LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125021.D
Acq On : 10 Aug 2021 1:55
Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125021.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	9	11	14	rBB	2103	2020	1.48%	0.190%
2	4.393	390	392	395	rBB	2150	1687	1.23%	0.159%
3	5.040	496	502	507	rBB	71910	91041	66.55%	8.560%
4	5.445	567	571	574	rBV	152418	134677	98.45%	12.663%
5	5.834	634	637	640	rBB	18359	14198	10.38%	1.335%
6	6.463	739	744	747	rBV	147723	133496	97.59%	12.552%
7	6.822	802	805	808	rBB	36655	28123	20.56%	2.644%
8	7.387	897	901	904	rBB	105959	85510	62.51%	8.040%
9	8.004	1003	1006	1009	rBV	40070	28352	20.73%	2.666%
10	8.104	1020	1023	1026	rBB	42215	33359	24.39%	3.137%
11	9.175	1202	1205	1209	rBB	157401	136798	100.00%	12.862%
12	9.857	1318	1321	1324	rBB	42225	30678	22.43%	2.884%
13	10.645	1452	1455	1458	rBV	88345	64255	46.97%	6.041%
14	11.339	1570	1573	1576	rBV	32280	26256	19.19%	2.469%
15	11.863	1660	1662	1665	rBB	5788	3992	2.92%	0.375%
16	12.551	1777	1779	1782	rBB	5292	4442	3.25%	0.418%
17	12.786	1816	1819	1821	rBB	6451	5321	3.89%	0.500%
18	12.927	1839	1843	1846	rBB	164915	129644	94.77%	12.190%
19	13.780	1983	1988	1990	rBV	1354	1626	1.19%	0.153%
20	13.816	1990	1994	2000	rVB	8442	9538	6.97%	0.897%
21	13.980	2018	2022	2025	rBV	37714	30964	22.63%	2.911%
22	14.004	2025	2026	2030	rVB	2073	1629	1.19%	0.153%
23	14.457	2098	2103	2106	rBV4	2118	3412	2.49%	0.321%
24	14.515	2109	2113	2115	rVB2	1630	1960	1.43%	0.184%
25	14.733	2147	2150	2154	rBV4	2354	3456	2.53%	0.325%
26	14.786	2156	2159	2160	rVV	1438	1747	1.28%	0.164%
27	14.815	2160	2164	2169	rVB4	2872	4874	3.56%	0.458%
28	14.933	2183	2184	2187	rBV3	1637	1721	1.26%	0.162%
29	15.010	2195	2197	2200	rBV3	2985	2968	2.17%	0.279%
30	15.280	2239	2243	2244	rVB2	1998	1685	1.23%	0.158%
31	15.374	2257	2259	2262	rVB2	2096	2233	1.63%	0.210%
32	15.439	2266	2270	2274	rBV	16462	20380	14.90%	1.916%
33	15.504	2278	2281	2284	rBV5	1302	1586	1.16%	0.149%
34	15.568	2291	2292	2295	rVB3	2297	2160	1.58%	0.203%
35	15.880	2341	2345	2348	rVB3	1238	1908	1.39%	0.179%
36	15.939	2348	2355	2358	rBV3	1800	3686	2.69%	0.347%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
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Acq On : 10 Aug 2021 1:55
Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.121	2383	2386	2388	rBV4	1904	1878	1.37%	0.177%
38	16.415	2433	2436	2439	rVB3	1484	1727	1.26%	0.162%
39	16.892	2514	2517	2519	rVB2	1994	1696	1.24%	0.159%
40	17.251	2574	2578	2583	rVB5	1309	2827	2.07%	0.266%
41	18.351	2760	2765	2766	rBV3	1390	1892	1.38%	0.178%
42	18.609	2807	2809	2814	rBV3	1394	2162	1.58%	0.203%

Sum of corrected areas: 1063564

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
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Acq On : 10 Aug 2021 1:55
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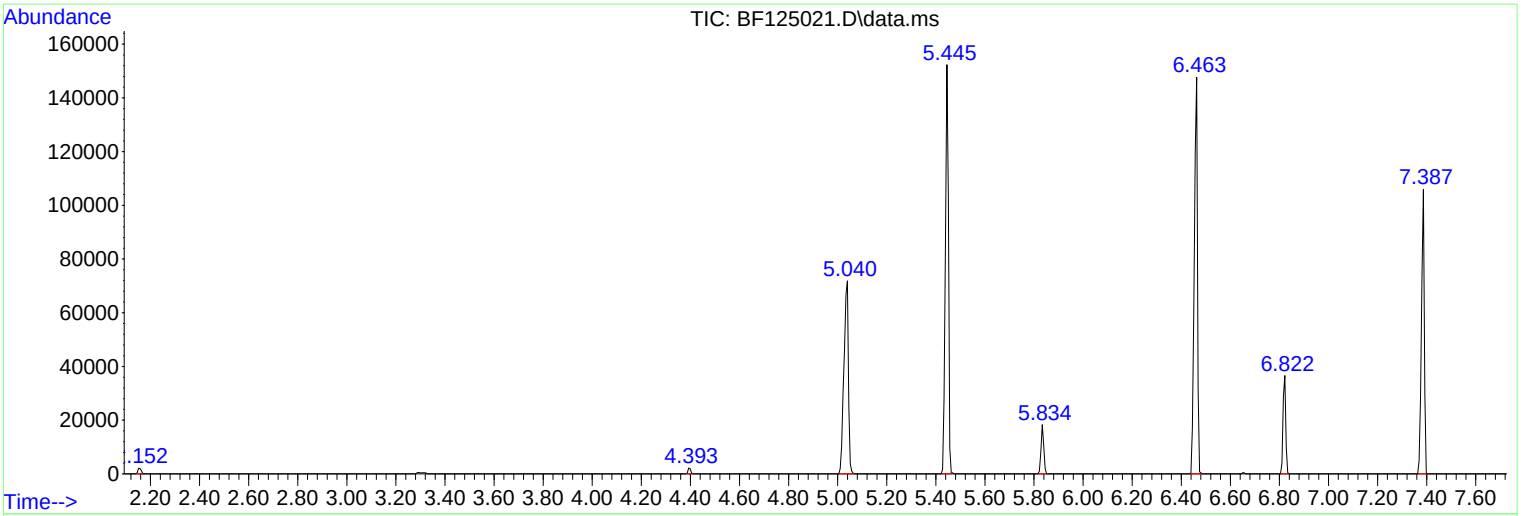
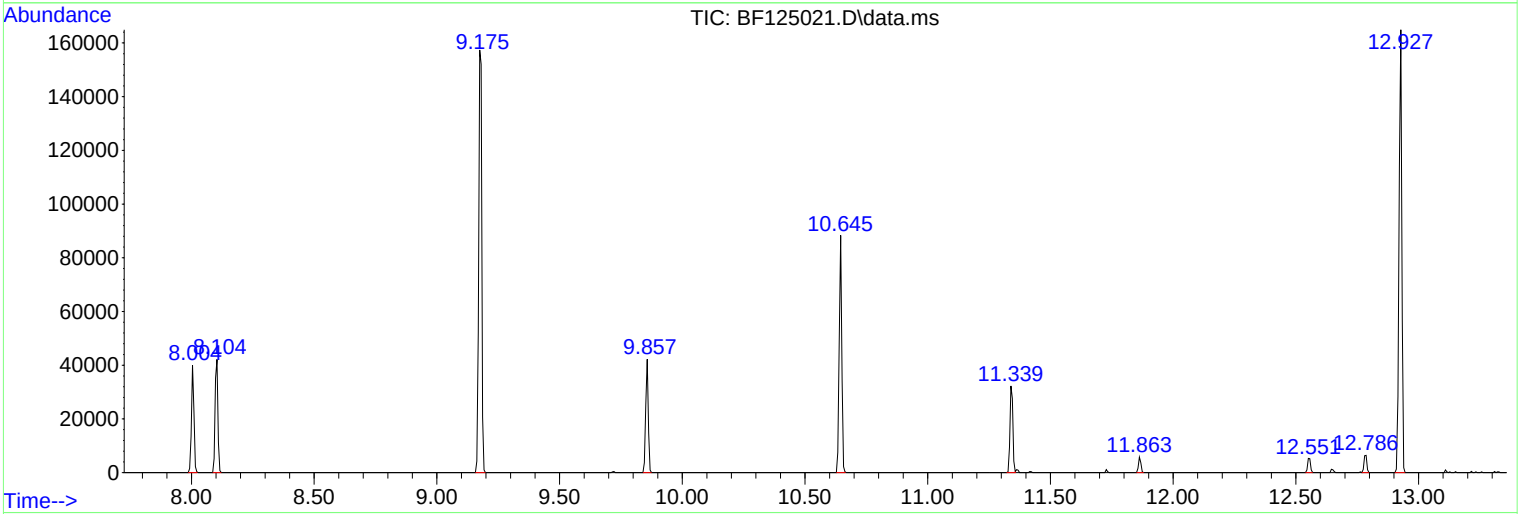
ALS Vial : 18 Sample Multiplier: 1

