LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071621

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-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124651.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	14	17	20	rBB	3023	3184	3.92%	0.476%
2	5.116	512	515	518	rBB	1809	1649	2.03%	0.247%
3	5.510	578	582	585	rBB	71939	59107	72.77%	8.845%
4	6.516	749	753	756	rBB	72938	60702	74.74%	9.084%
5	6.904	816	819	822	rBB	49671	36918	45.45%	5.525%
6	7.463	910	914	917	rBB	51537	38628	47.56%	5.781%
7	8.081	1017	1019	1021	rBB	3025	2000	2.46%	0.299%
8	8.186	1034	1037	1040	rBB	65667	47775	58.82%	7.149%
9	9.263	1217	1220	1223	rBB	96271	67020	82.52%	10.029%
10	9.945	1333	1336	1339	rBB	58916	42820	52.72%	6.408%
11	10.727	1467	1469	1472	rBB	31952	22112	27.23%	3.309%
12	11.433	1585	1589	1592	rBB	42993	33535	41.29%	5.018%
13	11.633	1620	1623	1626	rBB	2547	2238	2.76%	0.335%
14	11.945	1674	1676	1678	rBB	3508	2285	2.81%	0.342%
15	12.733	1809	1810	1813	rBB	2053	1210	1.49%	0.181%
16	12.886	1828	1836	1846	rBV	55669	81219	100.00%	12.154%
17	13.016	1855	1858	1861	rVB	67210	46801	57.62%	7.004%
18	13.210	1889	1891	1895	rVV	3059	3253	4.01%	0.487%
19	13.245	1895	1897	1899	rVB2	2472	1633	2.01%	0.244%
20	13.586	1953	1955	1957	rBV	2087	1717	2.11%	0.257%
21	13.786	1984	1989	1991	rBV2	993	1458	1.80%	0.218%
22	13.910	2007	2010	2014	rBV2	4427	5084	6.26%	0.761%
23	14.068	2034	2037	2040	rBV2	29059	26633	32.79%	3.986%
24	14.192	2054	2058	2061	rBV3	1126	2070	2.55%	0.310%
25	14.221	2061	2063	2064	rVV	1493	1316	1.62%	0.197%
26	14.233	2064	2065	2069	rVB	2109	1273	1.57%	0.191%
27	14.533	2113	2116	2121	rBV2	2018	2934	3.61%	0.439%
28	14.662	2137	2138	2142	rBV2	1071	946	1.16%	0.142%
29	14.810	2161	2163	2165	rVB	1225	1115	1.37%	0.167%
30	14.851	2165	2170	2172	rBV4	2622	4374	5.39%	0.655%
31	14.974	2189	2191	2194	rVB3	1199	1045	1.29%	0.156%
32	14.998	2194	2195	2199	rBV2	865	1075	1.32%	0.161%
33	15.198	2227	2229	2232	rVB	3502	3489	4.30%	0.522%
34	15.421	2264	2267	2270	rVB2	911	1260	1.55%	0.189%
35	15.474	2274	2276	2277	rBV2	1068	980	1.21%	0.147%
36	15.562	2286	2291	2294	rBV	15918	18774	23.12%	2.809%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071621

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-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.592	2294	2296	2299	rVB	2185	1872	2.30%	0.280%
38	15.715	2314	2317	2320	rBV2	1461	1720	2.12%	0.257%
39	15.768	2322	2326	2327	rBV2	1044	1310	1.61%	0.196%
40	16.045	2367	2373	2376	rBV3	2885	4214	5.19%	0.631%
41	16.080	2376	2379	2381	rBV2	1006	989	1.22%	0.148%
42	16.157	2389	2392	2394	rBV	1034	1255	1.55%	0.188%
43	16.209	2397	2401	2404	rVB2	1052	1094	1.35%	0.164%
44	16.256	2406	2409	2411	rBV3	921	1141	1.40%	0.171%
45	16.427	2435	2438	2440	rBV	856	1036	1.28%	0.155%
46	16.556	2459	2460	2465	rVB	1805	1859	2.29%	0.278%
47	16.715	2485	2487	2491	rVB2	640	920	1.13%	0.138%
48	16.786	2497	2499	2502	rVB2	1056	916	1.13%	0.137%
49	17.139	2555	2559	2560	rVB	1123	1393	1.72%	0.208%
50	17.162	2560	2563	2566	rBV2	1558	2462	3.03%	0.368%
51	17.192	2566	2568	2571	rVB2	1356	1583	1.95%	0.237%
52	17.256	2578	2579	2581	rBV	1133	970	1.19%	0.145%
53	17.333	2589	2592	2596	rBV3	692	931	1.15%	0.139%
54	17.621	2638	2641	2643	rBV2	1253	1690	2.08%	0.253%
55	17.656	2645	2647	2648	rBV	1173	980	1.21%	0.147%
56	17.715	2655	2657	2660	rVB	1412	1111	1.37%	0.166%
57	17.739	2660	2661	2664	rBV	1062	969	1.19%	0.145%
58	17.898	2686	2688	2693	rVB	1072	1729	2.13%	0.259%
59	18.345	2763	2764	2768	rVB	1546	1115	1.37%	0.167%
60	18.533	2794	2796	2799	rBV	1000	1011	1.24%	0.151%
61	18.762	2829	2835	2837	rBV	1211	2083	2.56%	0.312%
62	18.827	2843	2846	2848	rVB	810	1036	1.28%	0.155%
63	18.874	2852	2854	2857	rBV	1026	1213	1.49%	0.182%

