LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097618.D
Acq On : 12 Aug 2017 3:53
Operator : SJ/JU
Sample : I4727-01 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-012

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:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.987	49	51	55	rVB4	7590	8700	1.26%	0.105%
2	4.769	519	524	532	rBV3	6915	20892	3.03%	0.252%
3	5.463	639	642	664	rBV	82385	291550	42.27%	3.518%
4	7.104	918	921	932	rBV	83763	234417	33.99%	2.829%
5	7.192	932	936	955	rVB	162053	401627	58.23%	4.847%
6	7.510	986	990	1007	rBV	362359	504890	73.20%	6.093%
7	7.751	1027	1031	1051	rBV	154576	252430	36.60%	3.046%
8	8.439	1144	1148	1163	rBV	58243	161516	23.42%	1.949%
9	9.539	1331	1335	1361	rBV	472576	671540	97.36%	8.104%
10	11.316	1633	1637	1652	rBV	261192	342450	49.65%	4.132%
11	12.022	1753	1757	1761	rBV2	20342	28901	4.19%	0.349%
12	12.151	1775	1779	1786	rVB2	10494	14322	2.08%	0.173%
13	12.369	1811	1816	1829	rBV2	479932	679835	98.57%	8.204%
14	12.739	1874	1879	1884	rBV3	3482	7390	1.07%	0.089%
15	13.216	1954	1960	1964	rVB2	13862	18710	2.71%	0.226%
16	13.268	1964	1969	1978	rBB3	14788	25829	3.74%	0.312%
17	13.574	2012	2021	2026	rBV3	6642	14501	2.10%	0.175%
18	13.668	2033	2037	2050	rVB	79716	130682	18.95%	1.577%
19	13.986	2086	2091	2099	rBV2	13242	29587	4.29%	0.357%
20	14.604	2193	2196	2202	rVB2	5374	8170	1.18%	0.099%
21	14.721	2212	2216	2219	rBV2	10261	11357	1.65%	0.137%
22	14.762	2219	2223	2228	rVV2	425558	565201	81.95%	6.820%
23	14.804	2228	2230	2239	rVV	81478	105014	15.23%	1.267%
24	14.904	2242	2247	2253	rVB	14706	22161	3.21%	0.267%
25	15.210	2296	2299	2302	rBV2	6644	8509	1.23%	0.103%
26	15.304	2311	2315	2318	rBV2	5826	6927	1.00%	0.084%
27	15.398	2327	2331	2334	rBV3	8234	8807	1.28%	0.106%
28	15.562	2353	2359	2363	rBV3	25358	34441	4.99%	0.416%
29	15.610	2363	2367	2373	rVB	26100	29655	4.30%	0.358%
30	15.686	2376	2380	2382	rBV2	6105	9435	1.37%	0.114%
31	15.715	2382	2385	2390	rVV2	31013	44298	6.42%	0.535%
32	15.757	2390	2392	2397	rVB2	13837	18097	2.62%	0.218%
33	15.915	2414	2419	2422	rBV5	5840	7240	1.05%	0.087%
34	15.998	2428	2433	2434	rBV3	11664	13336	1.93%	0.161%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097618.D
Acq On : 12 Aug 2017 3:53
Operator : SJ/JU
Sample : I4727-01 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-012