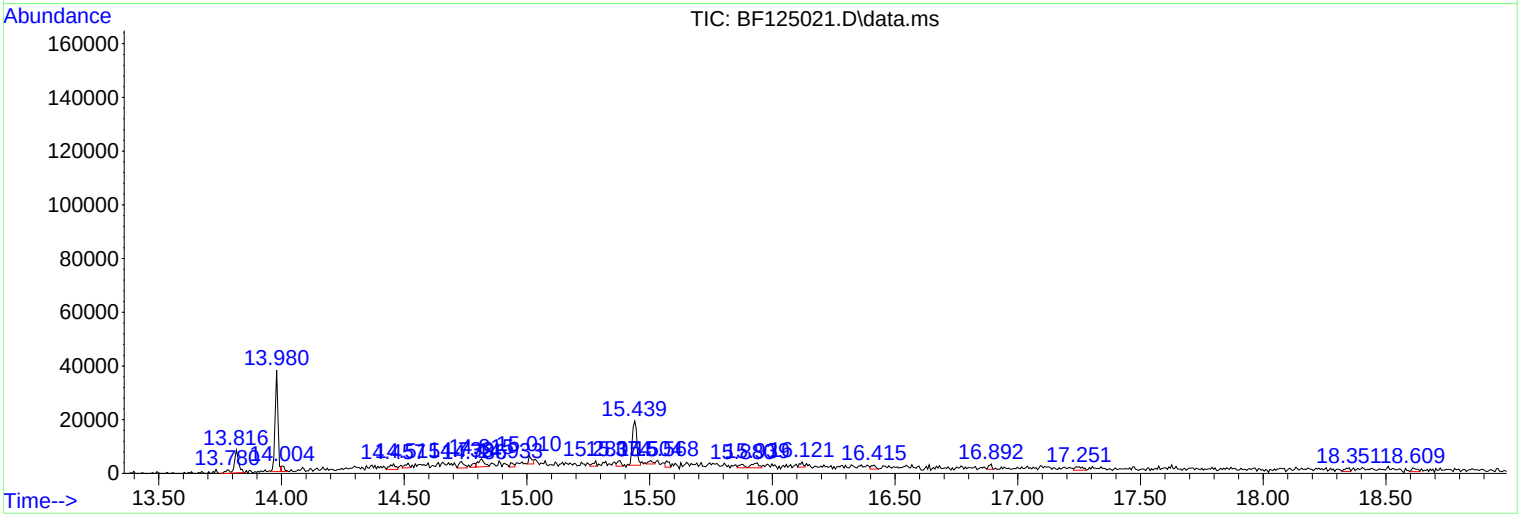
Instrument :
BNA_F
ClientSampleId :
FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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\BF080921\
Data File : BF125021.D
Acq On : 10 Aug 2021 1:55
Operator : JU/CG
Sample : M3295-01
Misc :
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Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

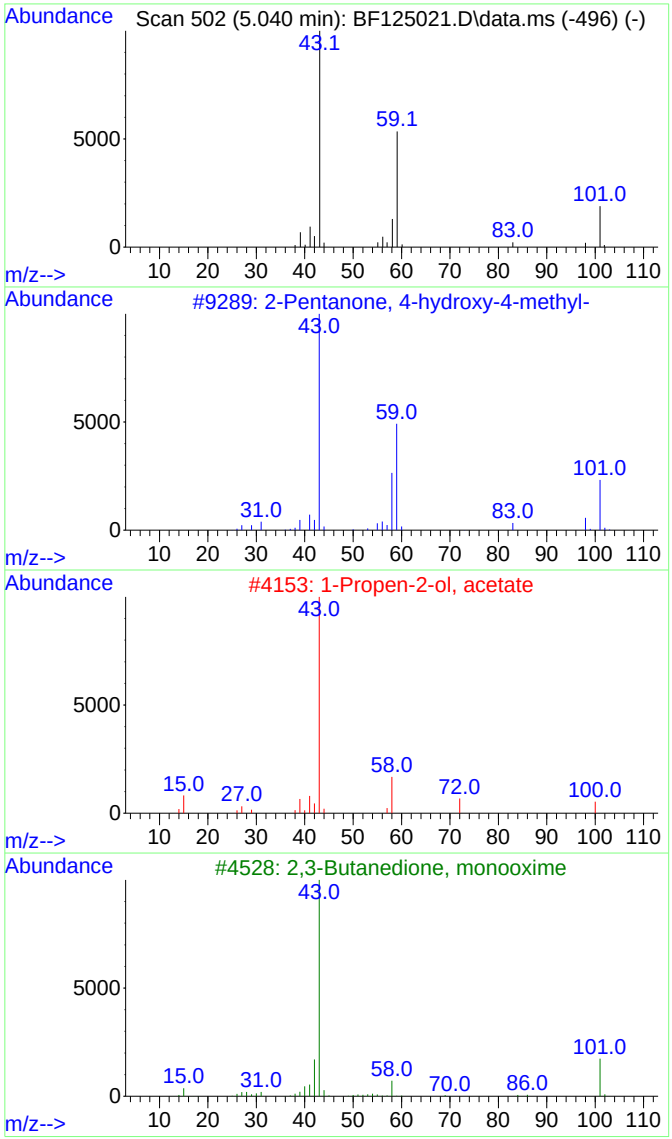
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