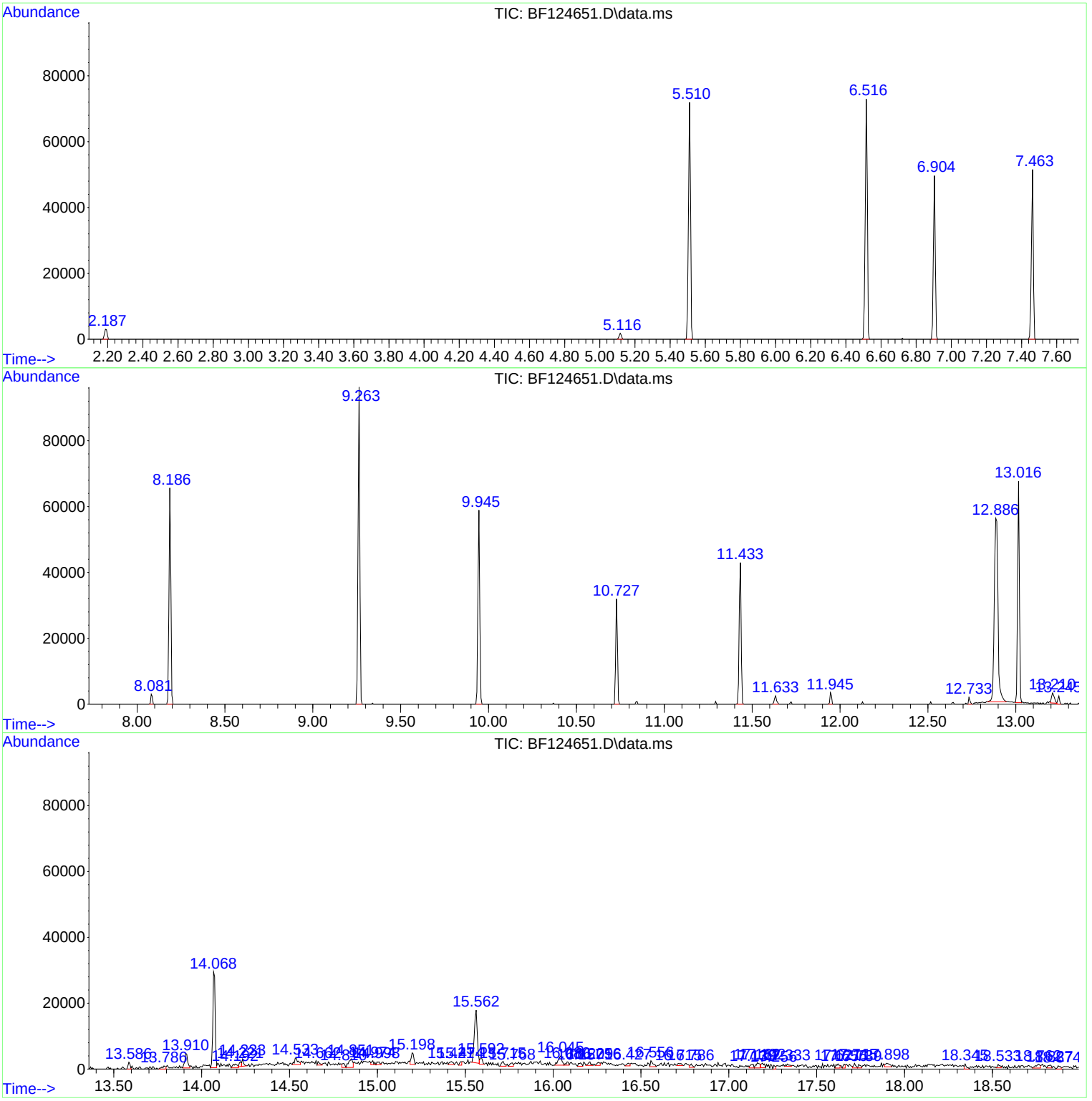
Sum of corrected areas: 668234

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-071621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-071621

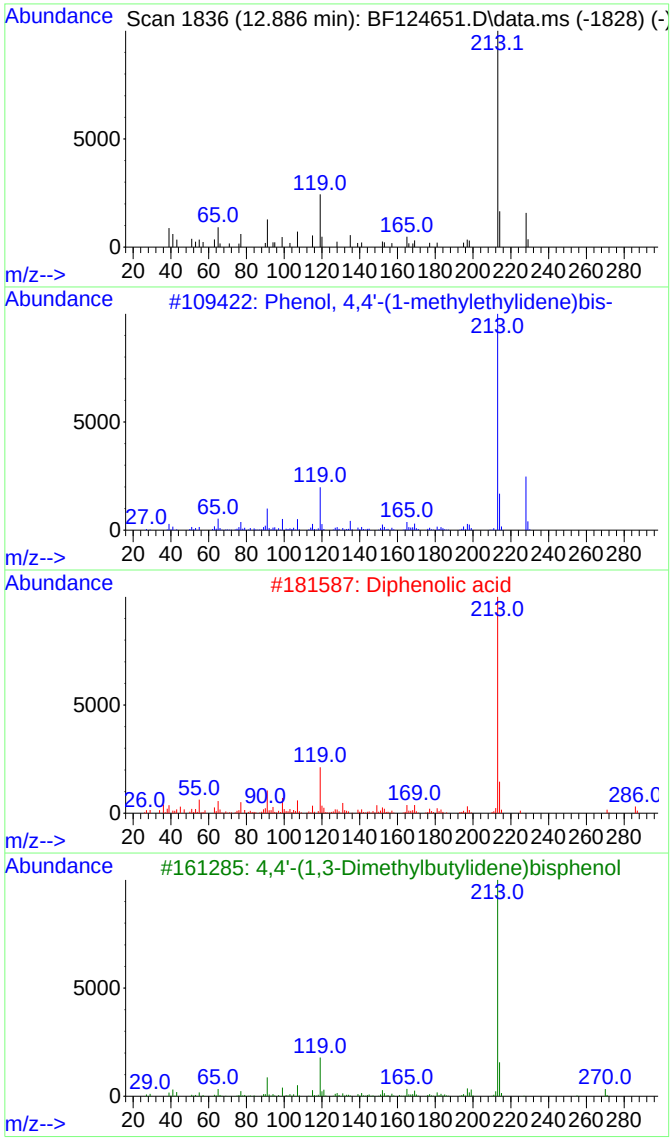
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