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:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.221	2469	2471	2475	rBV4	6814	10231	1.48%	0.123%
36	16.268	2476	2479	2483	rVB2	12263	14602	2.12%	0.176%
37	16.304	2483	2485	2489	rVB2	10547	11097	1.61%	0.134%
38	16.368	2491	2496	2499	rBV	36753	43542	6.31%	0.525%
39	16.409	2499	2503	2507	rBV5	25008	35544	5.15%	0.429%
40	16.445	2507	2509	2512	rVB3	12197	9777	1.42%	0.118%
41	16.486	2512	2516	2518	rBV3	19245	26831	3.89%	0.324%
42	16.515	2518	2521	2523	rVV	43289	43593	6.32%	0.526%
43	16.545	2523	2526	2527	rVV	35554	32504	4.71%	0.392%
44	16.568	2527	2530	2536	rVB	121495	145162	21.05%	1.752%
45	16.615	2536	2538	2542	rVB5	8570	9235	1.34%	0.111%
46	16.674	2545	2548	2551	rVB4	14291	13899	2.02%	0.168%
47	16.704	2551	2553	2557	rBV2	6984	8123	1.18%	0.098%
48	16.768	2561	2564	2567	rVB3	10699	13460	1.95%	0.162%
49	16.809	2567	2571	2573	rBV3	6253	8876	1.29%	0.107%
50	16.868	2577	2581	2588	rVB	183495	214816	31.15%	2.592%
51	16.939	2592	2593	2598	rBV4	11172	14490	2.10%	0.175%
52	16.992	2598	2602	2607	rVB3	17738	22519	3.26%	0.272%
53	17.051	2609	2612	2617	rBV4	10801	16650	2.41%	0.201%
54	17.115	2617	2623	2631	rVB	284728	332430	48.20%	4.011%
55	17.192	2633	2636	2640	rBV3	19580	30964	4.49%	0.374%
56	17.315	2652	2657	2658	rBV4	19291	28396	4.12%	0.343%
57	17.339	2658	2661	2666	rVB3	28612	42064	6.10%	0.508%
58	17.392	2666	2670	2672	rBV5	6889	8927	1.29%	0.108%
59	17.427	2672	2676	2680	rVB	20502	24813	3.60%	0.299%
60	17.474	2680	2684	2689	rBV2	37622	60100	8.71%	0.725%
61	17.515	2689	2691	2695	rVB3	12906	13588	1.97%	0.164%
62	17.586	2698	2703	2707	rBV2	29342	39863	5.78%	0.481%
63	17.627	2707	2710	2717	rVB2	25327	33019	4.79%	0.398%
64	17.698	2717	2722	2724	rBV5	7396	13393	1.94%	0.162%
65	17.980	2765	2770	2771	rBV4	9730	15473	2.24%	0.187%
66	18.086	2785	2788	2790	rBV3	15489	14881	2.16%	0.180%
67	18.139	2794	2797	2800	rVV2	21981	30808	4.47%	0.372%
68	18.168	2800	2802	2806	rVB3	20037	21483	3.11%	0.259%
69	18.203	2806	2808	2811	rBV2	11687	12389	1.80%	0.150%
70	18.386	2833	2839	2844	rBV9	15798	31698	4.60%	0.383%
71	18.462	2846	2852	2856	rBV	555161	689724	100.00%	8.323%

LSC Area Percent Report

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Misc :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	18.498	2856	2858	2866	rVV	57885	84845	12.30%	1.024%
73	18.586	2870	2873	2876	rVB5	17108	22453	3.26%	0.271%
74	18.968	2936	2938	2942	rVB	23714	27772	4.03%	0.335%
75	19.733	3065	3068	3071	rBV2	43183	63430	9.20%	0.765%
76	20.080	3125	3127	3130	rVB	46827	40705	5.90%	0.491%
77	20.133	3132	3136	3144	rVB	452681	540865	78.42%	6.527%
78	21.050	3290	3292	3296	rBV4	47403	73803	10.70%	0.891%
79	21.403	3350	3352	3353	rBV2	39962	38212	5.54%	0.461%
80	21.715	3401	3405	3406	rBV3	43982	62513	9.06%	0.754%
81	22.121	3472	3474	3476	rBV3	34422	45454	6.59%	0.549%
82	22.274	3498	3500	3509	rVB10	40743	83828	12.15%	1.012%
83	22.338	3509	3511	3512	rBV	43975	43130	6.25%	0.520%
84	22.944	3613	3614	3618	rVB4	28699	20726	3.00%	0.250%
85	22.974	3618	3619	3620	rBV	41599	27901	4.05%	0.337%
86	23.168	3649	3652	3655	rBV4	25297	46265	6.71%	0.558%
87	23.262	3664	3668	3672	rBV7	34212	72829	10.56%	0.879%
88	23.433	3692	3697	3700	rBV6	27667	60258	8.74%	0.727%
89	23.503	3706	3709	3710	rBV3	24213	26605	3.86%	0.321%
90	23.621	3727	3729	3733	rVB4	29232	33973	4.93%	0.410%