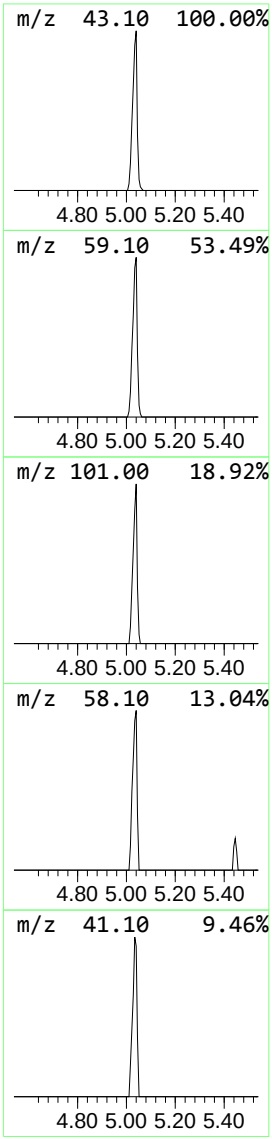
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	64.74 ng	91041	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





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Operator : JU/CG
Sample : M3295-01
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Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

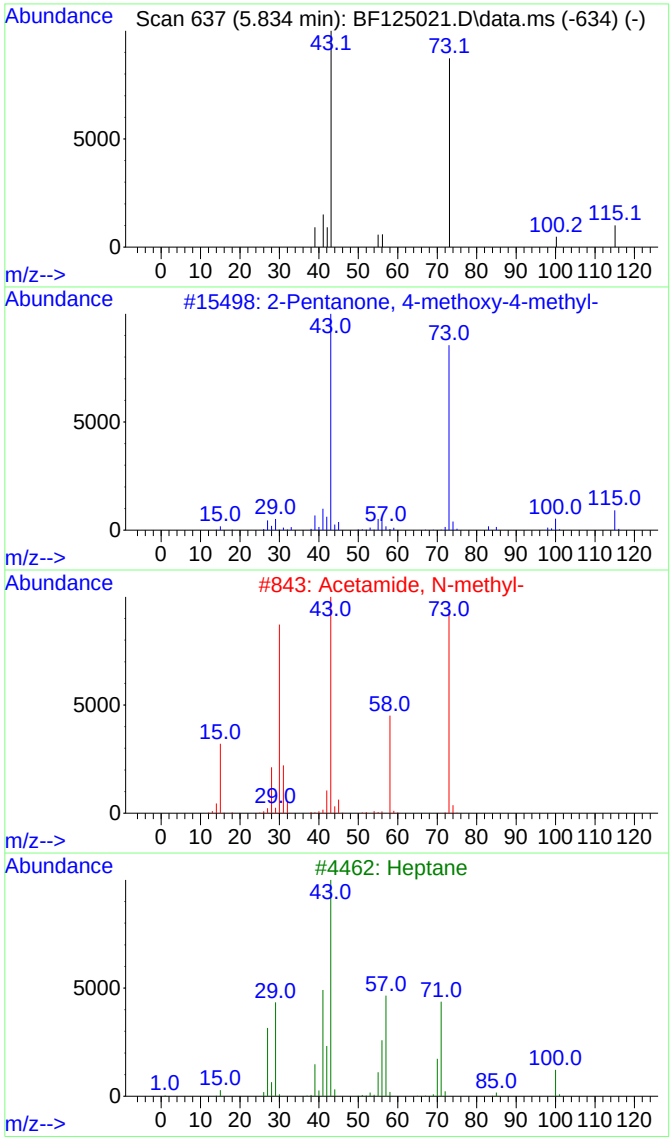
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

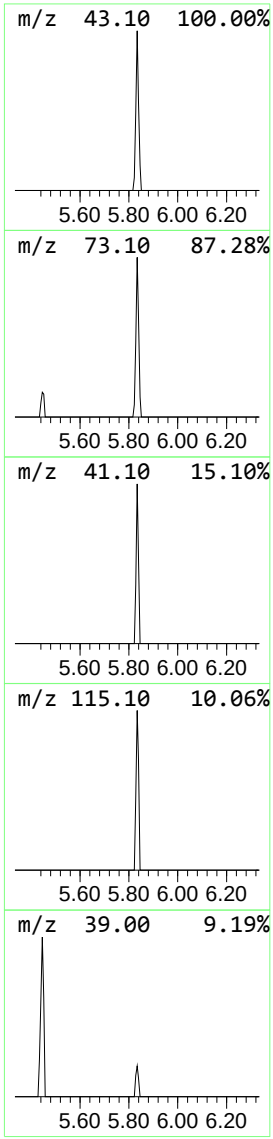
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	10.10 ng	14198	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	74
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	7
3	Heptane	100	C7H16	000142-82-5	4
4	1-Amino-3,3-dimethyl-2-butanone	115	C6H13NO	082962-91-2	4
5	Acetamide, N-(2-methylpropyl)-	115	C6H13NO	001540-94-9	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125021.D
Acq On : 10 Aug 2021 1:55
Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

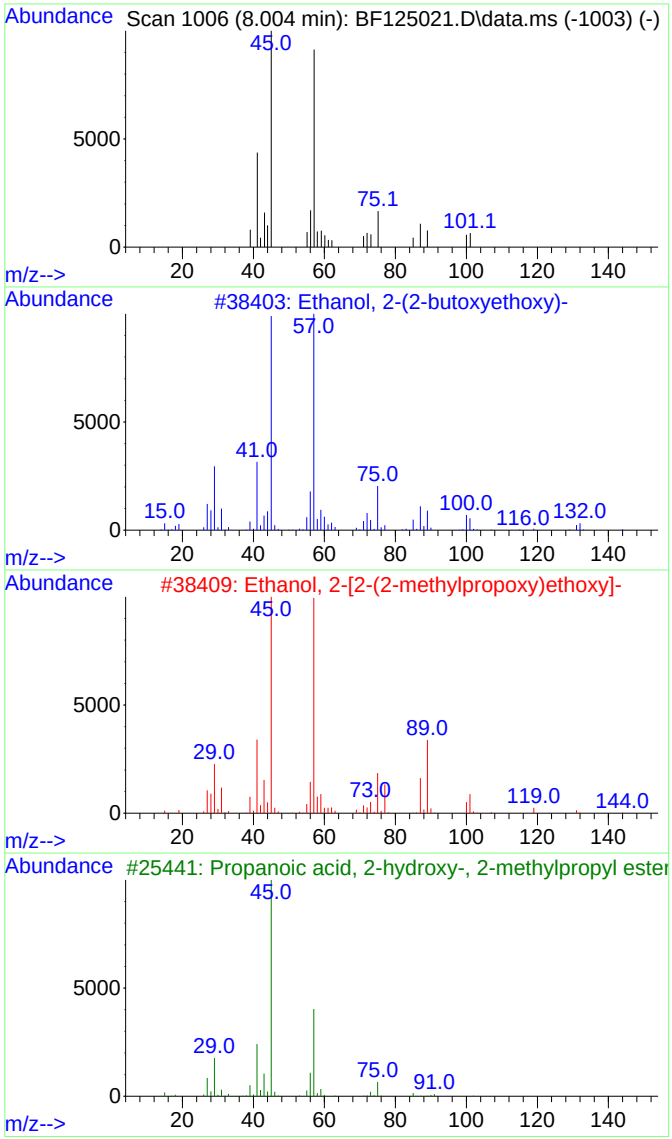
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

