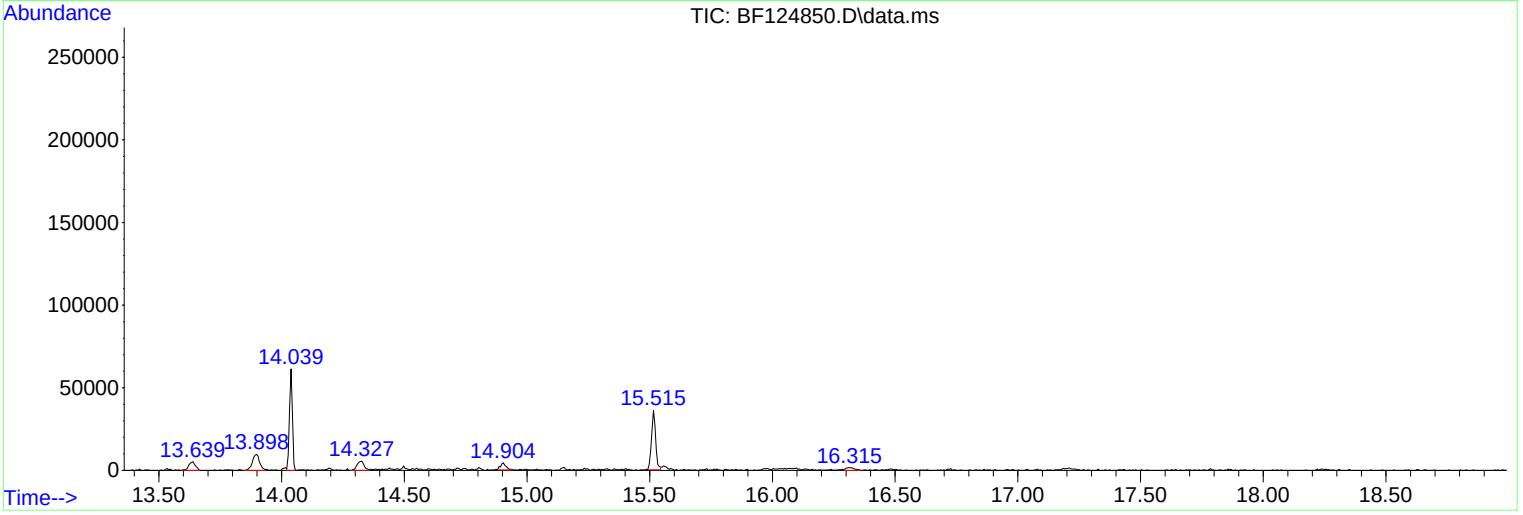
Instrument :
BNA_F
ClientSampleId :
20210581-COM-4

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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Operator : JU/CG
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Instrument :
BNA_F
ClientSampleId :
20210581-COM-4

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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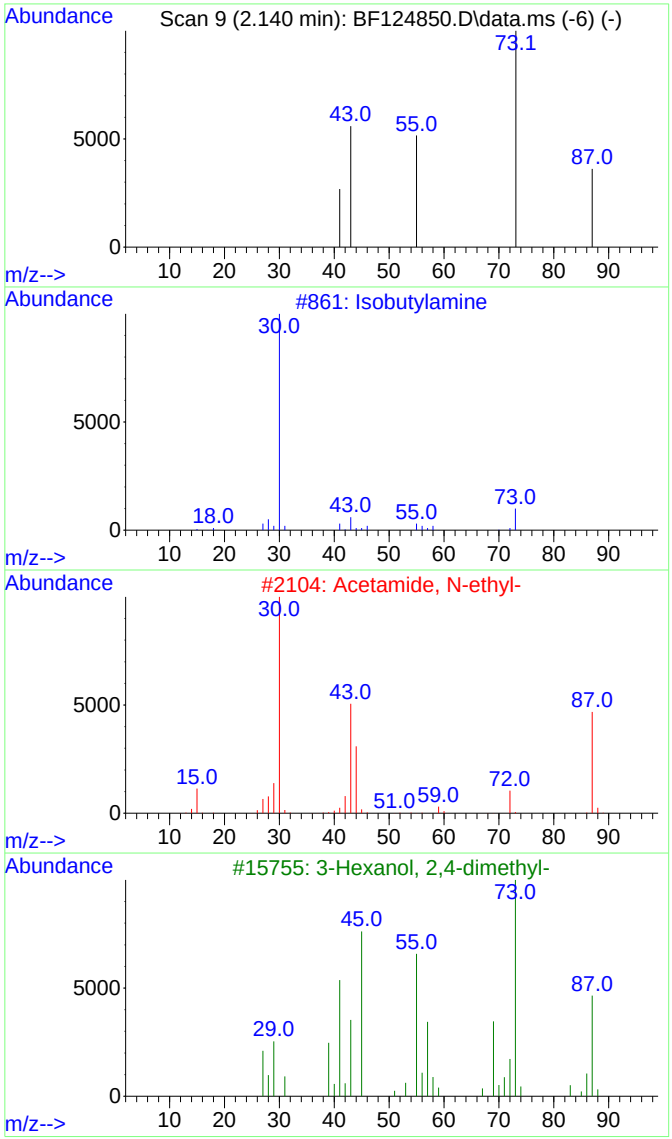
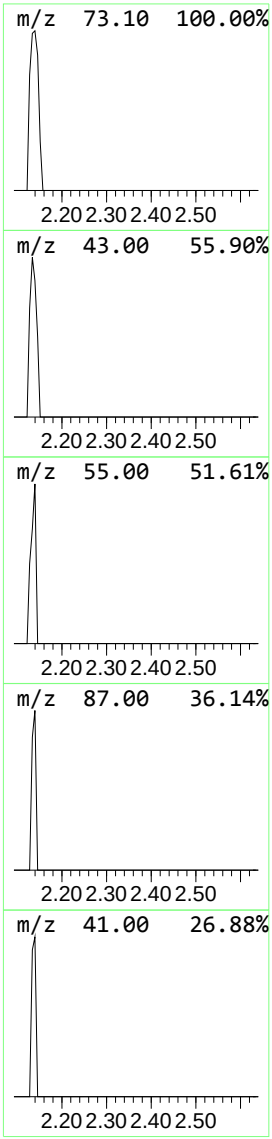
Peak Number 1 unknown2.140 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	2.56 ng	3770	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutylamine	73	C4H11N	000078-81-9	4
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	4
3	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	4