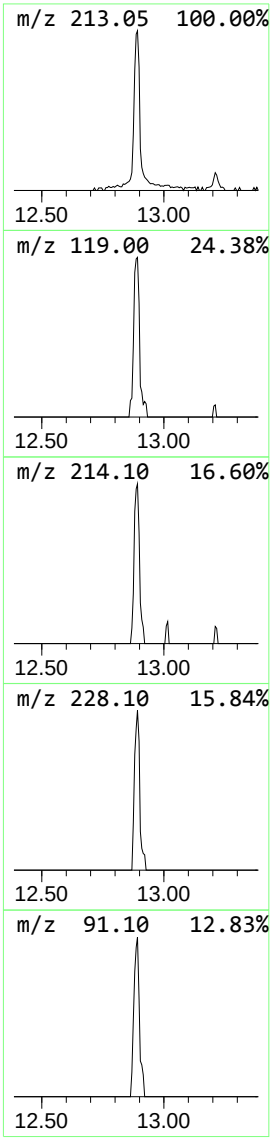
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Phenol, 4,4'-(1-methylethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	60.99 ng	81219	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	Diphenolic acid	286	C17H18O4	000126-00-1	72
3	4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	72
4	5-Fluoro-2-nitrophenylamine, TMS...	228	C9H13FN2O2Si	1000484-54-5	59
5	2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-071621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

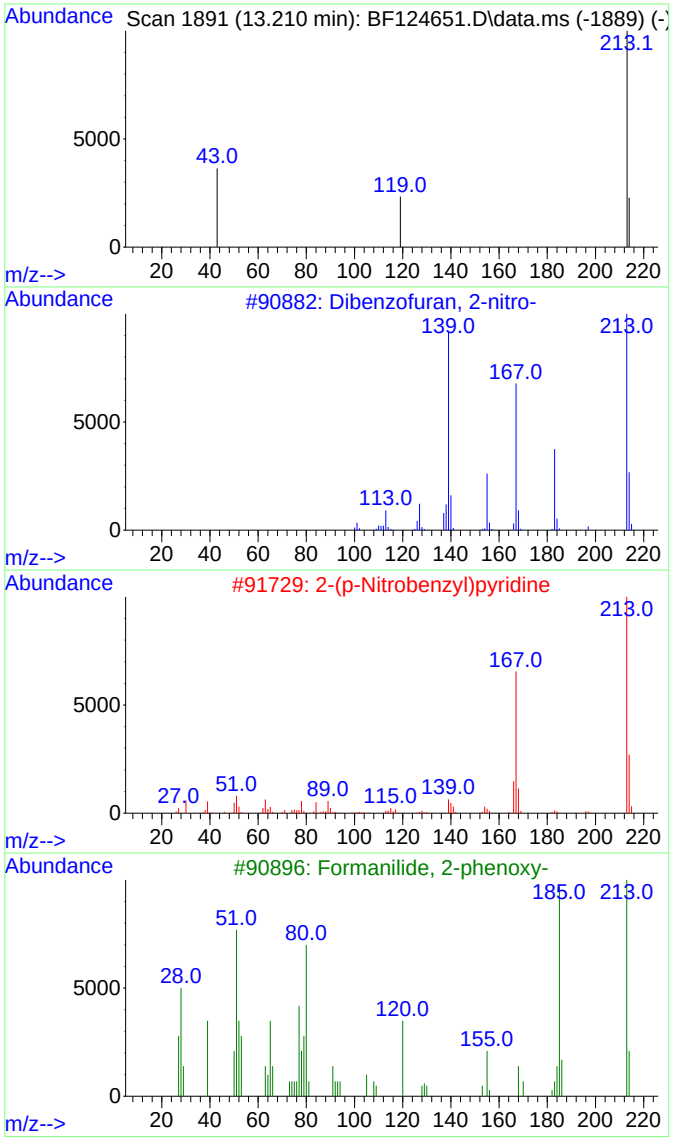
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

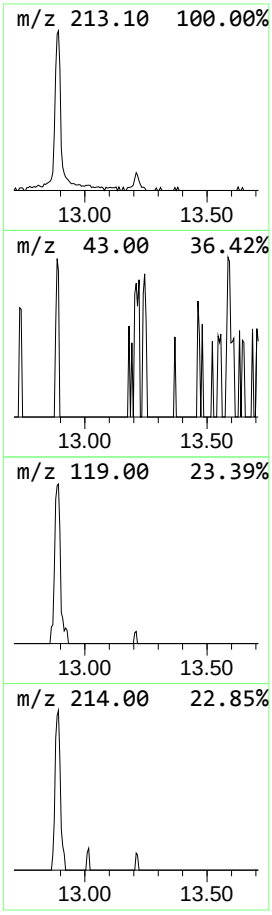
****

Peak Number 2 unknown13.210 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.210	2.44 ng	3253	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzofuran, 2-nitro-	213	C12H7NO3	020927-95-1	5
2	2-(p-Nitrobenzyl)pyridine	214	C12H10N2O2	000620-87-1	5
3	Formanilide, 2-phenoxy-	213	C13H11NO2	002770-12-9	5
4	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	5
5	benzenamine, 4-[2-(2-furanyl)eth...	213	C14H15NO	1000400-66-9	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-071621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