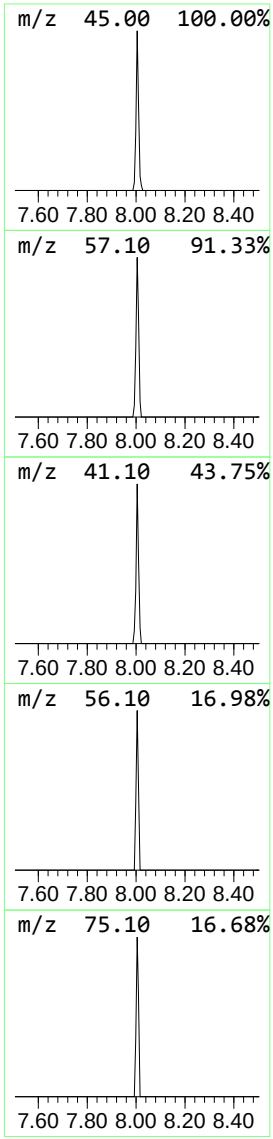
****

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	17.00 ng	28352	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53
4	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47
5	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40





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Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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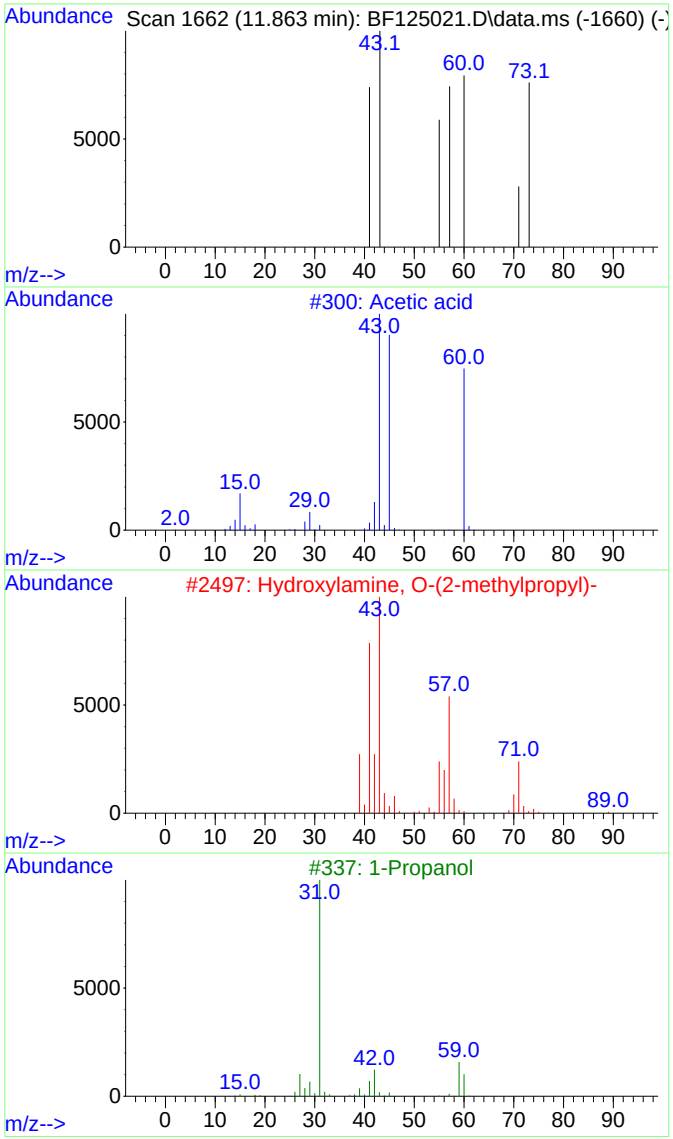
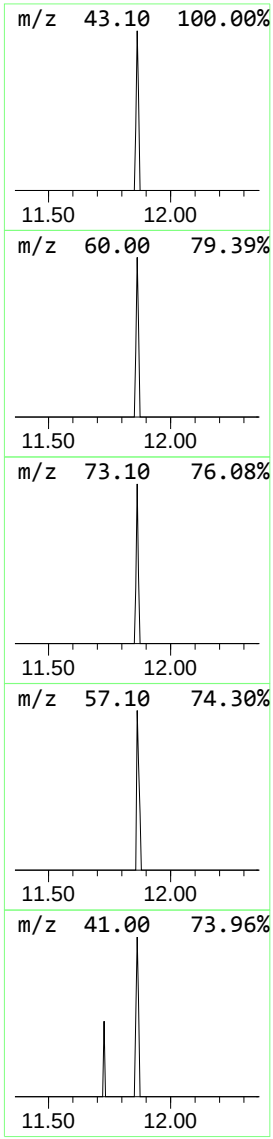
****

Peak Number 4 unknown11.863 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	3.04 ng	3992	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	4
2	Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	4
3	1-Propanol	60	C3H8O	000071-23-8	3
4	Isobutylamine	73	C4H11N	000078-81-9	3
5	Urea	60	CH4N2O	000057-13-6	2





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

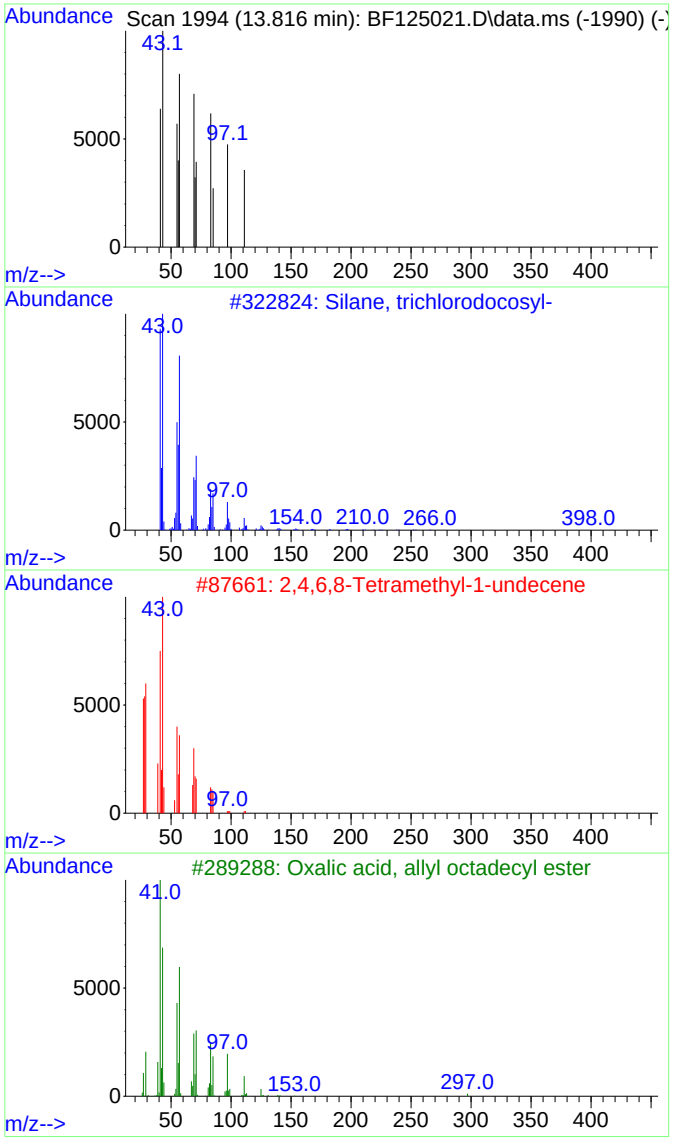
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