4	2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	4
5	1-Butanamine	73	C4H11N	000109-73-9	3





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Operator : JU/CG
Sample : M3206-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210581-COM-4

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

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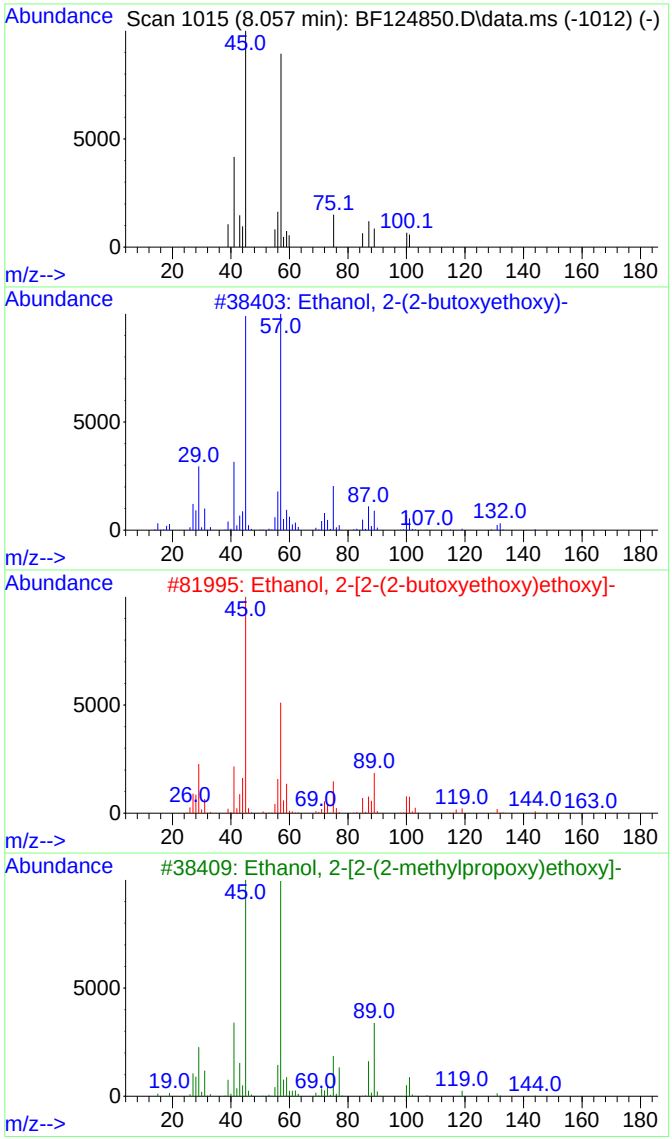
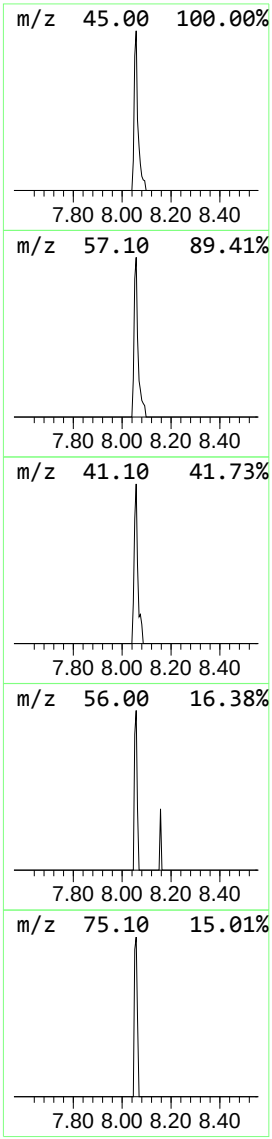
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.057	11.13 ng	22129	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	42
5	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	42





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Sample : M3206-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210581-COM-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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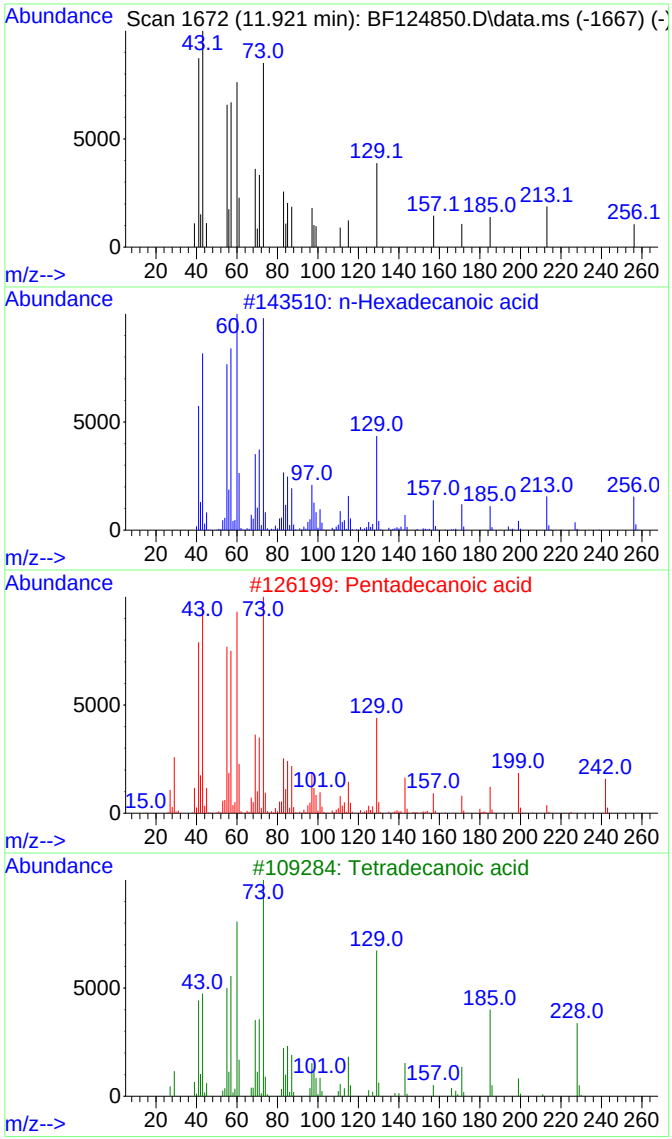