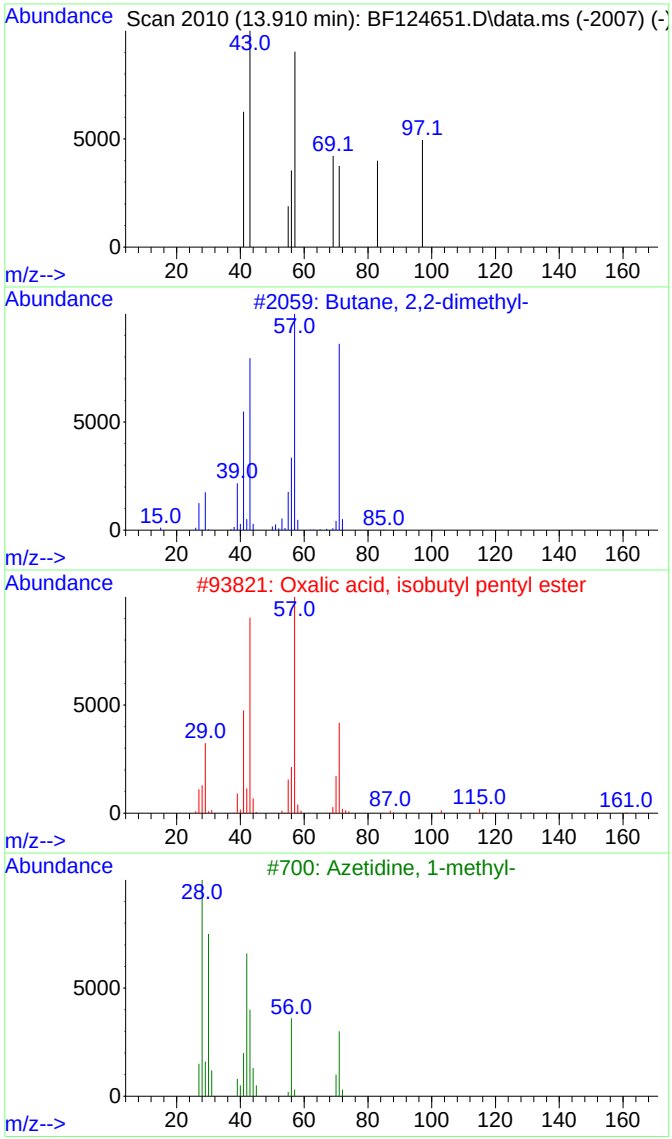
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

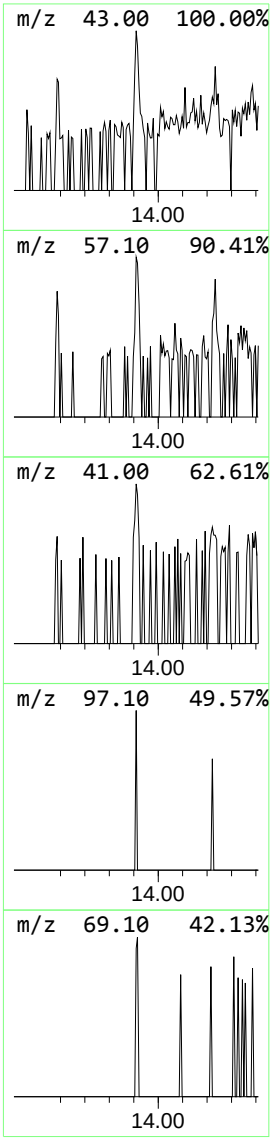
****

Peak Number 3 unknown13.910 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	3.82 ng	5084	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
2	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	9
3	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	4
4	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	4
5	Azetidine	57	C3H7N	000503-29-7	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-071621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

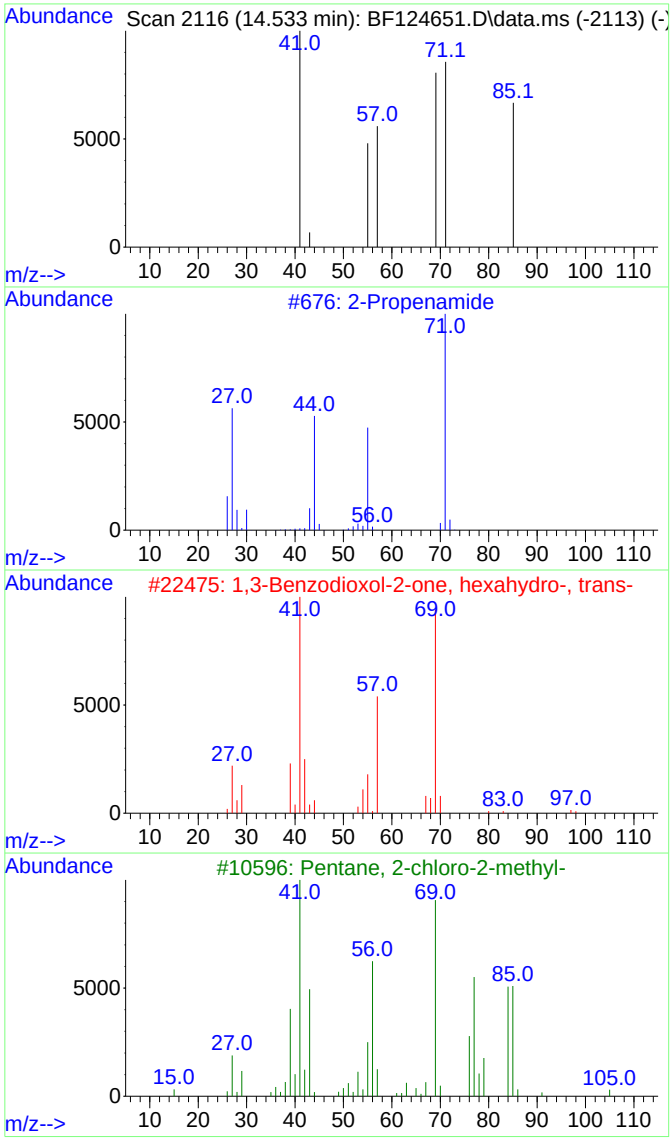
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

