LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124755.D
Acq On : 24 Jul 2021 19:18
Operator : JU/CG
Sample : M3117-09 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NJ-CLEAN-9

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: BF124755.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	5	8	12	rBB	4971	5440	8.15%	0.913%
2	2.481	64	67	70	rBB	2773	2251	3.37%	0.378%
3	5.081	507	509	511	rBB	1334	1060	1.59%	0.178%
4	5.481	573	577	580	rBB	69507	58712	87.94%	9.849%
5	6.487	745	748	751	rBB	65733	59747	89.49%	10.022%
6	6.875	811	814	816	rBB	45608	39006	58.42%	6.543%
7	7.428	905	908	911	rBB	44158	38915	58.29%	6.528%
8	8.051	1012	1014	1017	rBB	16582	10997	16.47%	1.845%
9	8.157	1028	1032	1035	rBB	64334	50964	76.33%	8.549%
10	9.228	1211	1214	1217	rBV	96630	66764	100.00%	11.199%
11	9.910	1327	1330	1333	rBB	64631	46771	70.05%	7.846%
12	10.692	1461	1463	1466	rBB	31334	23738	35.56%	3.982%
13	11.398	1579	1583	1586	rBV	43926	35397	53.02%	5.938%
14	12.610	1787	1789	1791	rBB	1846	1243	1.86%	0.209%
15	12.839	1826	1828	1830	rBB	1541	1118	1.67%	0.188%
16	12.980	1849	1852	1855	rBB	57072	42444	63.57%	7.120%
17	13.880	2002	2005	2007	rBV4	2608	2389	3.58%	0.401%
18	14.033	2027	2031	2034	rBV	33565	29432	44.08%	4.937%
19	14.092	2039	2041	2045	rBV	1409	1591	2.38%	0.267%
20	14.192	2055	2058	2062	rBV	1659	2048	3.07%	0.344%
21	14.268	2068	2071	2074	rBV2	901	1174	1.76%	0.197%
22	14.315	2076	2079	2080	rBV2	1345	1100	1.65%	0.185%
23	14.504	2107	2111	2112	rBV	2326	2099	3.14%	0.352%
24	14.639	2133	2134	2137	rBV2	1936	1771	2.65%	0.297%
25	14.710	2145	2146	2150	rVB3	1281	961	1.44%	0.161%
26	14.763	2153	2155	2158	rVB3	1257	1094	1.64%	0.184%
27	14.868	2171	2173	2174	rBV2	1478	966	1.45%	0.162%
28	15.074	2205	2208	2210	rBV3	1535	1815	2.72%	0.304%
29	15.151	2219	2221	2225	rVB	2912	2722	4.08%	0.457%
30	15.192	2225	2228	2230	rBV2	851	1222	1.83%	0.205%
31	15.227	2230	2234	2237	rVV2	1488	2636	3.95%	0.442%
32	15.292	2241	2245	2248	rVB5	1735	2433	3.64%	0.408%
33	15.439	2268	2270	2273	rVB3	1009	1075	1.61%	0.180%
34	15.510	2278	2282	2285	rVV2	17649	21351	31.98%	3.582%
35	15.533	2285	2286	2288	rVV2	2798	1933	2.90%	0.324%
36	15.586	2291	2295	2298	rVV3	1222	1702	2.55%	0.286%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124755.D
Acq On : 24 Jul 2021 19:18
Operator : JU/CG
Sample : M3117-09 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NJ-CLEAN-9