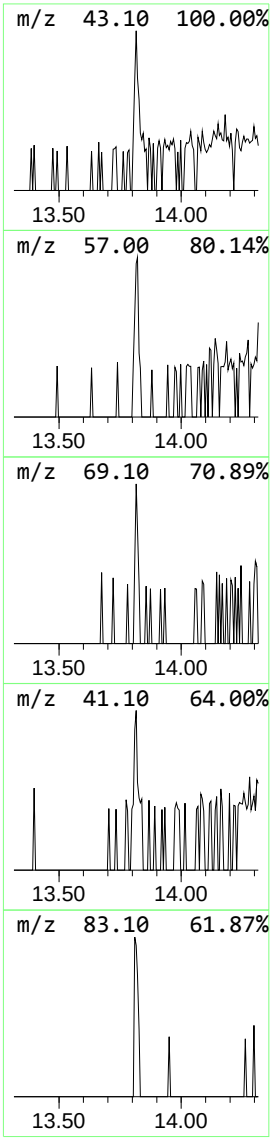
****

Peak Number 5 Silane, trichlorodocosyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	6.16 ng	9538	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	64
2	2,4,6,8-Tetramethyl-1-undecene	210	C15H30	059920-26-2	37
3	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	33
4	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	28
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	28





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Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

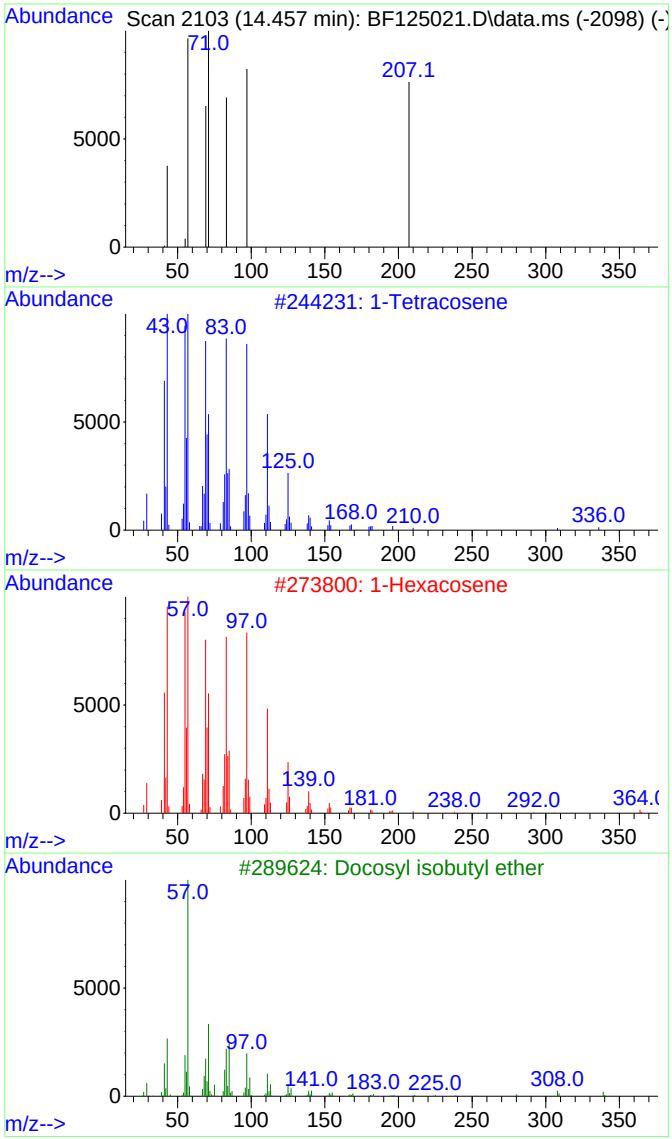
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

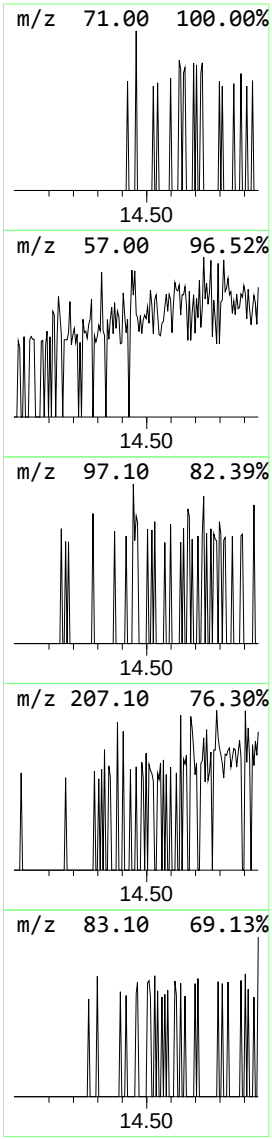
****

Peak Number 6 unknown14.457 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	2.20 ng	3412	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	28
2	1-Hexacosene	364	C26H52	018835-33-1	28
3	Docosyl isobutyl ether	382	C26H54O	1000406-33-1	9
4	Silane, [(11-chloroundecyl)oxy]t...	278	C14H31ClOSi	026305-82-8	9
5	11-Bromo-1-undecanol, TMS deriva...	322	C14H31BrOSi	026305-83-9	9





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Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

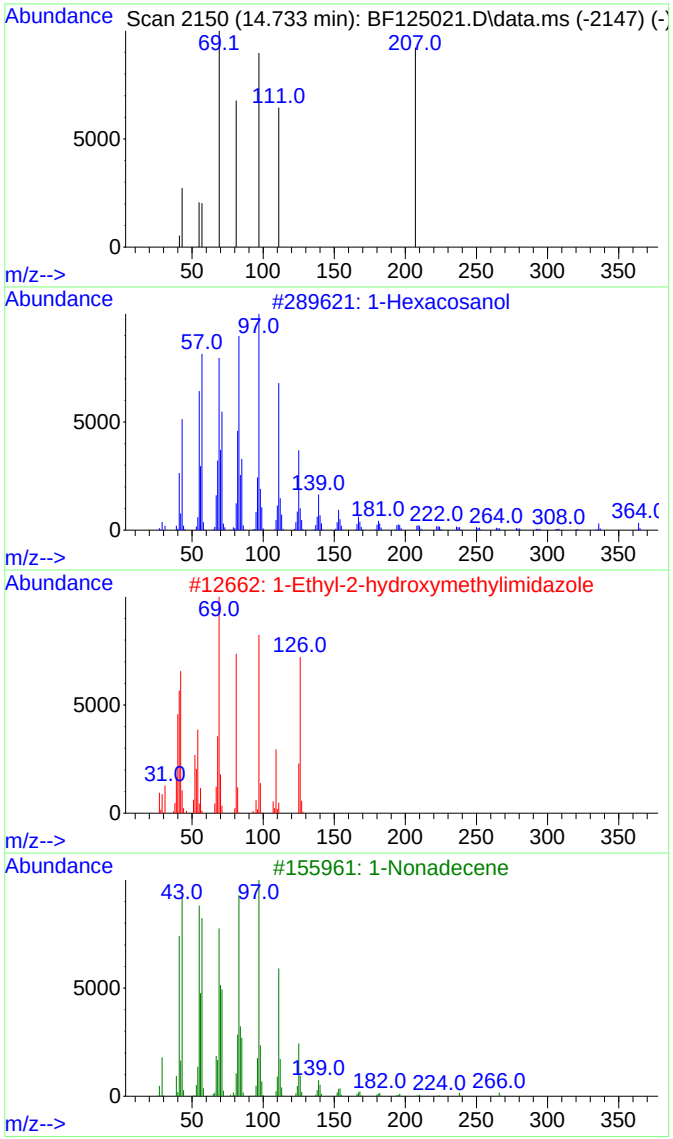
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