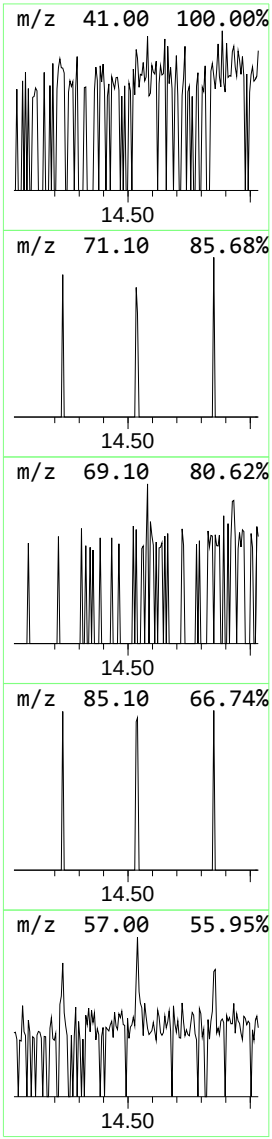
****

Peak Number 4 unknown14.533 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	2.20 ng	2934	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide	71	C3H5NO	000079-06-1	5
2	1,3-Benzodioxol-2-one, hexahydro...	142	C7H10O3	020192-66-9	4
3	Pentane, 2-chloro-2-methyl-	120	C6H13Cl	004325-48-8	4
4	2,2,6,6-Tetramethylheptane	156	C11H24	040117-45-1	4
5	3H-1,2,4-Triazol-3-one, 1,2-dihy...	85	C2H3N3O	000930-33-6	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-071621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

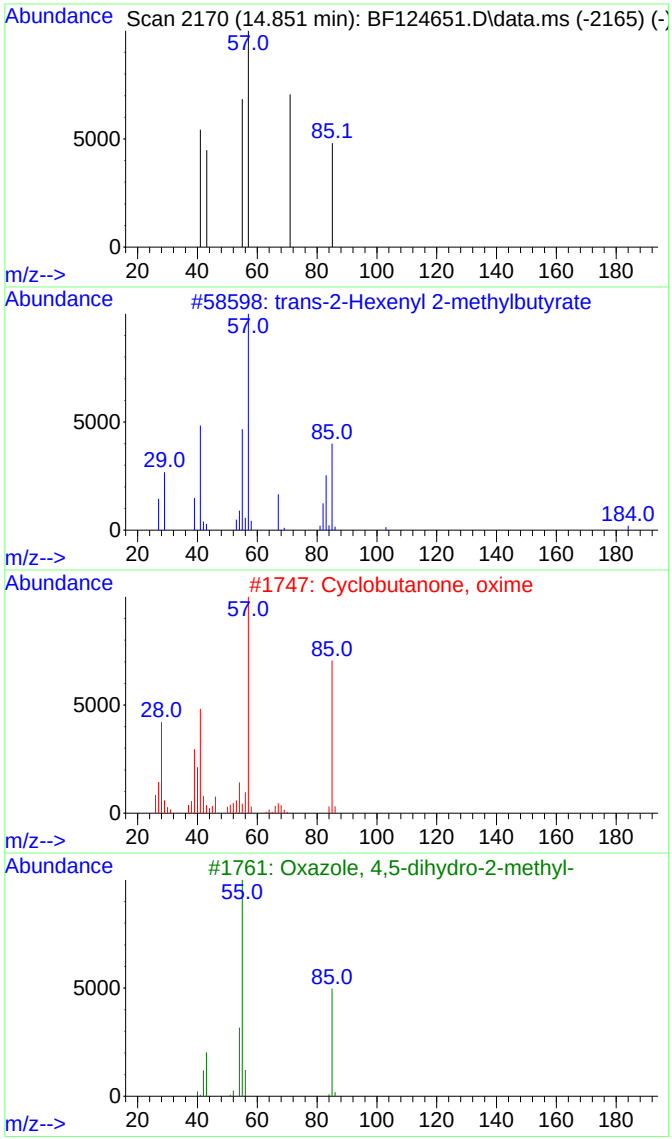
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