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

37	15.610	2298	2299	2303	rVB	1334	1247	1.87%	0.209%
38	15.745	2319	2322	2325	rVB	1449	1413	2.12%	0.237%
39	15.974	2358	2361	2369	rVB2	2599	4145	6.21%	0.695%
40	16.098	2379	2382	2385	rVB3	1124	1205	1.80%	0.202%
41	16.221	2401	2403	2407	rBV3	1696	1725	2.58%	0.289%
42	16.286	2411	2414	2417	rVB3	1326	1396	2.09%	0.234%
43	16.357	2424	2426	2428	rBV2	1309	1406	2.11%	0.236%
44	16.480	2445	2447	2453	rVB3	1103	1545	2.31%	0.259%
45	16.786	2498	2499	2504	rVB2	1433	1899	2.84%	0.319%
46	17.174	2560	2565	2567	rBV2	1343	1914	2.87%	0.321%
47	17.286	2581	2584	2585	rVB2	1892	1386	2.08%	0.232%
48	17.562	2629	2631	2632	rBV	1107	1135	1.70%	0.190%
49	17.721	2655	2658	2660	rBV3	1285	1327	1.99%	0.223%
50	17.786	2667	2669	2672	rBV2	1006	993	1.49%	0.167%
51	18.003	2701	2706	2708	rBV	764	1028	1.54%	0.172%
52	18.239	2743	2746	2748	rVB2	1025	1053	1.58%	0.177%
53	18.380	2768	2770	2774	rVB2	821	961	1.44%	0.161%
54	18.433	2776	2779	2782	rBV3	1026	1314	1.97%	0.220%
55	18.545	2795	2798	2801	rBV2	848	1269	1.90%	0.213%
56	18.927	2860	2863	2867	rBV3	999	1703	2.55%	0.286%