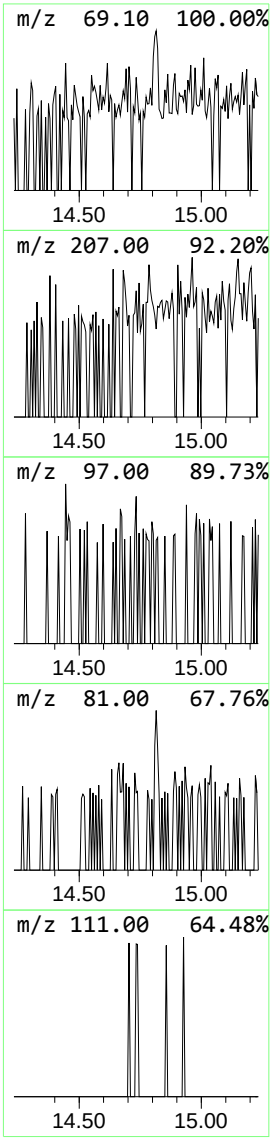
****

Peak Number 7 unknown14.733 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	3.39 ng	3456	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	9
2	1-Ethyl-2-hydroxymethylimidazole	126	C6H10N2O	063634-44-6	9
3	1-Nonadecene	266	C19H38	018435-45-5	9
4	2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	9
5	1-Hexadecanol	242	C16H34O	036653-82-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125021.D
Acq On : 10 Aug 2021 1:55
Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

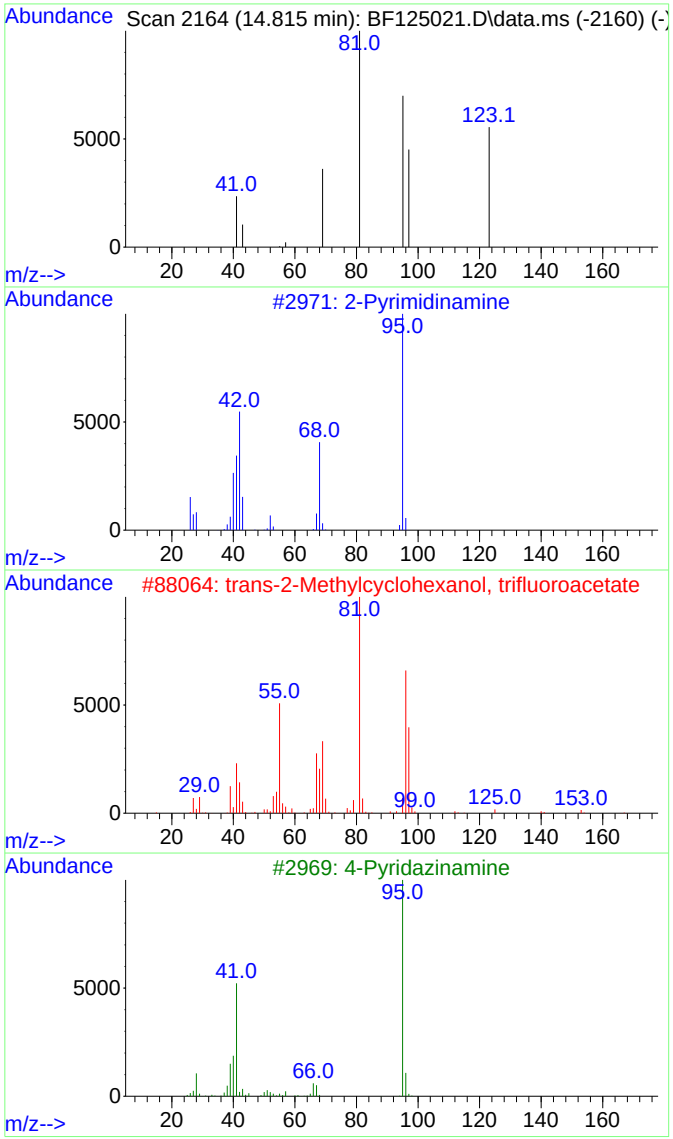
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

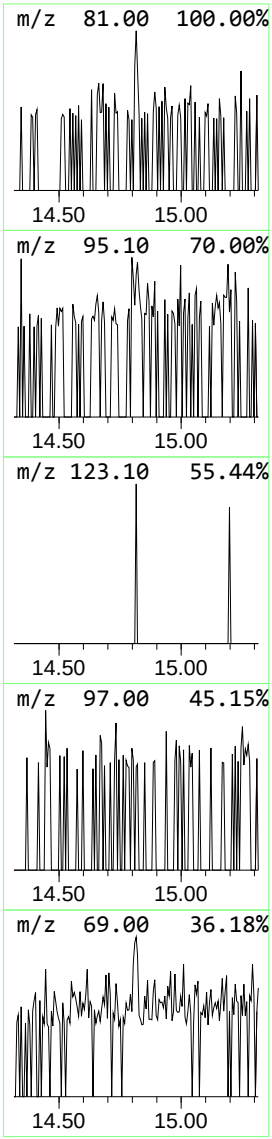
****

Peak Number 8 unknown14.816 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	4.78 ng	4874	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrimidinamine	95	C4H5N3	000109-12-6	4
2	trans-2-Methylcyclohexanol, trif...	210	C9H13F3O2	1000364-13-3	4
3	4-Pyridazinamine	95	C4H5N3	020744-39-2	3
4	1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	3
5	Ethanamine, 2-bromo-	123	C2H6BrN	000107-09-5	3





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Data File : BF125021.D
Acq On : 10 Aug 2021 1:55
Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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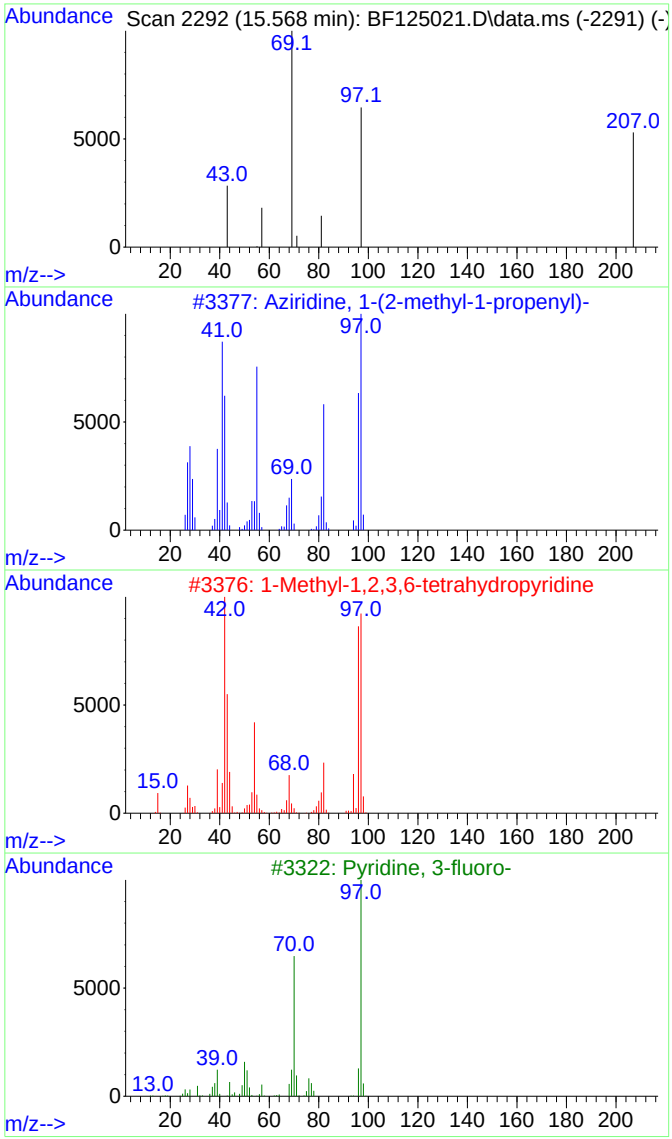
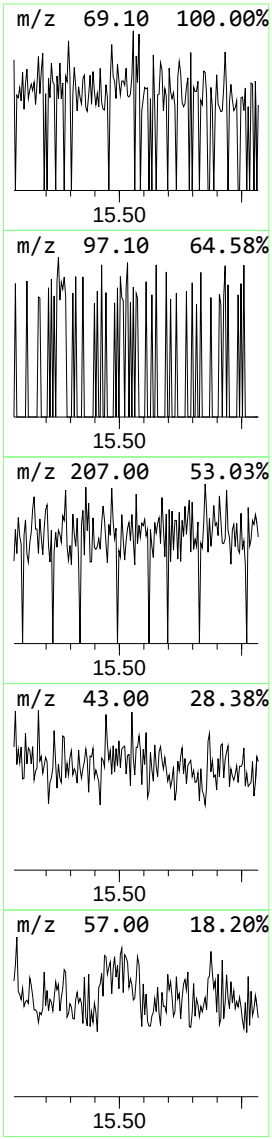
Peak Number 9 unknown15.568 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.568	2.12 ng	2160	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 1-(2-methyl-1-propenyl)-	97	C6H11N	080839-93-6	4
2	1-Methyl-1,2,3,6-tetrahydropyridine	97	C6H11N	000694-55-3	4
3	Pyridine, 3-fluoro-	97	C5H4FN	000372-47-4	4
4	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	4
5	1-Methylpyrazol-4-amine	97	C4H7N3	069843-13-6	4