Sum of corrected areas: 8286948

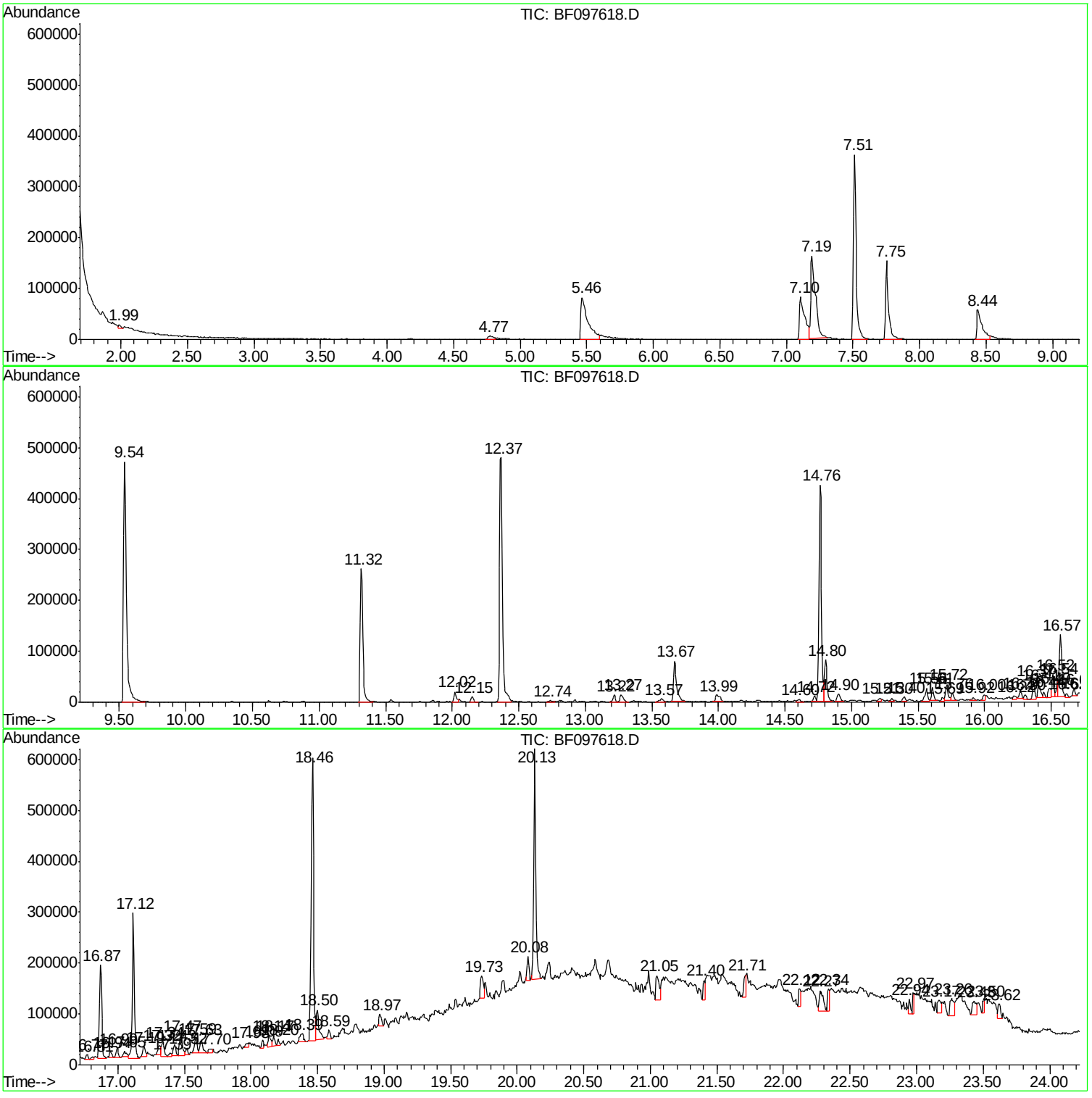
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097618.D
Acq On : 12 Aug 2017 3:53
Operator : SJ/JU
Sample : I4727-01 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097618.D
Acq On : 12 Aug 2017 3:53
Operator : SJ/JU
Sample : I4727-01 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