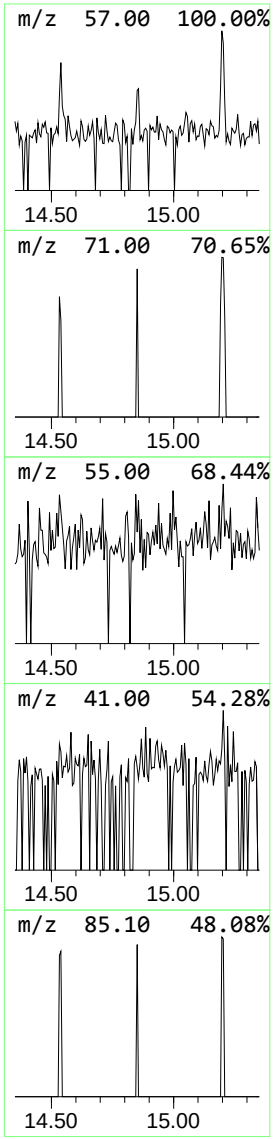
****

Peak Number 5 unknown14.851 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	4.66 ng	4374	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
2	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
3	Oxazole, 4,5-dihydro-2-methyl-	85	C4H7NO	001120-64-5	4
4	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
5	(E)-But-2-en-1-yl 2-methylbutanoate	156	C9H16O2	1000372-81-0	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

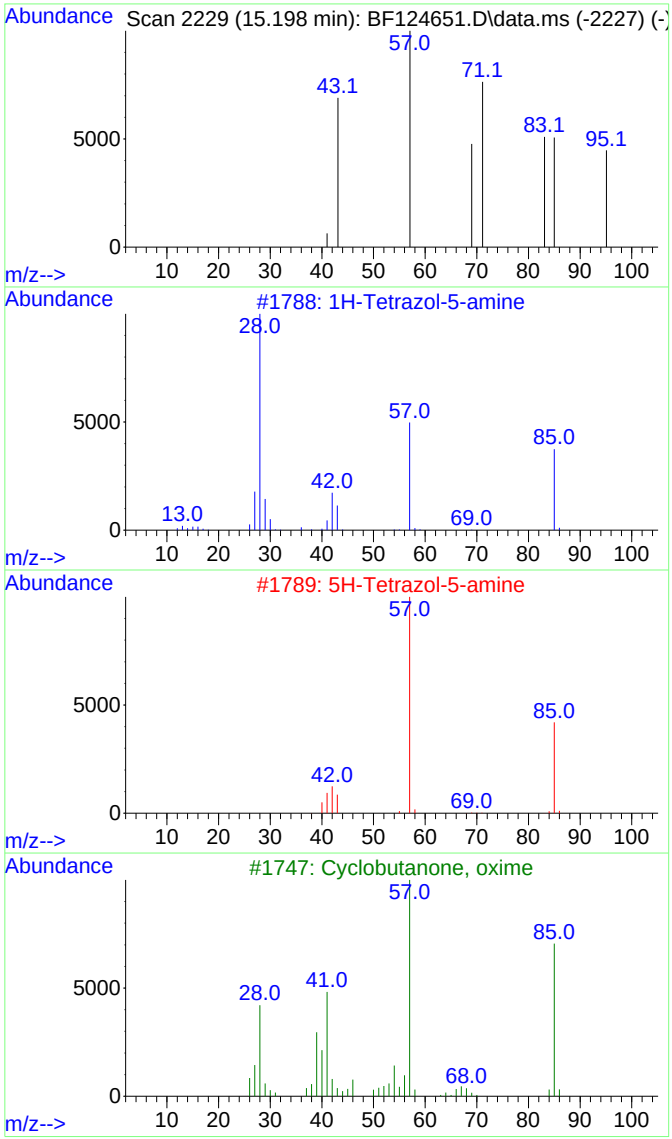
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

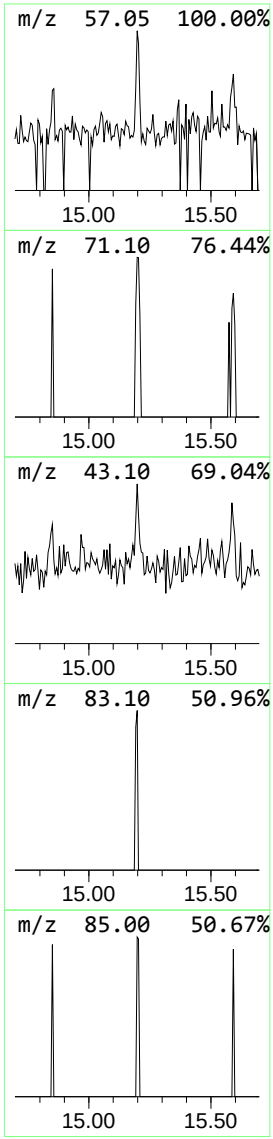
****

Peak Number 6 unknown15.198 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	3.72 ng	3489	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
2	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
3	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
4	Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	4
5	Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