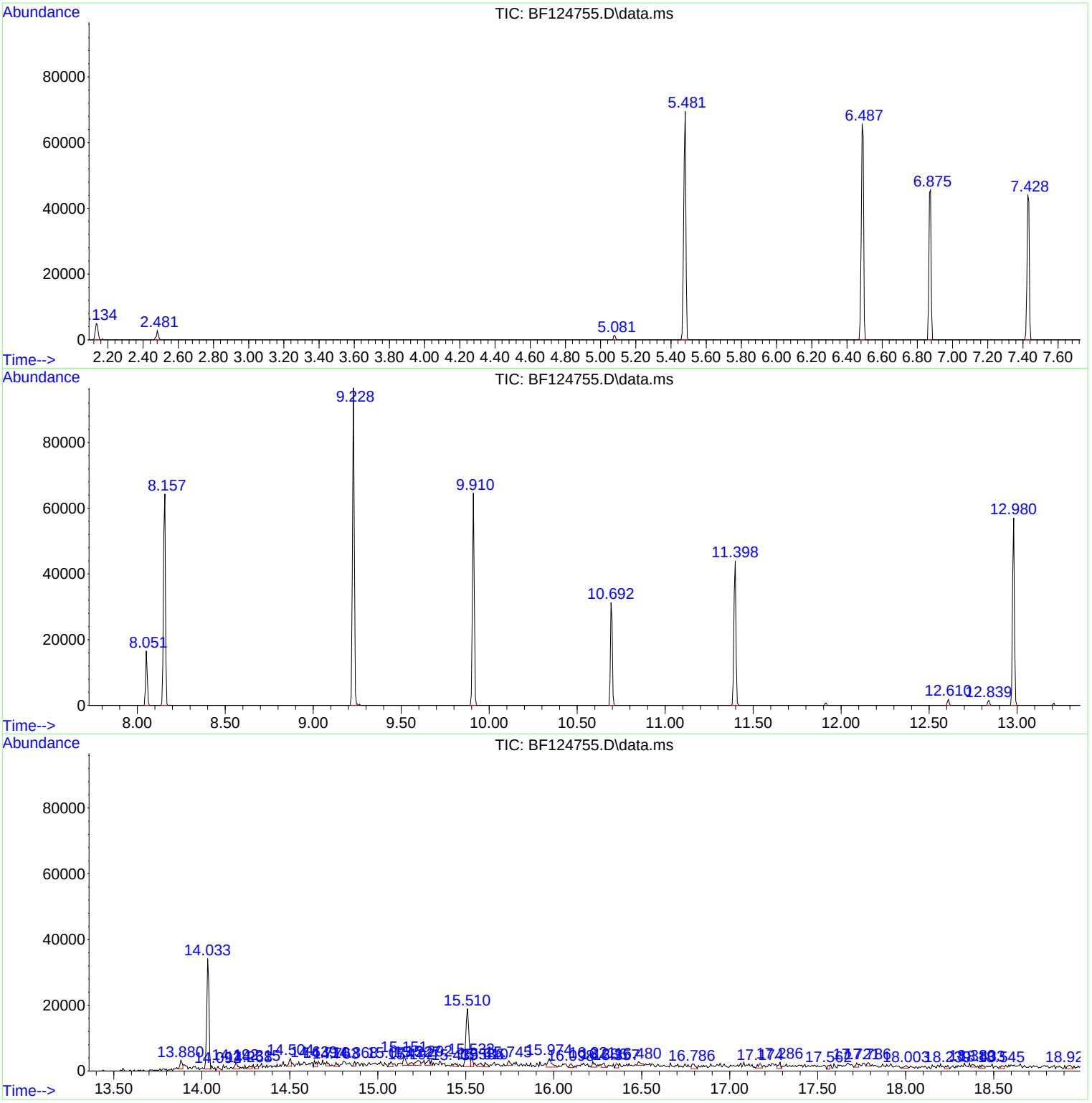
Sum of corrected areas: 596145

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124755.D
Acq On : 24 Jul 2021 19:18
Operator : JU/CG
Sample : M3117-09 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

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\BF072421\
Data File : BF124755.D
Acq On : 24 Jul 2021 19:18
Operator : JU/CG
Sample : M3117-09 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

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

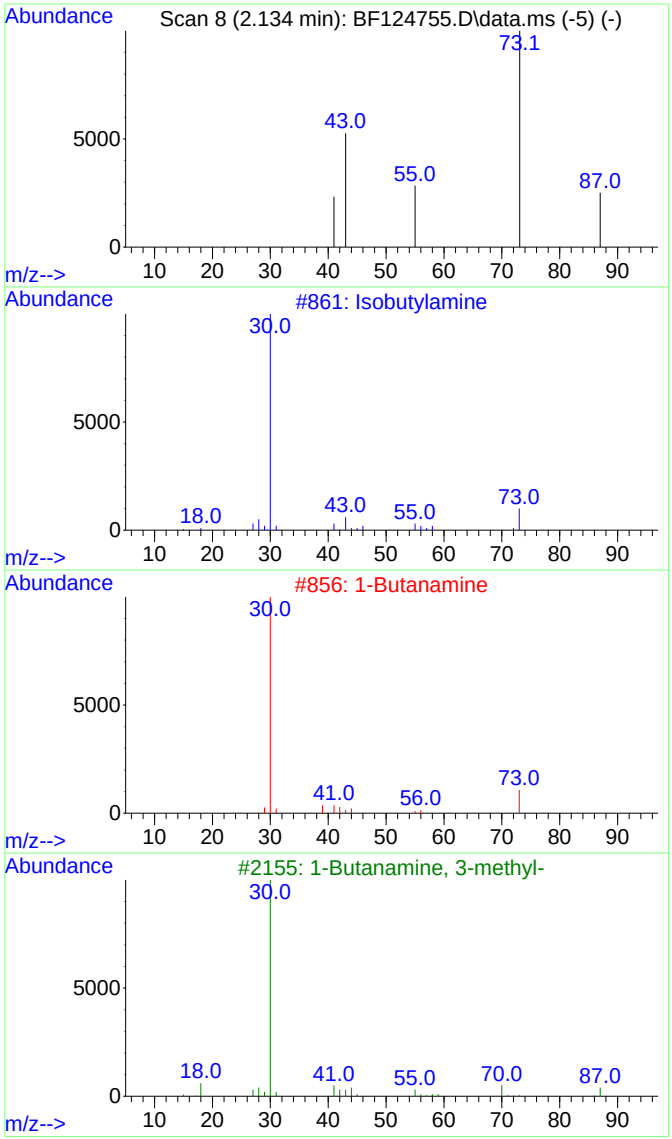
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

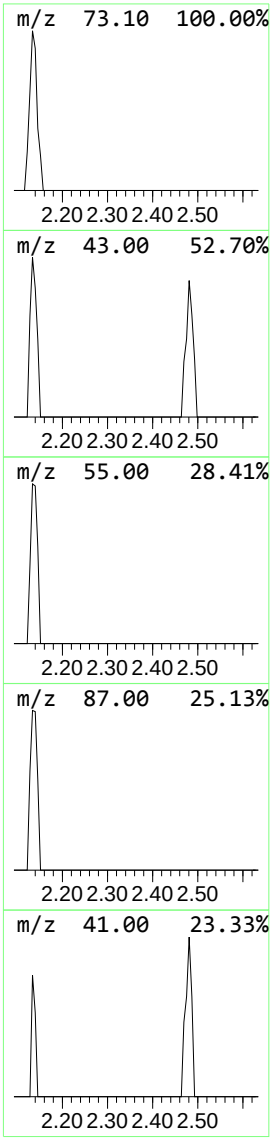
****

Peak Number 1 unknown2.134 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	2.79 ng	5440	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutylamine	73	C4H11N	000078-81-9	5
2	1-Butanamine	73	C4H11N	000109-73-9	3
3	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	3
4	1-Pentanamine	87	C5H13N	000110-58-7	3
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124755.D
Acq On : 24 Jul 2021 19:18
Operator : JU/CG
Sample : M3117-09 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