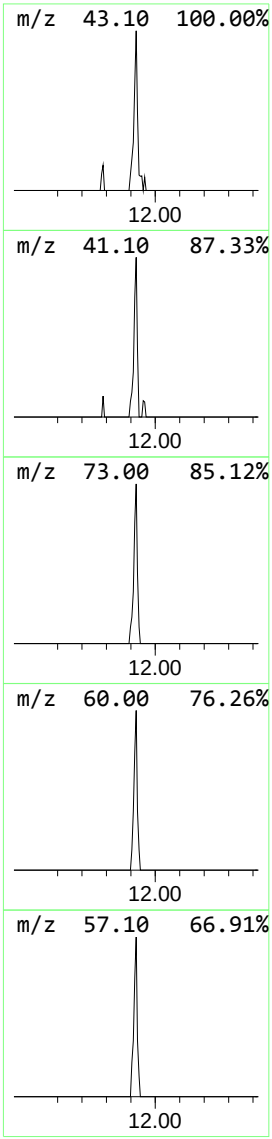
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	9.92 ng	27875	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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Sample : M3206-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210581-COM-4

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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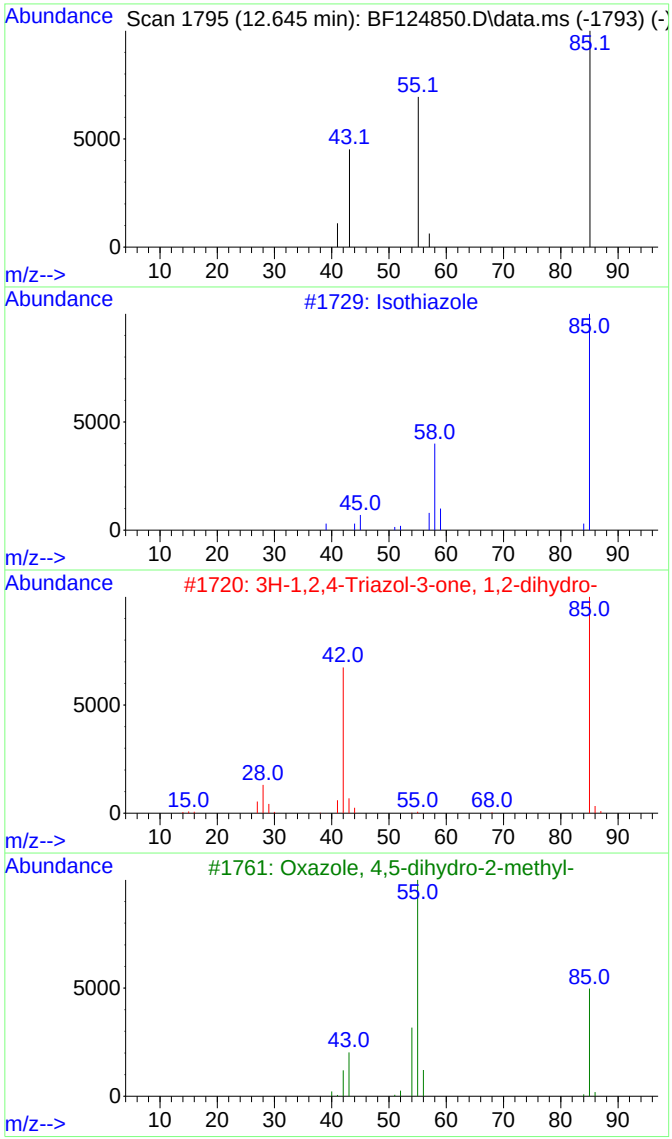
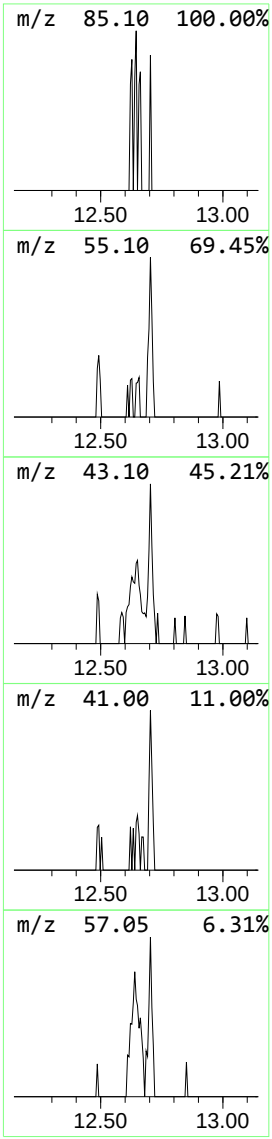
Peak Number 4 unknown12.645 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.19 ng	6163	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isothiazole	85	C3H3NS	000288-16-4	4
2	3H-1,2,4-Triazol-3-one, 1,2-dihy...	85	C2H3N3O	000930-33-6	3