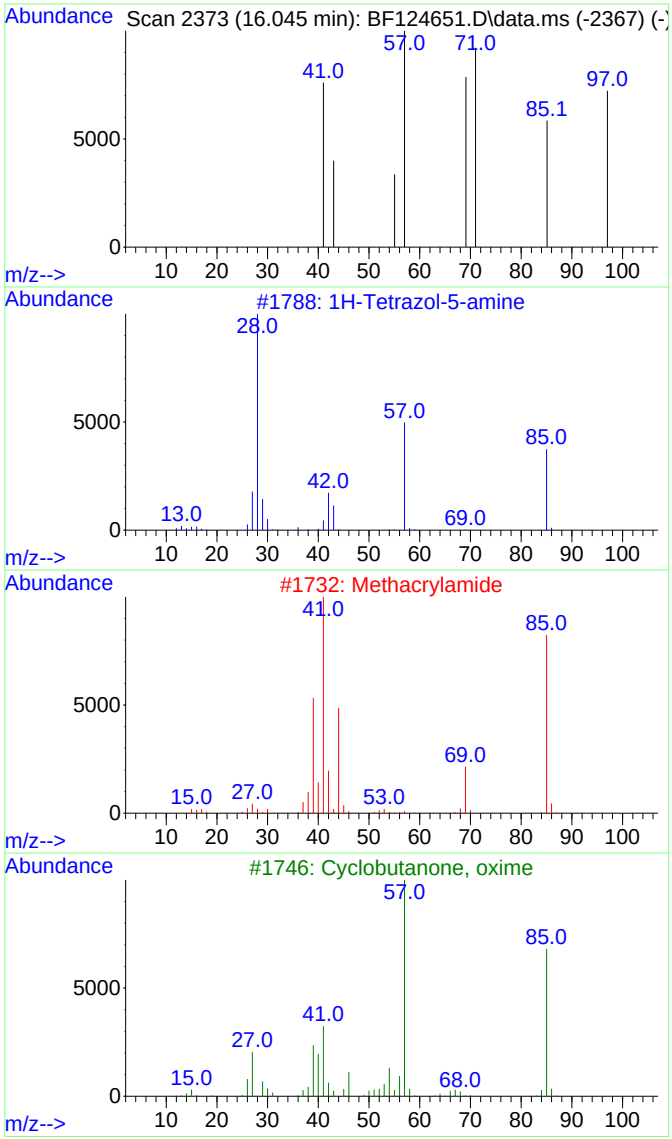
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

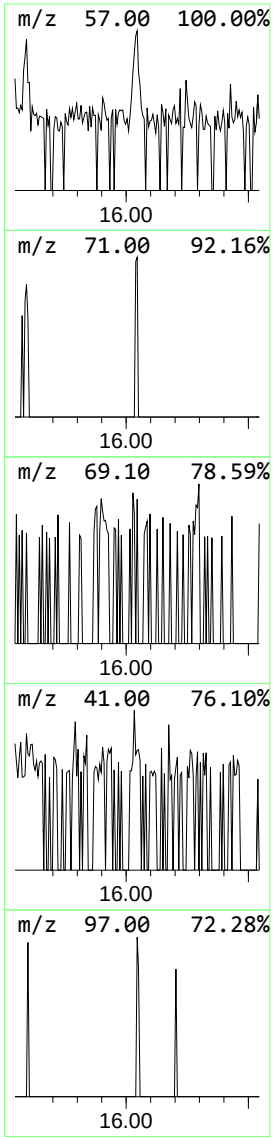
****

Peak Number 7 unknown16.045 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.045	4.49 ng	4214	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
2	Methacrylamide	85	C4H7NO	000079-39-0	4
3	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
4	trans-Crotonamide	85	C4H7NO	000625-37-6	4
5	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

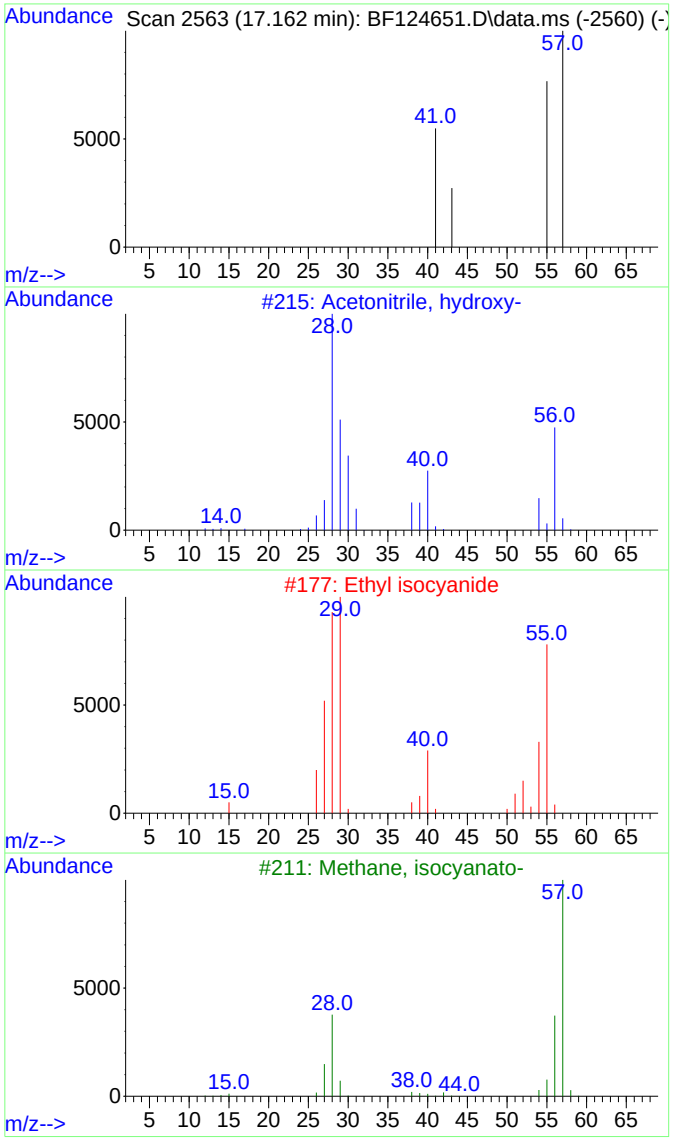
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