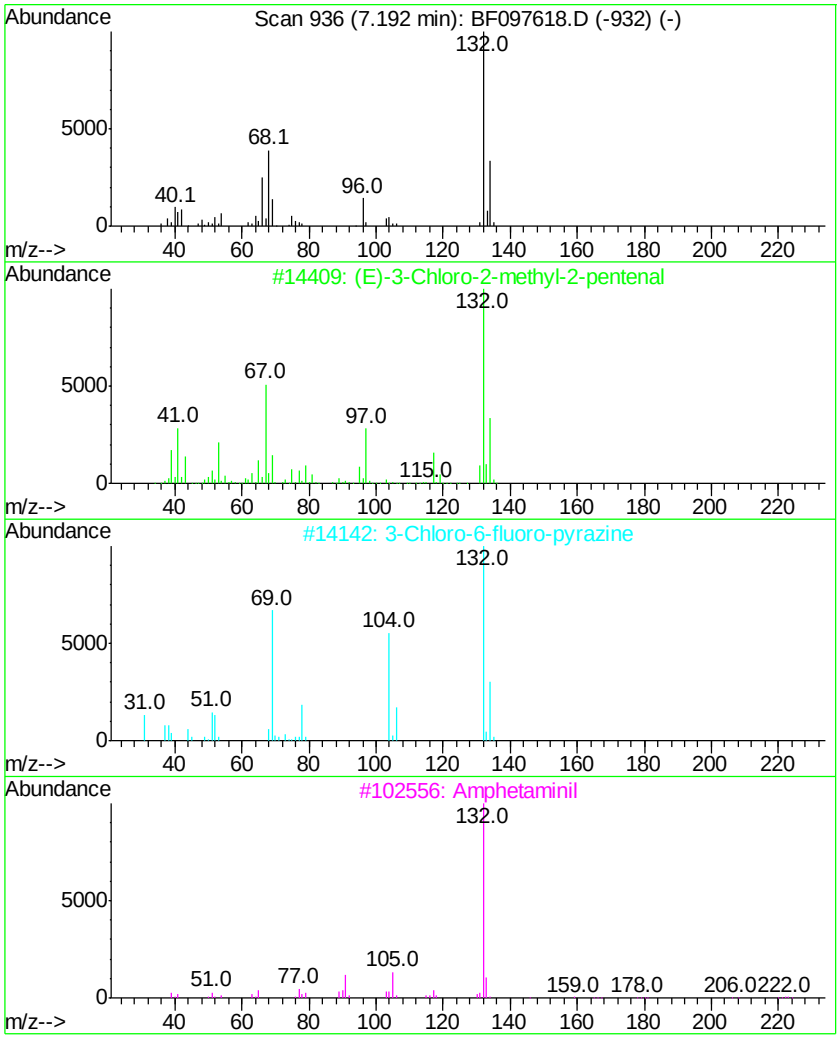
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

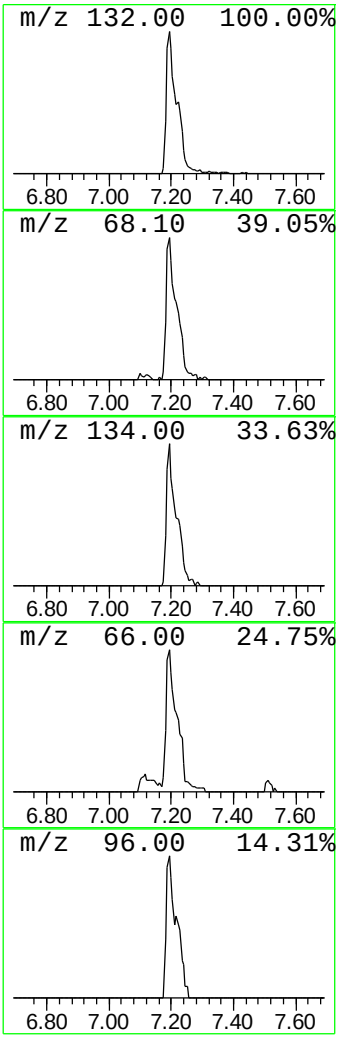
****

Peak Number 1 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	15.91 ng	401627	1,4-Dichlorobenzene-d4	7.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097618.D
Acq On : 12 Aug 2017 3:53
Operator : SJ/JU
Sample : I4727-01 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