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

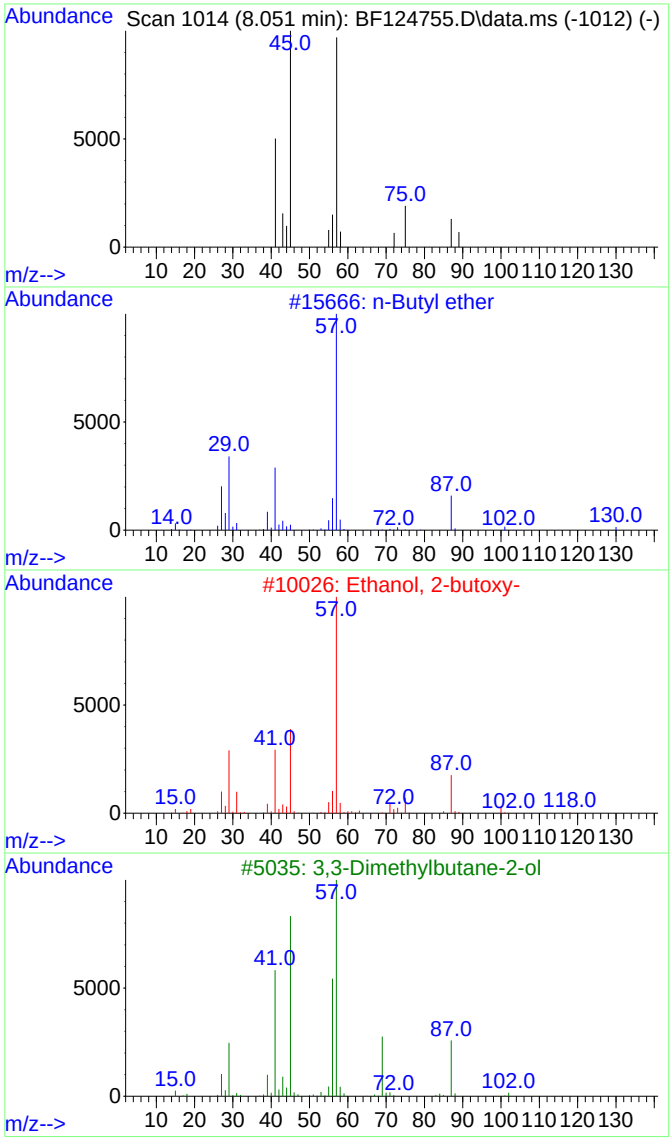
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

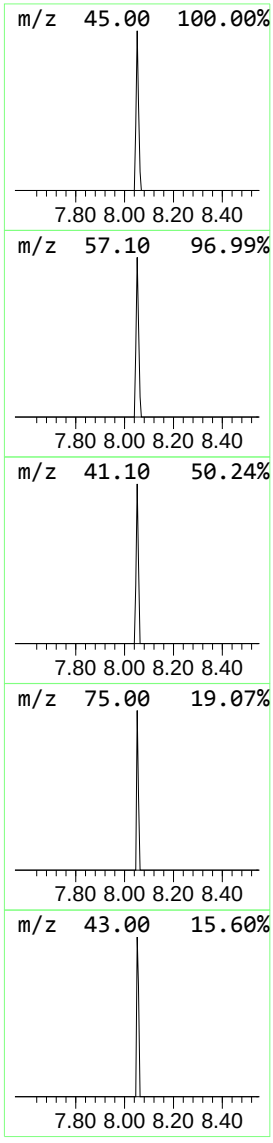
****

Peak Number 2 unknown8.051 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	4.32 ng	10997	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl ether	130	C8H18O	000142-96-1	9
2	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	9
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	9
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	9
5	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124755.D
Acq On : 24 Jul 2021 19:18
Operator : JU/CG
Sample : M3117-09 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NJ-CLEAN-9