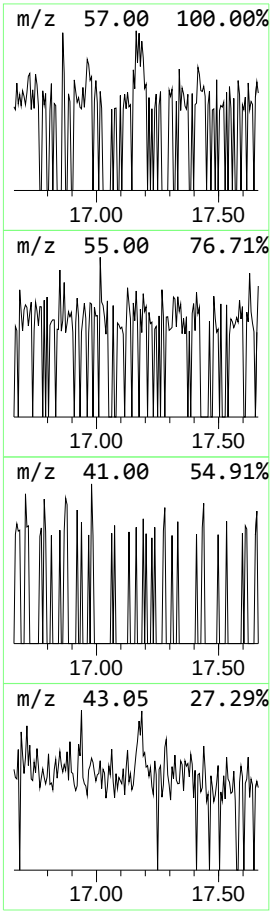
****

Peak Number 8 unknown17.162 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.162	2.62 ng	2462	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
2	Ethyl isocyanide	55	C3H5N	000624-79-3	1
3	Methane, isocyanato-	57	C2H3NO	000624-83-9	1
4	Azetidine	57	C3H7N	000503-29-7	1
5	Oxalic acid, butyl propyl ester	188	C9H16O4	1000309-25-6	1





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-071621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

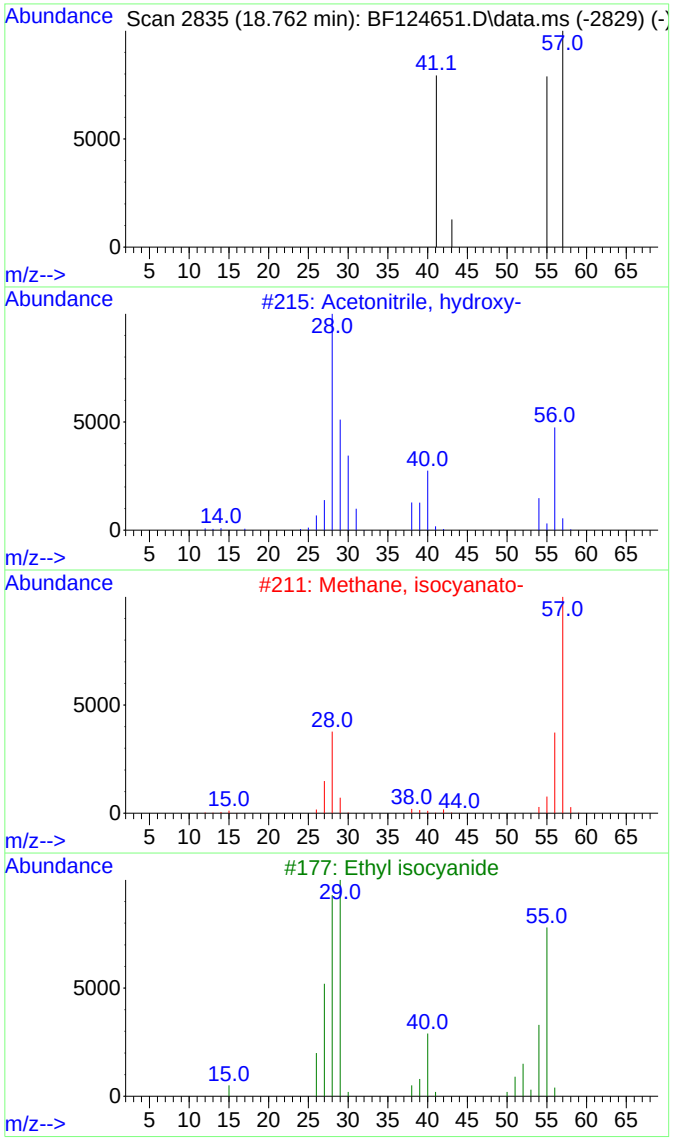
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

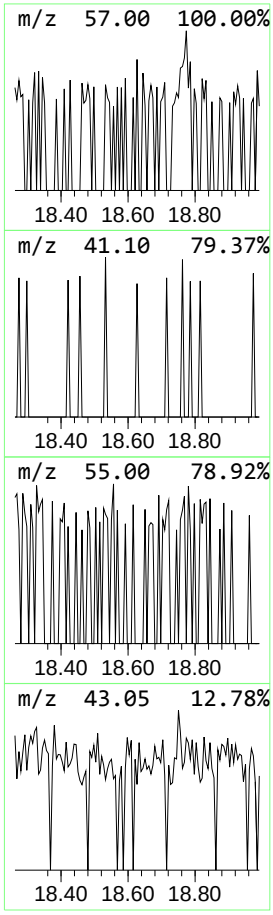
****

Peak Number 9 unknown18.762 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.762	2.22 ng	2083	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
2	Methane, isocyanato-	57	C2H3NO	000624-83-9	1
3	Ethyl isocyanide	55	C3H5N	000624-79-3	1
4	Azetidine	57	C3H7N	000503-29-7	1
5	Oxalic acid, butyl propyl ester	188	C9H16O4	1000309-25-6	1





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124651.D
Acq On : 21 Jul 2021 4:13
Operator : JU/CG
Sample : M3074-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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
Phenol, 4,4'-(1...	12.886	61.0	ng	81219	5	14.068	26633	20.0
unknown13.210	13.210	2.4	ng	3253	5	14.068	26633	20.0
unknown13.910	13.910	3.8	ng	5084	5	14.068	26633	20.0
unknown14.533	14.533	2.2	ng	2934	5	14.068	26633	20.0
unknown14.851	14.851	4.7	ng	4374	6	15.562	18774	20.0
unknown15.198	15.198	3.7	ng	3489	6	15.562	18774	20.0
unknown16.045	16.045	4.5	ng	4214	6	15.562	18774	20.0
unknown17.162	17.162	2.6	ng	2462	6	15.562	18774	20.0
unknown18.762	18.762	2.2	ng	2083	6	15.562	18774	20.0