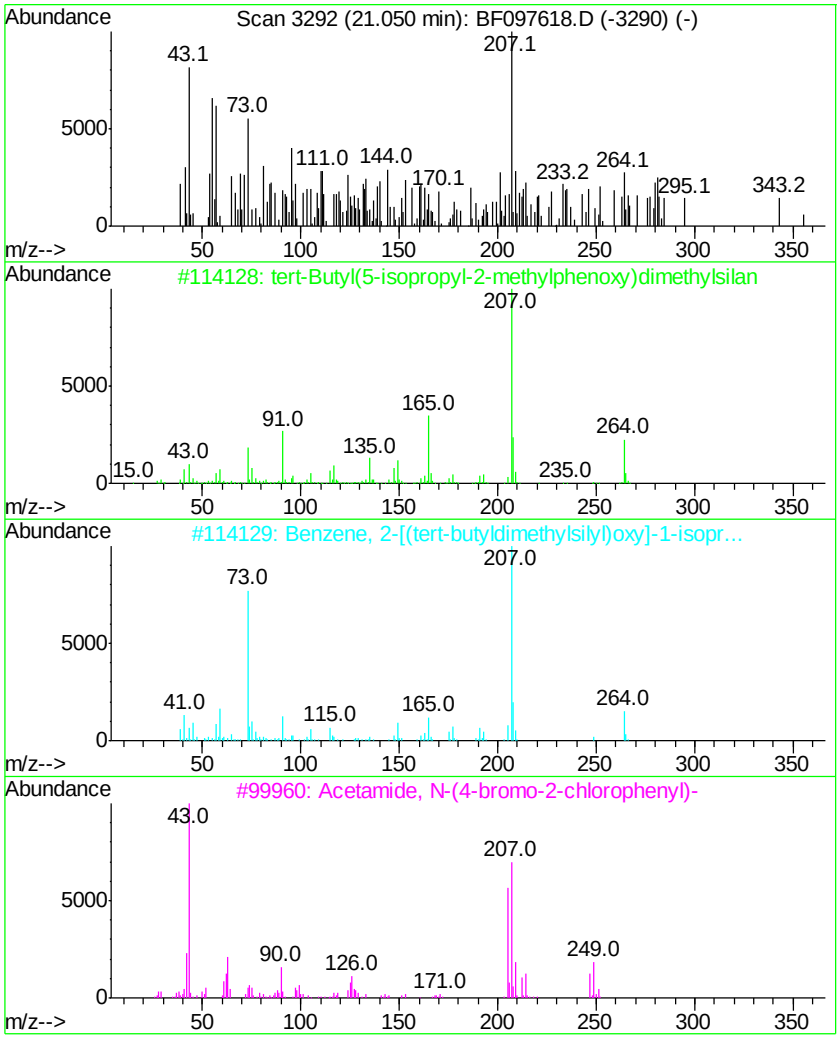
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

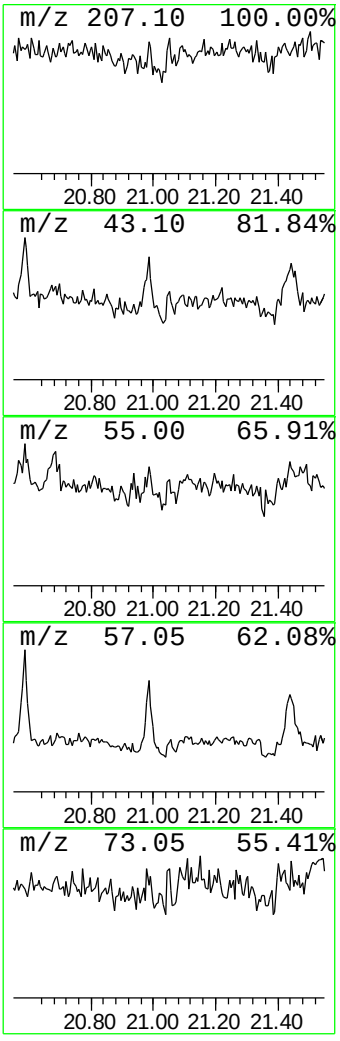
****

Peak Number 3 unknown21.05 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.05	2.73 ng	73803	Perylene-d12	20.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	tert-Butyl(5-isopropyl-2-methylp...	264	C16H28OSi	1000367-02-3	25
2	Benzene, 2-[(tert-butyldimethyls...	264	C16H28OSi	330455-64-6	22
3	Acetamide, N-(4-bromo-2-chlorph...	247	C8H7BrClNO	003460-23-9	22
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	18
5	1H-Indole, 5-methyl-2-phenyl-	207	C15H13N	013228-36-9	18