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

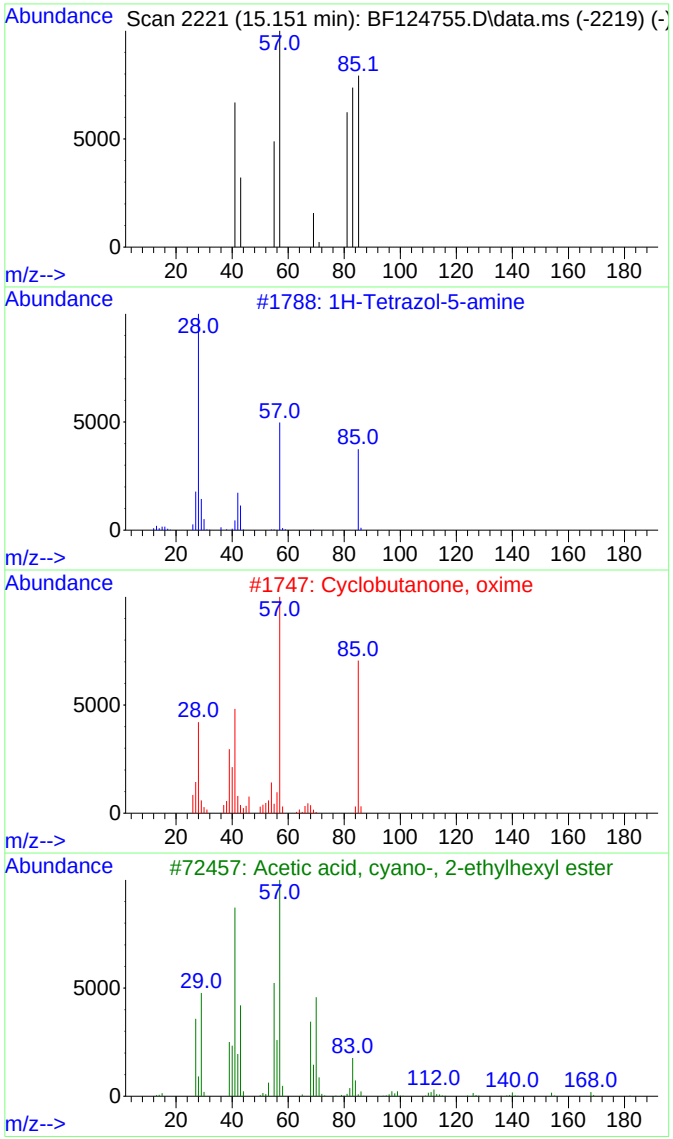
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

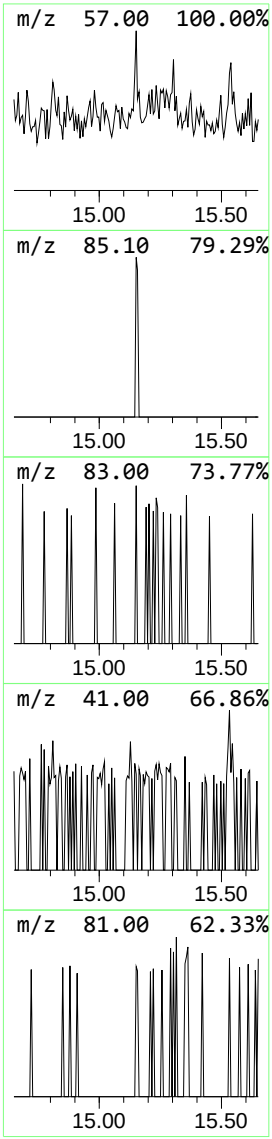
****

Peak Number 3 unknown15.151 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	2.55 ng	2722	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	7
2	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
3	Acetic acid, cyano-, 2-ethylhexy...	197	C11H19NO2	013361-34-7	4
4	S-Methyl 3-methylbutanethioate	132	C6H12OS	023747-45-7	4
5	1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124755.D
Acq On : 24 Jul 2021 19:18
Operator : JU/CG
Sample : M3117-09 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