3	Oxazole, 4,5-dihydro-2-methyl-	85	C4H7NO	001120-64-5	3
4	Phosphoramidous difluoride	85	F2H2NP	025757-74-8	2
5	Oxalic acid, cyclobutyl isohexyl...	228	C12H20O4	1000309-69-6	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
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Acq On : 29 Jul 2021 14:30
Operator : JU/CG
Sample : M3206-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210581-COM-4

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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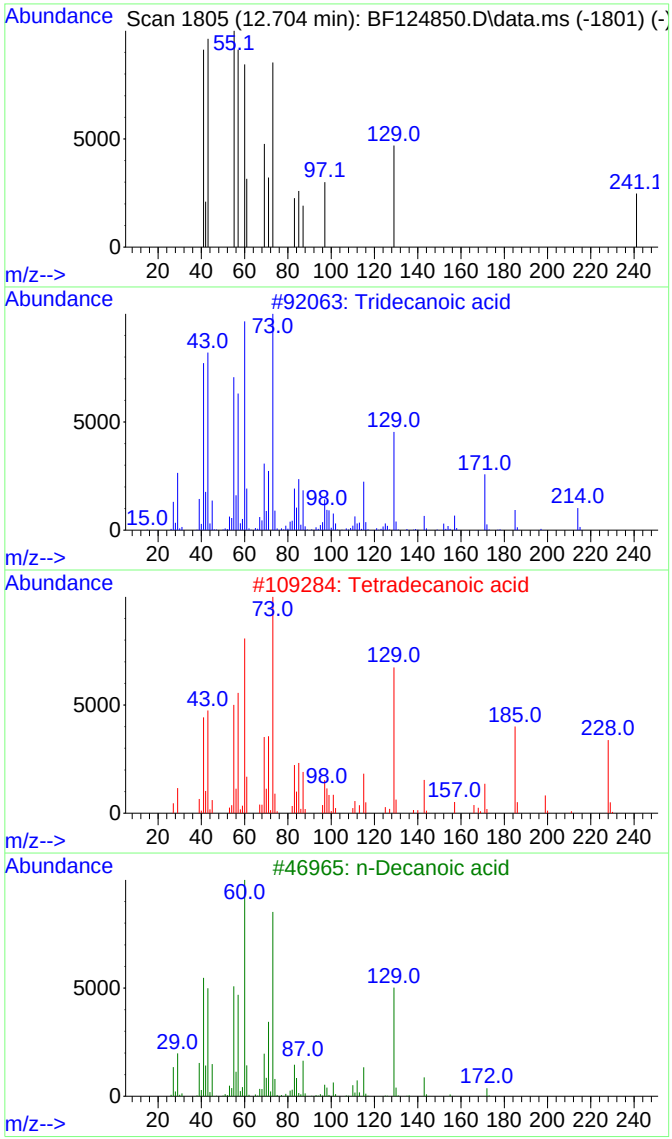
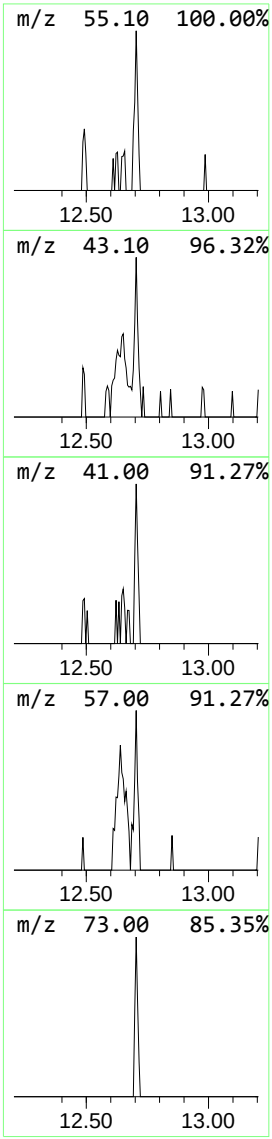
Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	4.22 ng	11846	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	72
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53