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

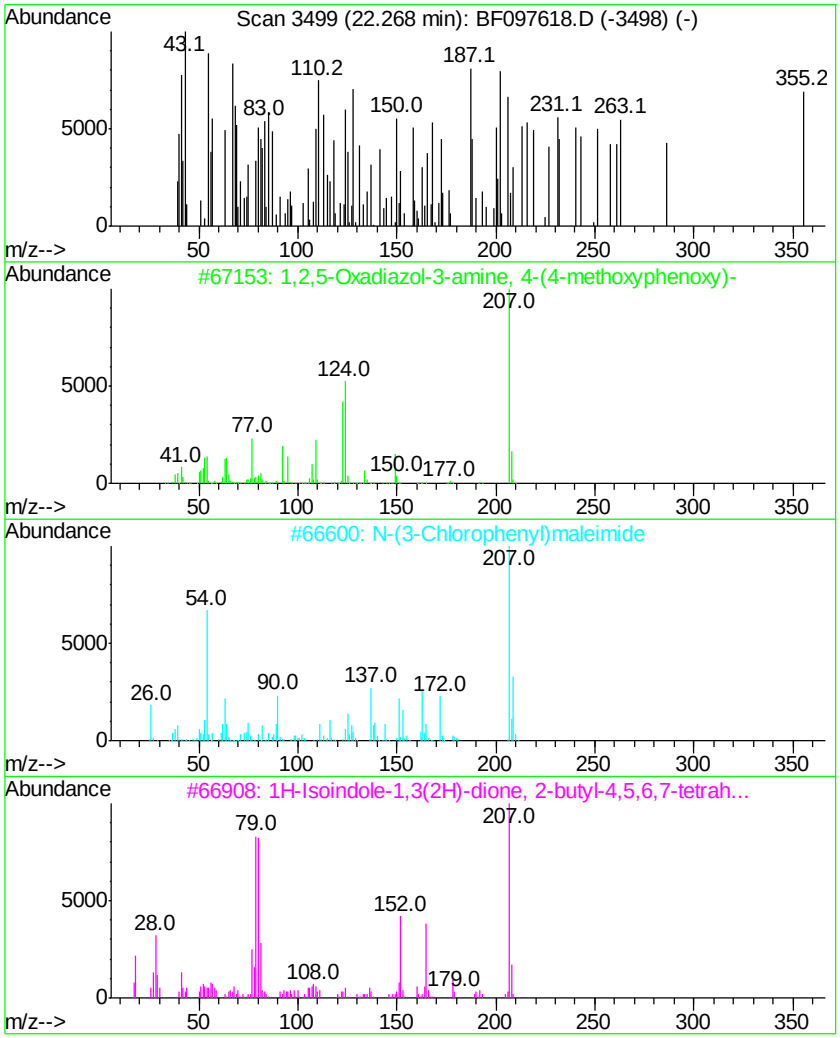
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

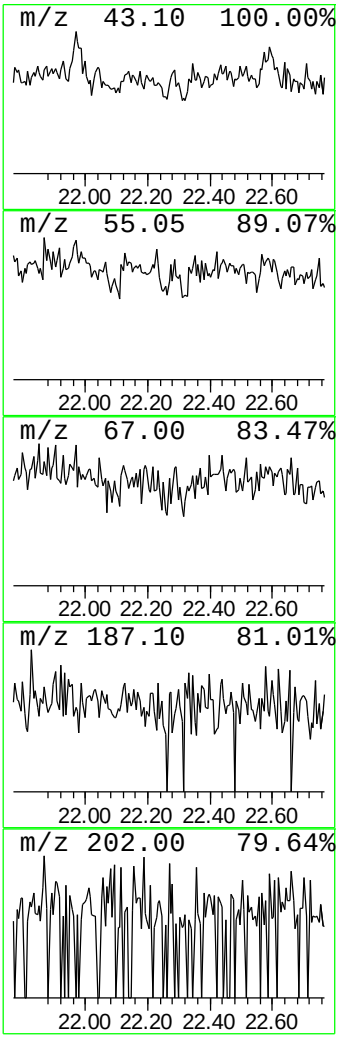
****

Peak Number 5 unknown22.27 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.27	3.10 ng	83828	Perylene-d12	20.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,5-Oxadiazol-3-amine, 4-(4-me...	207	C9H9N3O3	1000351-72-7	18
2	N-(3-Chlorophenyl)maleimide	207	C10H6ClNO2	1000341-21-1	14
3	1H-Isoindole-1,3(2H)-dione, 2-bu...	207	C12H17NO2	054934-85-9	14
4	1H-Pyrazole, 1-(3-methylbutyl)-4...	264	C14H25BN2O2	1000319-70-0	14
5	4-Cyclohexene-1,2-dicarboximide,...	207	C12H17NO2	028916-00-9	14





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Operator : SJ/JU
Sample : I4727-01 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