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

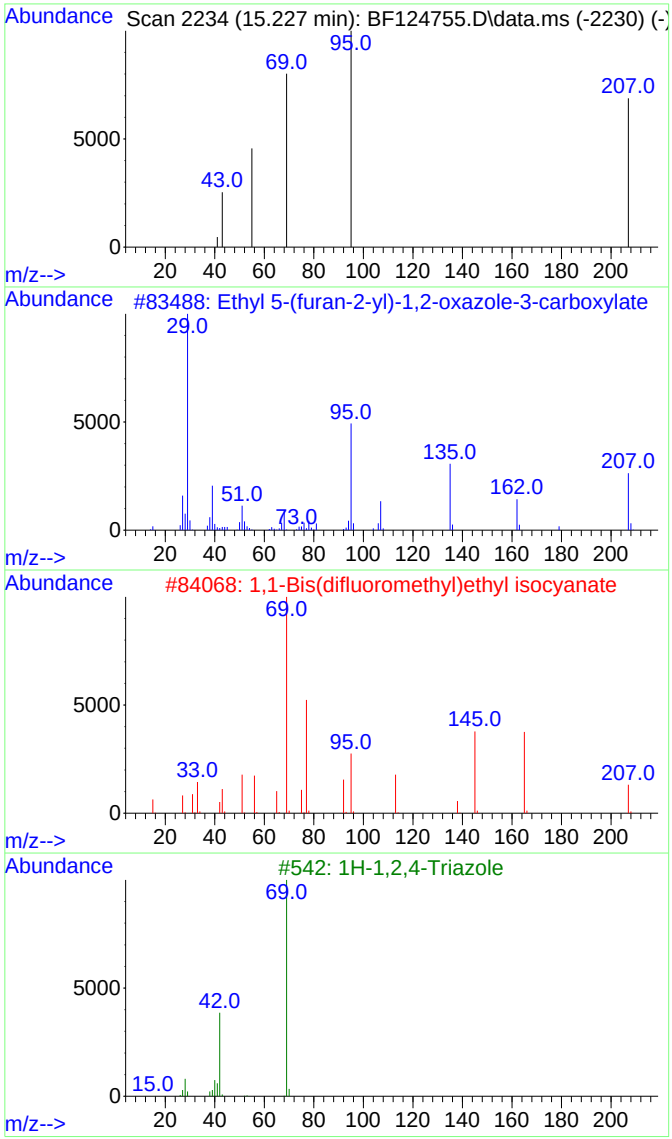
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

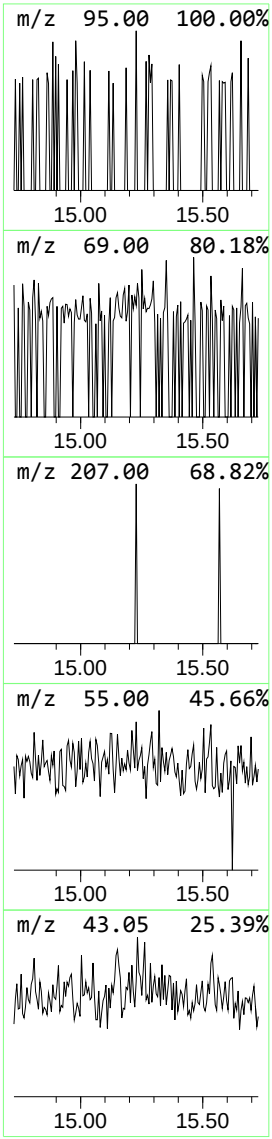
****

Peak Number 4 unknown15.2272 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	2.47 ng	2636	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl 5-(furan-2-yl)-1,2-oxazole...	207	C10H9NO4	1000411-40-9	4
2	1,1-Bis(difluoromethyl)ethyl iso...	207	C5H3F6NO	1000305-84-0	4
3	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	3
4	4-Pyridazinamine	95	C4H5N3	020744-39-2	2
5	4-Aminopyrimidine	95	C4H5N3	000591-54-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124755.D
Acq On : 24 Jul 2021 19:18
Operator : JU/CG
Sample : M3117-09 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