5	Methyl 6-O-[1-methylpropyl]-.bet...	250	C11H22O6	1010126-15-7	50





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Misc :
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Instrument : BNA_F
ClientSampleId : 20210581-COM-4

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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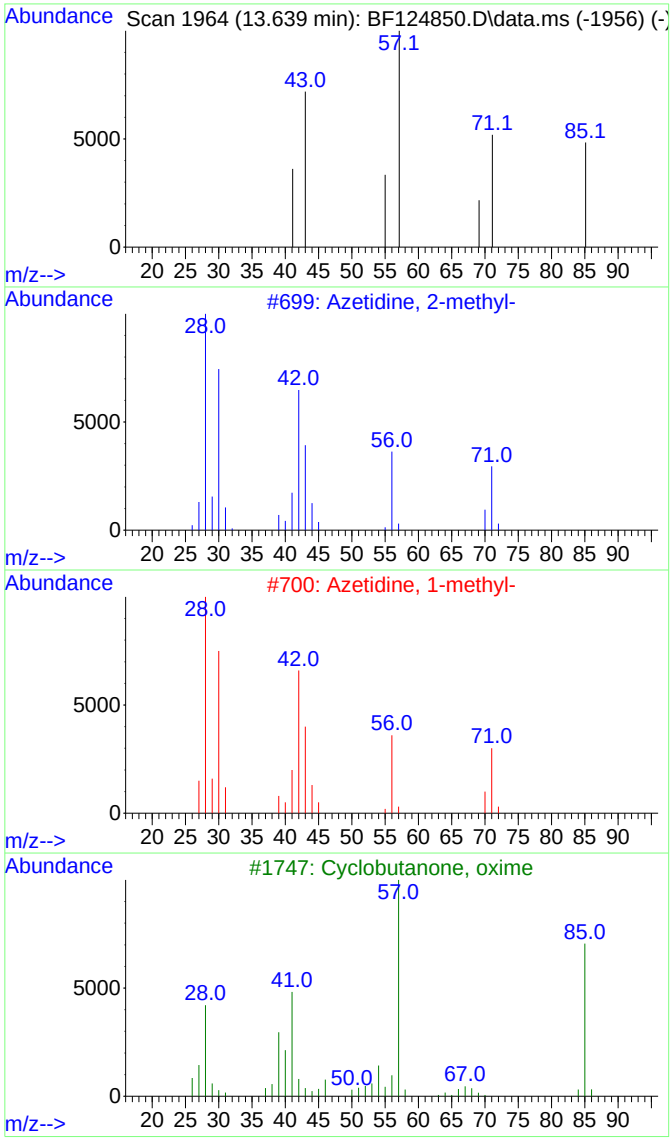
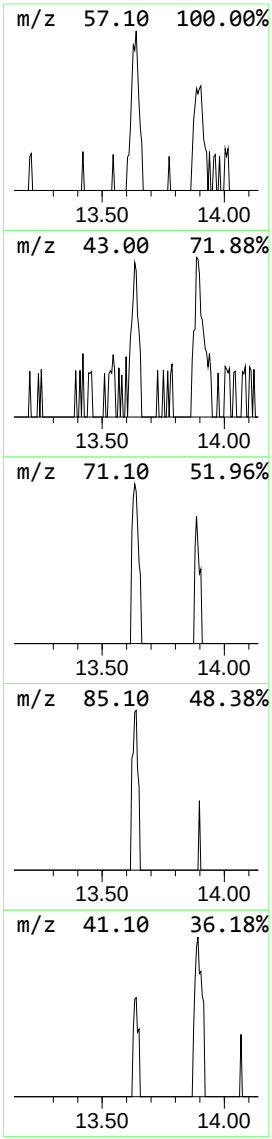
Peak Number 6 unknown13.639 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.639	3.90 ng	10000	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	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
4	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
5	2-Propenamide	71	C3H5NO	000079-06-1	4





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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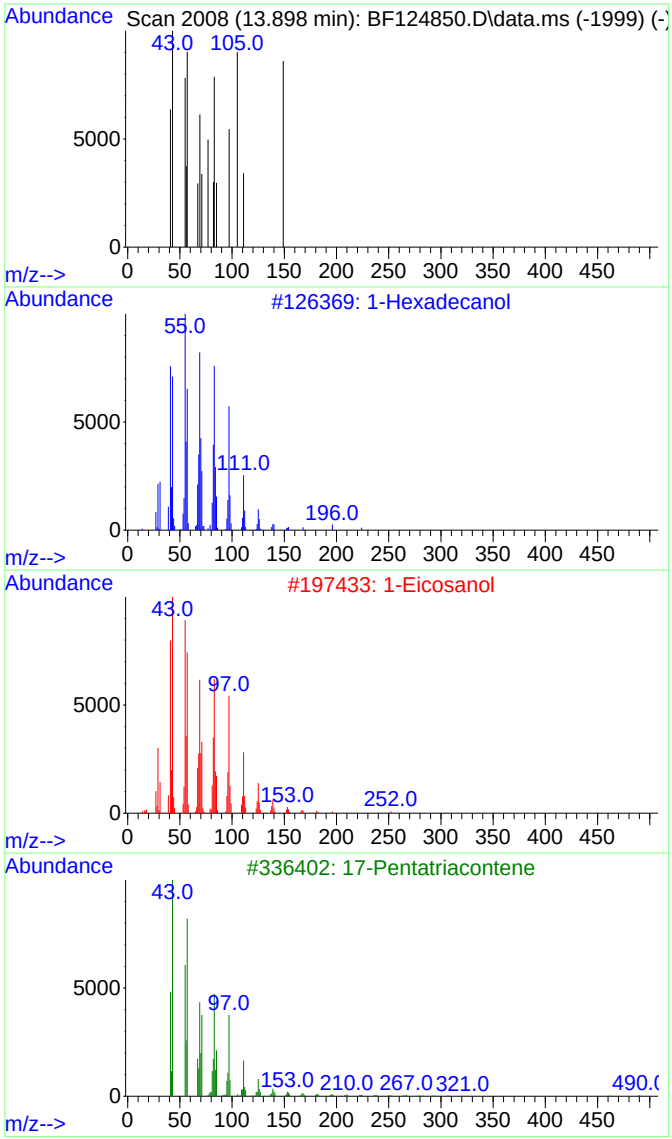