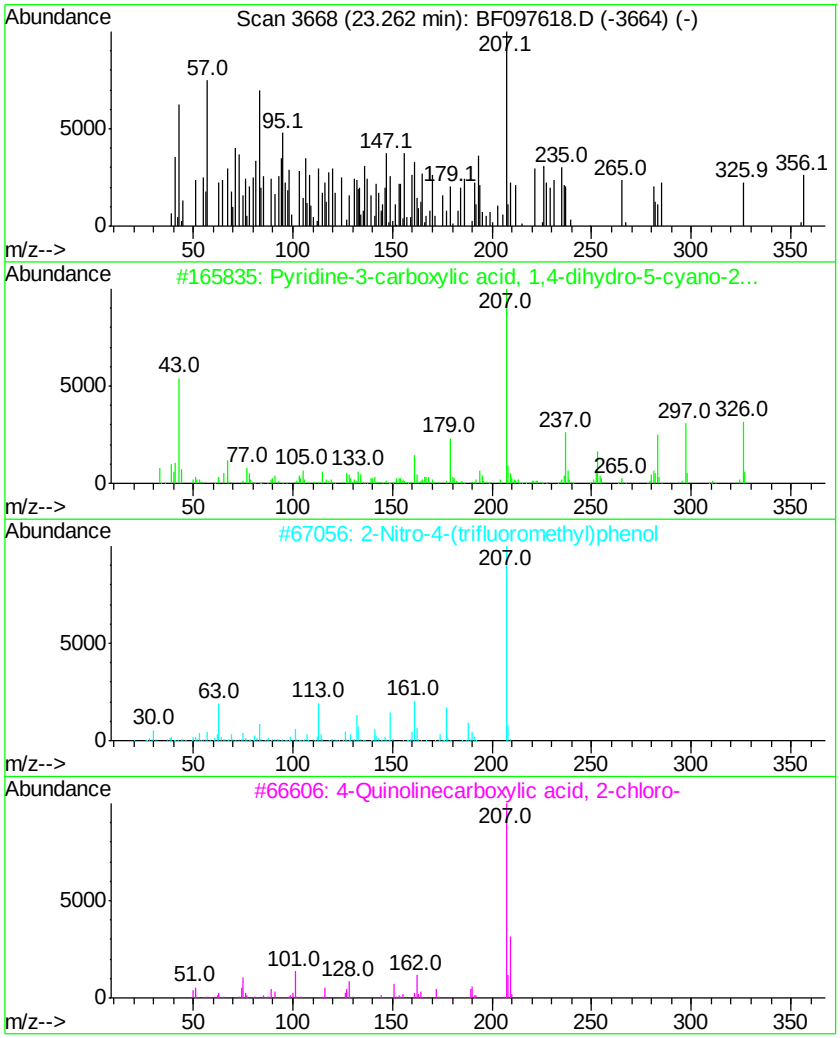
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

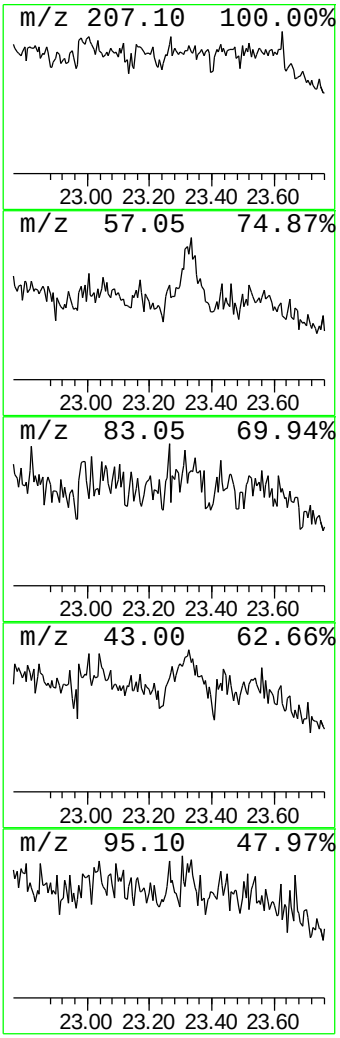
****

Peak Number 6 unknown23.26 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.26	2.69 ng	72829	Perylene-d12	20.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-3-carboxylic acid, 1,4-...	326	C19H22N2O3	350795-31-2	38
2	2-Nitro-4-(trifluoromethyl)phenol	207	C7H4F3NO3	000400-99-7	18
3	4-Quinolinecarboxylic acid, 2-ch...	207	C10H6ClNO2	005467-57-2	18
4	Propanamide, N-(3-methoxyphenyl)...	207	C12H17NO2	056619-93-3	18
5	2,3,4-Trimethoxyphenylacetonitrile	207	C11H13NO3	068913-85-9	18





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Operator : SJ/JU
Sample : I4727-01 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