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Data File : BF125021.D
Acq On : 10 Aug 2021 1:55
Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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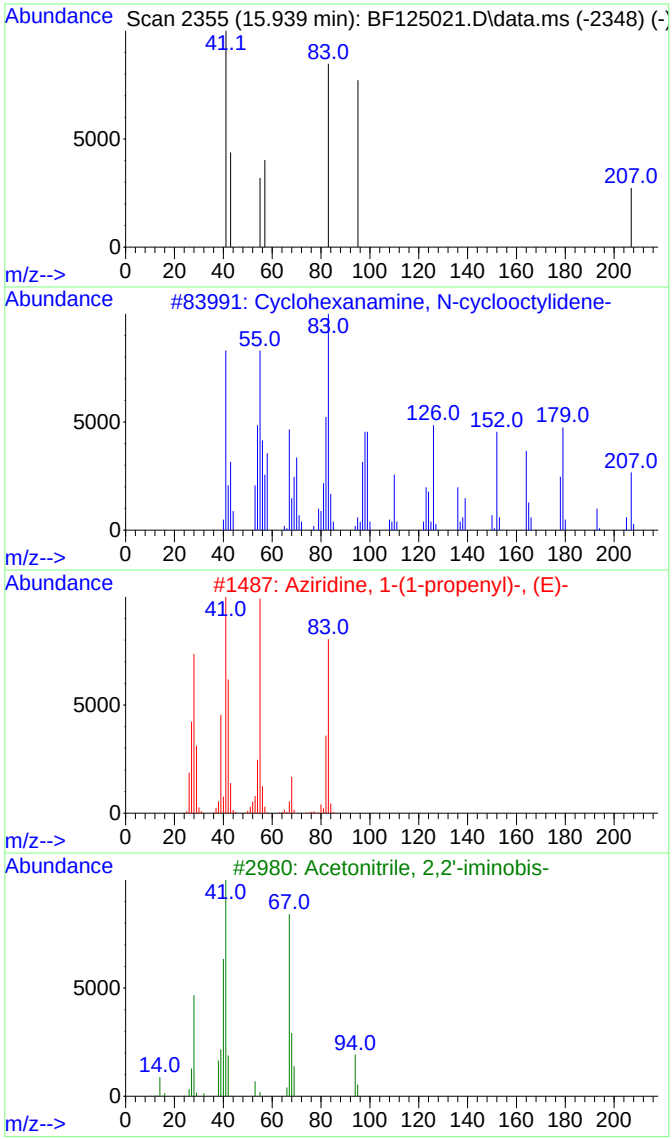
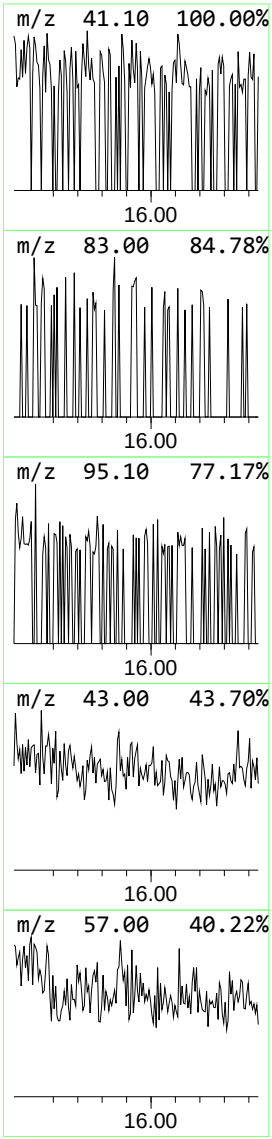
Peak Number 10 unknown15.939 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.939	3.62 ng	3686	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N-cyclooctylidene-	207	C14H25N	054699-42-2	4
2	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	4
3	Acetonitrile, 2,2'-iminobis-	95	C4H5N3	000628-87-5	3
4	4-Pyridinol	95	C5H5NO	000626-64-2	2
5	4-Pyridazinamine	95	C4H5N3	020744-39-2	2