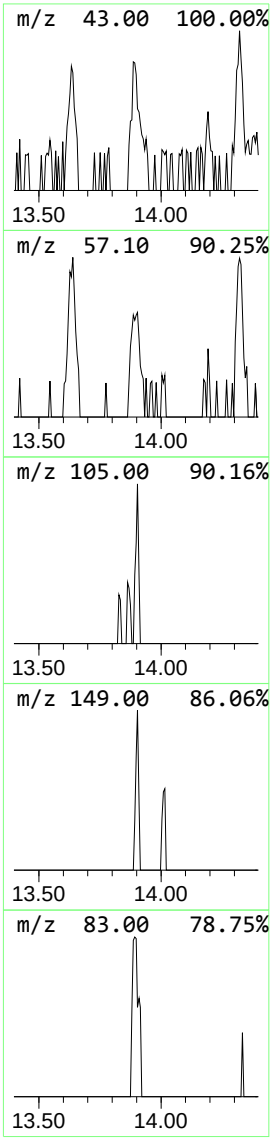
Peak Number 7 unknown13.898 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	7.79 ng	19956	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	43
2	1-Eicosanol	298	C20H42O	000629-96-9	43
3	17-Pentatriacontene	491	C35H70	006971-40-0	43
4	1-Docosene	308	C22H44	001599-67-3	38
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	38





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TIC Library : C:\Database\NIST20.L
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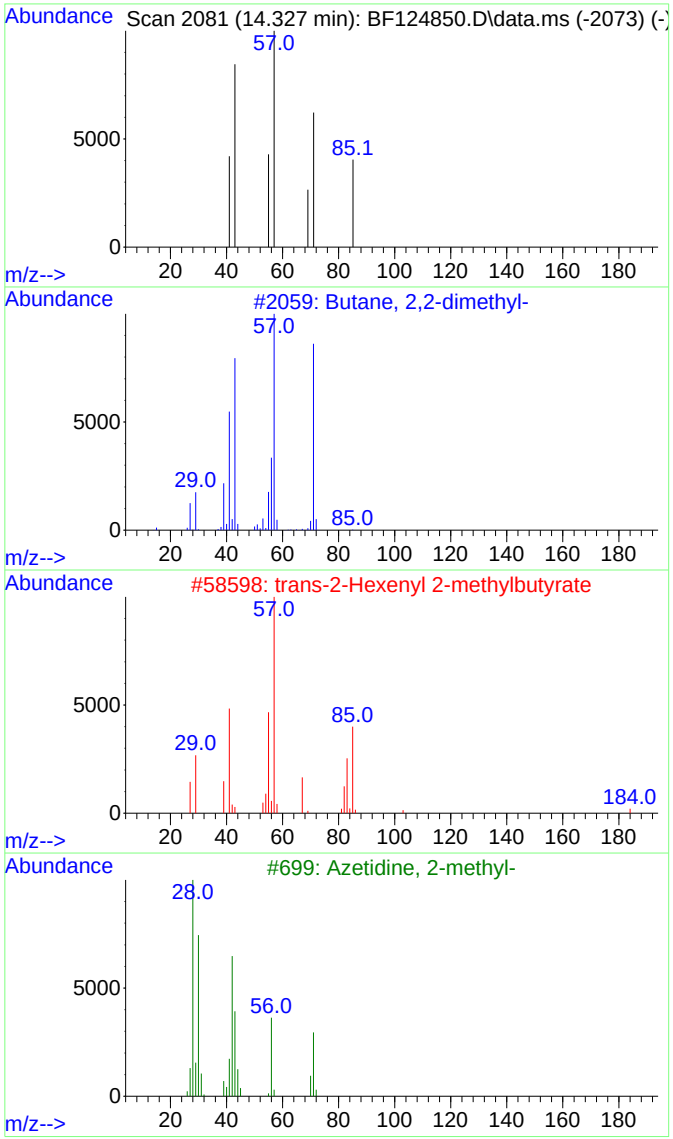
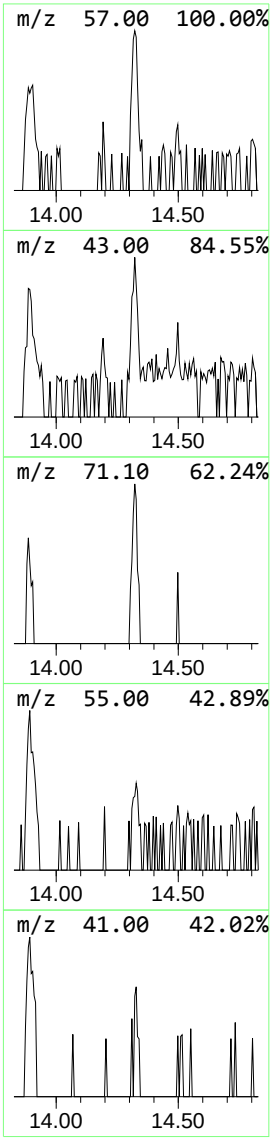
Peak Number 8 unknown14.327 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	4.40 ng	11272	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