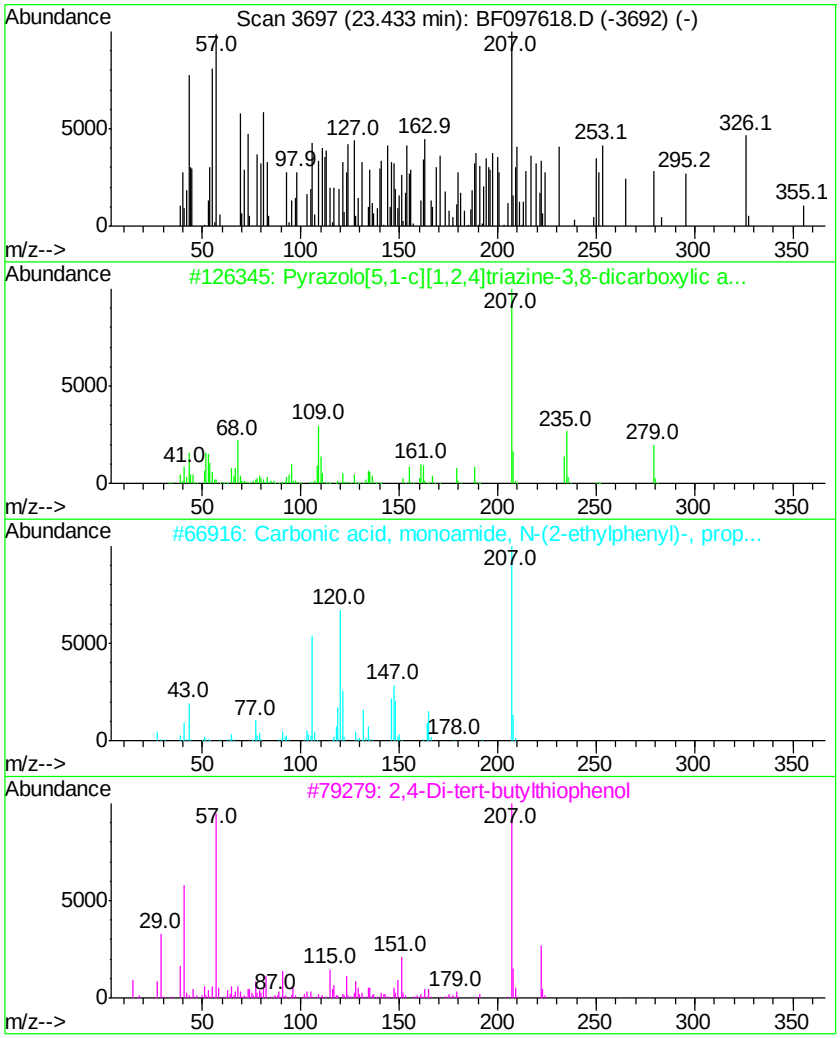
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

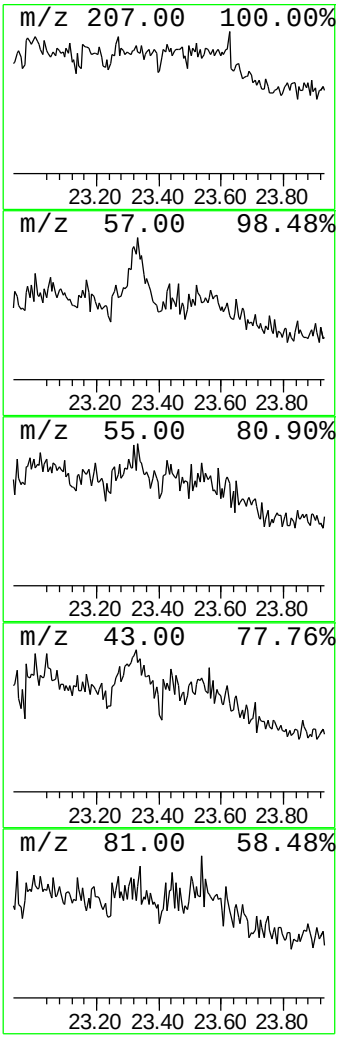
****

Peak Number 7 unknown23.43 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.43	2.23 ng	60258	Perylene-d12	20.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazolo[5,1-c][1,2,4]triazine-3...	279	C11H13N5O4	1000302-77-3	35
2	Carbonic acid, monoamide, N-(2-e...	207	C12H17NO2	1000340-19-1	25
3	2,4-Di-tert-butylthiophenol	222	C14H22S	019728-43-9	25
4	5H-Benzo[b]pyran-8-ol, 2,3,5,5,8...	222	C14H22O2	097306-66-6	25
5	5,6,7-Trimethoxy-1-indanone	222	C12H14O4	038472-90-1	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
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Acq On : 12 Aug 2017 3:53
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Misc :
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Instrument : BNA_F
ClientSampleId : FK-PS-01-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.19	7.19	15.9	ng	401627	1	7.51	504890	20.0
unknown21.05	21.05	2.7	ng	73803	6	20.13	540865	20.0
unknown22.27	22.27	3.1	ng	83828	6	20.13	540865	20.0
unknown23.26	23.26	2.7	ng	72829	6	20.13	540865	20.0
unknown23.43	23.43	2.2	ng	60258	6	20.13	540865	20.0