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Data File : BF125021.D
Acq On : 10 Aug 2021 1:55
Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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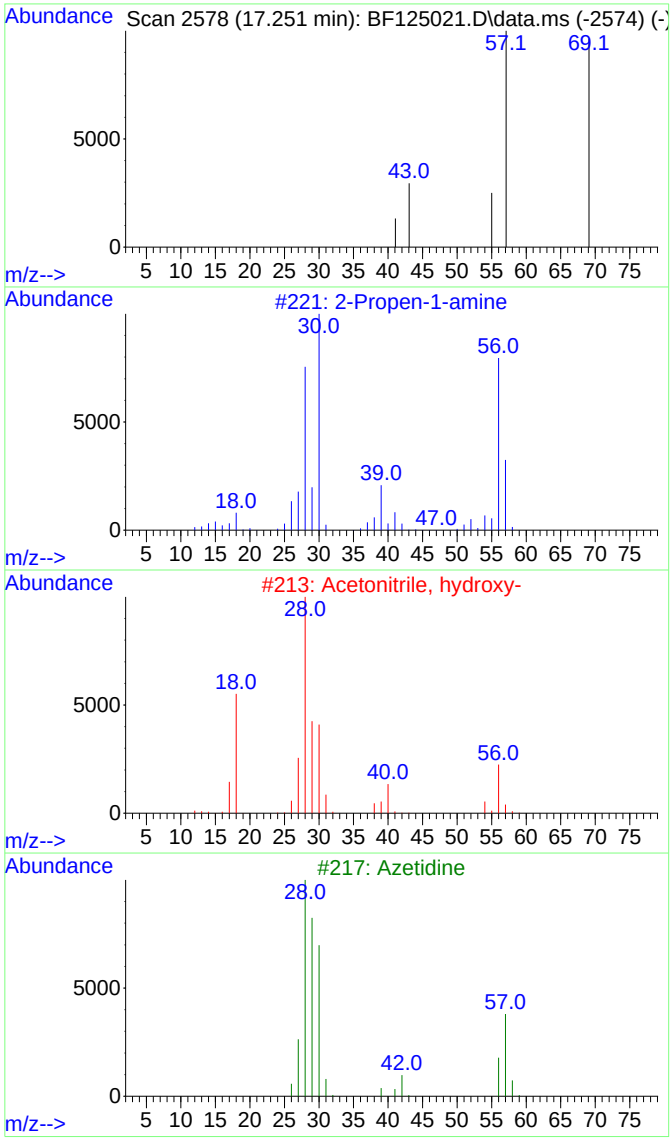
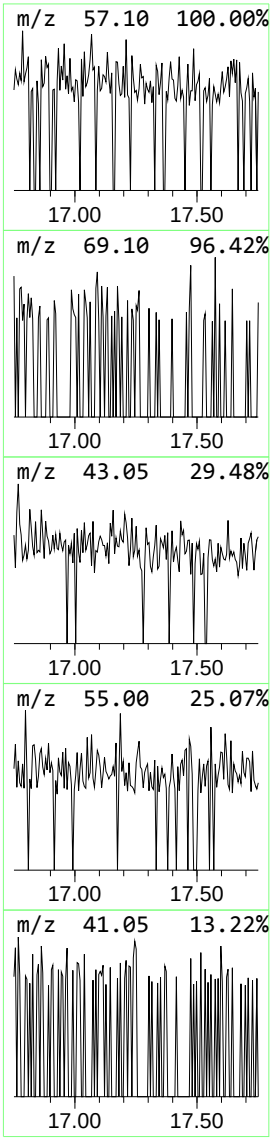
Peak Number 11 unknown17.251 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.251	2.77 ng	2827	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propen-1-amine	57	C3H7N	000107-11-9	3
2	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
3	Azetidine	57	C3H7N	000503-29-7	2
4	2-Propynenitrile, 3-fluoro-	69	C3FN	032038-83-8	2
5	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125021.D
Acq On : 10 Aug 2021 1:55
Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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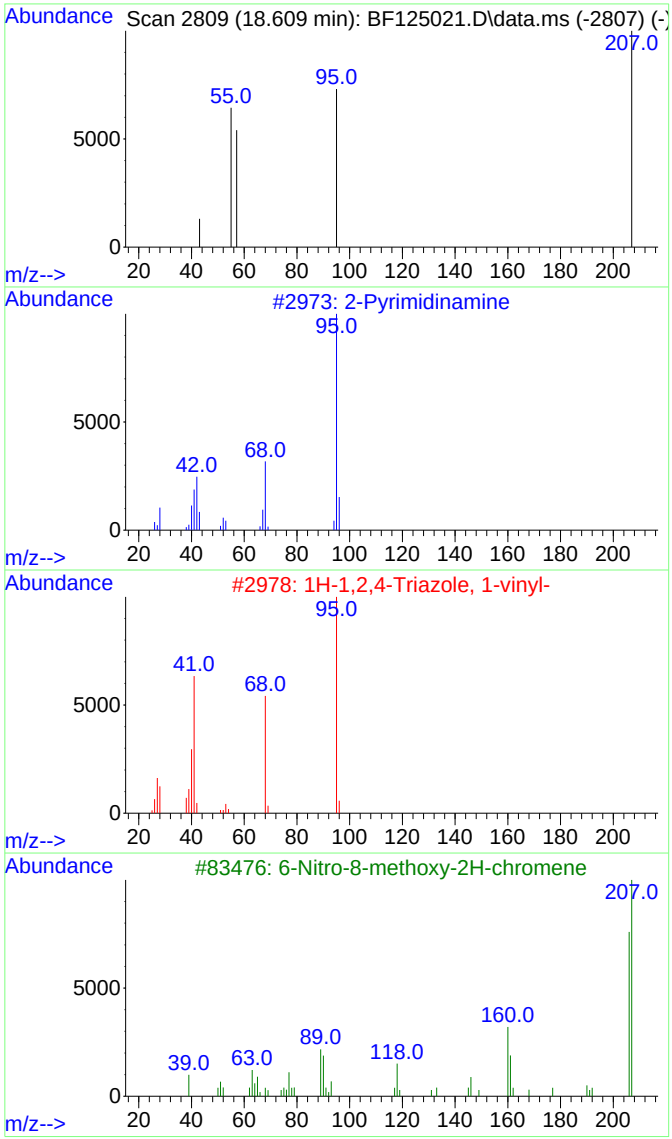
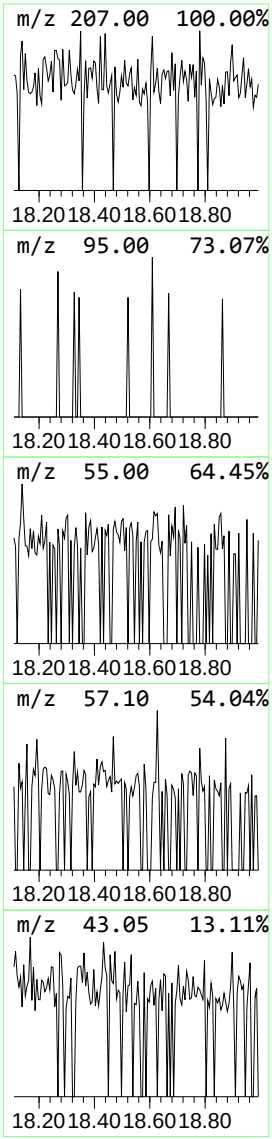
Peak Number 12 unknown18.609 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.609	2.12 ng	2162	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrimidinamine	95	C4H5N3	000109-12-6	3
2	1H-1,2,4-Triazole, 1-vinyl-	95	C4H5N3	002764-83-2	2
3	6-Nitro-8-methoxy-2H-chromene	207	C10H9NO4	062063-07-4	2
4	4-Pyridinol	95	C5H5NO	000626-64-2	2
5	2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125021.D
Acq On : 10 Aug 2021 1:55
Operator : JU/CG
Sample : M3295-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-022-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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
2-Pentanone, 4-...	5.040	64.7	ng	91041	1	6.822	28123	20.0
2-Pentanone, 4-...	5.834	10.1	ng	14198	1	6.822	28123	20.0
Ethanol, 2-(2-b...	8.004	17.0	ng	28352	2	8.104	33359	20.0
unknown11.863	11.863	3.0	ng	3992	4	11.339	26256	20.0
Silane, trichlo...	13.816	6.2	ng	9538	5	13.980	30964	20.0
unknown14.457	14.457	2.2	ng	3412	5	13.980	30964	20.0
unknown14.733	14.733	3.4	ng	3456	6	15.439	20380	20.0
unknown14.816	14.816	4.8	ng	4874	6	15.439	20380	20.0
unknown15.568	15.568	2.1	ng	2160	6	15.439	20380	20.0
unknown15.939	15.939	3.6	ng	3686	6	15.439	20380	20.0
unknown17.251	17.251	2.8	ng	2827	6	15.439	20380	20.0
unknown18.609	18.609	2.1	ng	2162	6	15.439	20380	20.0