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

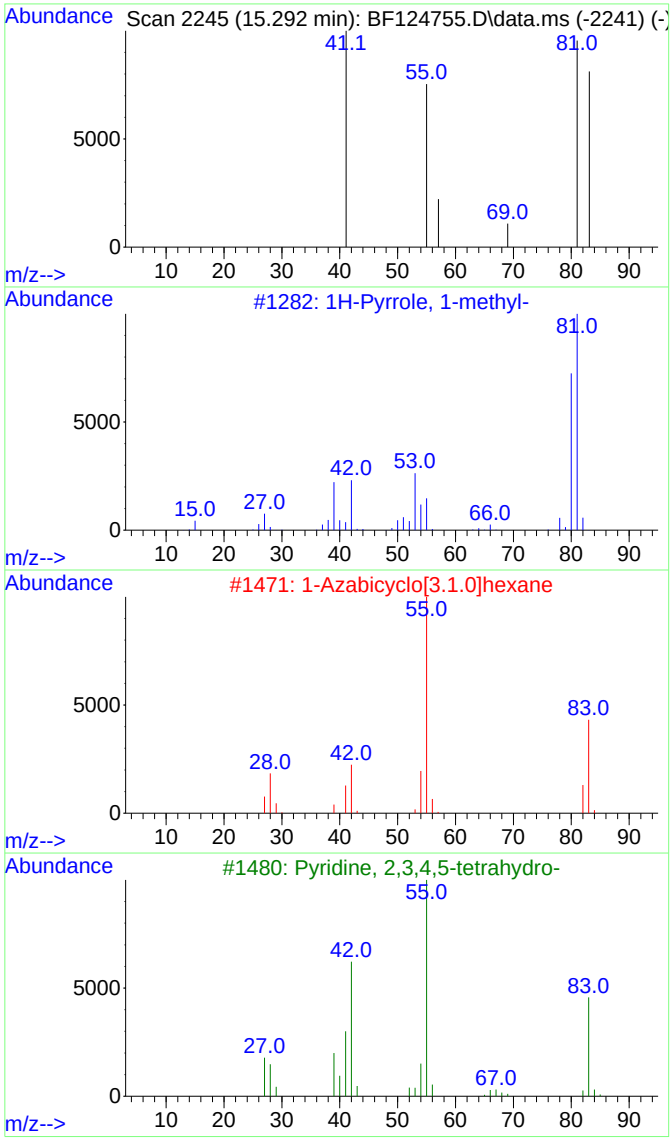
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

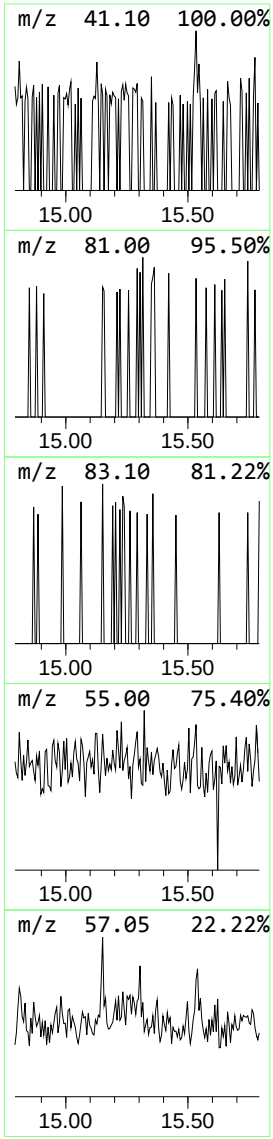
****

Peak Number 5 unknown15.292 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	2.28 ng	2433	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrrole, 1-methyl-	81	C5H7N	000096-54-8	2
2	1-Azabicyclo[3.1.0]hexane	83	C5H9N	000285-76-7	2
3	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	2
4	Cyclohexene 3-(tert-butyl)peroxide	170	C10H18O2	051437-25-3	1
5	1-Hexyne, 5-methyl-	96	C7H12	002203-80-7	1





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124755.D
Acq On : 24 Jul 2021 19:18
Operator : JU/CG
Sample : M3117-09 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