2	trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
3	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
4	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
5	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4





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Sample : M3206-02
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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210581-COM-4

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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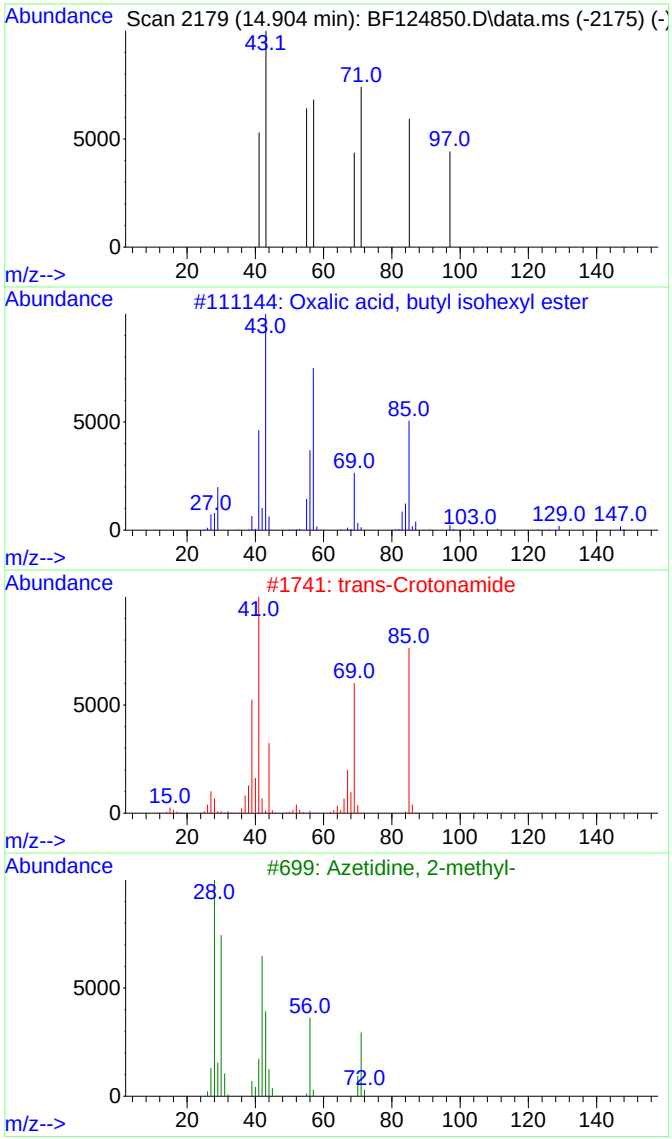
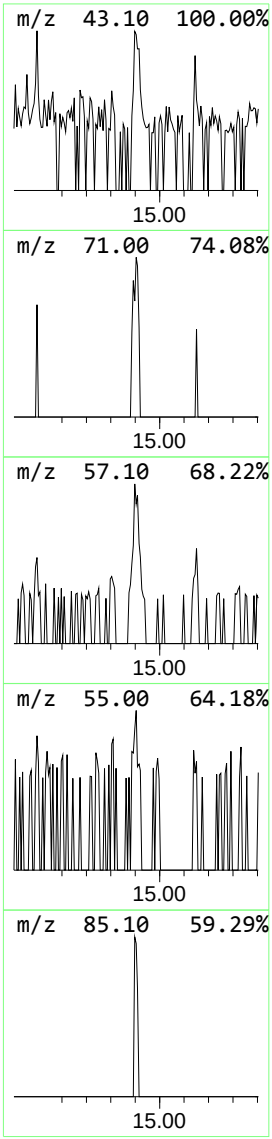
Peak Number 9 unknown14.904 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	3.16 ng	6668	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	9
2	trans-Crotonamide	85	C4H7NO	000625-37-6	7
3	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
4	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
5	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
Data File : BF124850.D
Acq On : 29 Jul 2021 14:30
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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.140	2.140	2.6	ng	3770	1	6.869	29509	20.0
Ethanol, 2-(2-b...	8.057	11.1	ng	22129	2	8.157	39781	20.0
n-Hexadecanoic ...	11.922	9.9	ng	27875	4	11.398	56206	20.0
unknown12.645	12.645	2.2	ng	6163	4	11.398	56206	20.0
Tridecanoic acid	12.704	4.2	ng	11846	4	11.398	56206	20.0
unknown13.639	13.639	3.9	ng	10000	5	14.039	51254	20.0
unknown13.898	13.898	7.8	ng	19956	5	14.039	51254	20.0
unknown14.327	14.327	4.4	ng	11272	5	14.039	51254	20.0
unknown14.904	14.904	3.2	ng	6668	6	15.515	42201	20.0