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

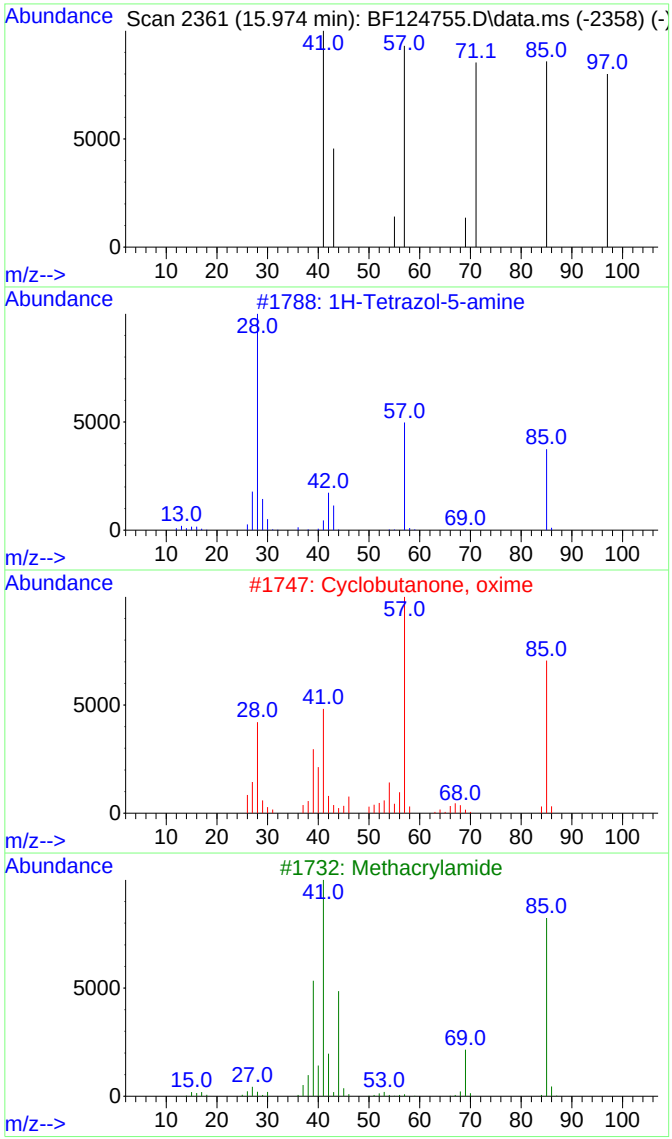
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

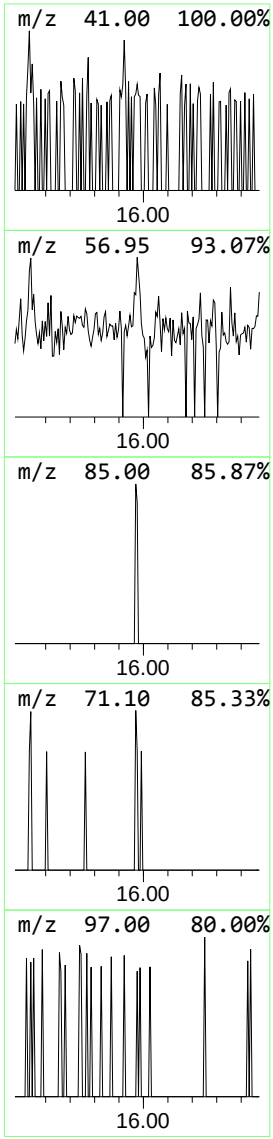
****

Peak Number 6 unknown15.974 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	3.88 ng	4145	Perylene-d12	15.509

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	Methacrylamide	85	C4H7NO	000079-39-0	4
4	trans-Crotonamide	85	C4H7NO	000625-37-6	4
5	2,2-Dimethylpropionic acid, 4-me...	186	C11H22O2	150588-62-8	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124755.D
Acq On : 24 Jul 2021 19:18
Operator : JU/CG
Sample : M3117-09 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NJ-CLEAN-9

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	2.8	ng	5440	1	6.875	39006	20.0
unknown8.051	8.051	4.3	ng	10997	2	8.157	50964	20.0
unknown15.151	15.151	2.5	ng	2722	6	15.509	21351	20.0
unknown15.2272	15.227	2.5	ng	2636	6	15.509	21351	20.0
unknown15.292	15.292	2.3	ng	2433	6	15.509	21351	20.0
unknown15.974	15.974	3.9	ng	4145	6	15.509	21351	20.0