LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095945.D
Acq On : 15 Jun 2017 3:17
Operator : SJ/MA
Sample : I3635-13 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-061217-E

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-BF060517.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	4.504	493	496	510	rBV2	21533	50941	6.74%	0.640%
2	5.234	617	620	648	rBV	206804	571460	75.64%	7.184%
3	6.910	902	905	917	rBV	212844	503146	66.59%	6.325%
4	6.998	917	920	939	rVB	402803	755537	100.00%	9.498%
5	7.334	973	977	988	rBV	293316	376106	49.78%	4.728%
6	7.569	1013	1017	1033	rBV	390734	518375	68.61%	6.516%
7	8.251	1130	1133	1160	rBV	201750	358658	47.47%	4.509%
8	9.369	1318	1323	1339	rBV	345469	479994	63.53%	6.034%
9	11.145	1620	1625	1636	rBV	582372	729270	96.52%	9.168%
10	11.845	1740	1744	1750	rBV	39062	49341	6.53%	0.620%
11	12.186	1797	1802	1808	rBV2	376081	447013	59.16%	5.619%
12	12.233	1808	1810	1815	rVB3	9526	12634	1.67%	0.159%
13	13.045	1942	1948	1953	rBB	10980	13426	1.78%	0.169%
14	13.486	2019	2023	2038	rBB	176029	264256	34.98%	3.322%
15	13.816	2075	2079	2086	rBV2	9556	17456	2.31%	0.219%
16	14.539	2199	2202	2205	rBV2	6119	7862	1.04%	0.099%
17	14.580	2205	2209	2213	rVV	306984	378492	50.10%	4.758%
18	14.621	2213	2216	2223	rVB2	38589	55829	7.39%	0.702%
19	14.721	2228	2233	2238	rBV	9707	14113	1.87%	0.177%
20	15.121	2297	2301	2305	rBV2	6410	9556	1.26%	0.120%
21	15.221	2316	2318	2325	rVB3	5537	7799	1.03%	0.098%
22	15.392	2343	2347	2351	rVV3	8086	8753	1.16%	0.110%
23	15.439	2351	2355	2359	rVB2	9401	11835	1.57%	0.149%
24	15.545	2370	2373	2377	rVV2	11348	16717	2.21%	0.210%
25	15.604	2377	2383	2393	rVB6	20735	39505	5.23%	0.497%
26	15.845	2419	2424	2427	rBV4	6076	9792	1.30%	0.123%
27	16.204	2479	2485	2488	rBV2	10483	11893	1.57%	0.150%
28	16.239	2488	2491	2496	rBV5	5164	8989	1.19%	0.113%
29	16.321	2501	2505	2513	rVV5	17885	32112	4.25%	0.404%
30	16.404	2513	2519	2524	rVV	115646	146313	19.37%	1.839%
31	16.515	2534	2538	2541	rBV4	6417	8944	1.18%	0.112%
32	16.645	2556	2560	2565	rBV6	4357	10631	1.41%	0.134%
33	16.704	2566	2570	2576	rBV	136831	165598	21.92%	2.082%
34	16.910	2602	2605	2608	rVB5	5680	8104	1.07%	0.102%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.951	2608	2612	2620	rBV	510548	576588	76.31%	7.248%
36	17.033	2622	2626	2631	rVB5	8132	12314	1.63%	0.155%
37	17.151	2641	2646	2648	rBV6	13899	20726	2.74%	0.261%
38	17.180	2648	2651	2655	rVB	16315	21488	2.84%	0.270%
39	17.262	2662	2665	2670	rBV2	13393	15704	2.08%	0.197%
40	17.315	2670	2674	2679	rBV5	18521	33821	4.48%	0.425%
41	17.427	2690	2693	2696	rVB2	7395	8050	1.07%	0.101%
42	17.474	2697	2701	2704	rVV3	7987	11112	1.47%	0.140%
43	17.515	2706	2708	2711	rVB2	10865	8454	1.12%	0.106%
44	17.609	2722	2724	2727	rBV4	11315	14689	1.94%	0.185%
45	17.674	2732	2735	2737	rBV3	8672	10569	1.40%	0.133%
46	17.751	2745	2748	2752	rBV6	7577	11159	1.48%	0.140%
47	17.880	2767	2770	2773	rBV3	8960	12137	1.61%	0.153%
48	17.980	2784	2787	2789	rBV3	8840	9254	1.22%	0.116%
49	18.009	2789	2792	2795	rVB3	12683	14589	1.93%	0.183%
50	18.086	2802	2805	2808	rVB5	10151	11152	1.48%	0.140%
51	18.151	2814	2816	2819	rVB3	15294	15690	2.08%	0.197%
52	18.221	2824	2828	2832	rBV5	32432	57680	7.63%	0.725%
53	18.298	2836	2841	2845	rBV2	351492	483707	64.02%	6.081%
54	18.333	2845	2847	2852	rVB	39934	54866	7.26%	0.690%
55	18.433	2862	2864	2868	rVB3	17865	16516	2.19%	0.208%
56	19.574	3055	3058	3061	rBV	66587	84580	11.19%	1.063%
57	19.862	3105	3107	3113	rVB	37581	44770	5.93%	0.563%
58	19.921	3115	3117	3121	rBV	47370	57338	7.59%	0.721%
59	19.974	3123	3126	3131	rBV	212489	247413	32.75%	3.110%

Sum of corrected areas: 7954816

LSC Report - Integrated Chromatogram

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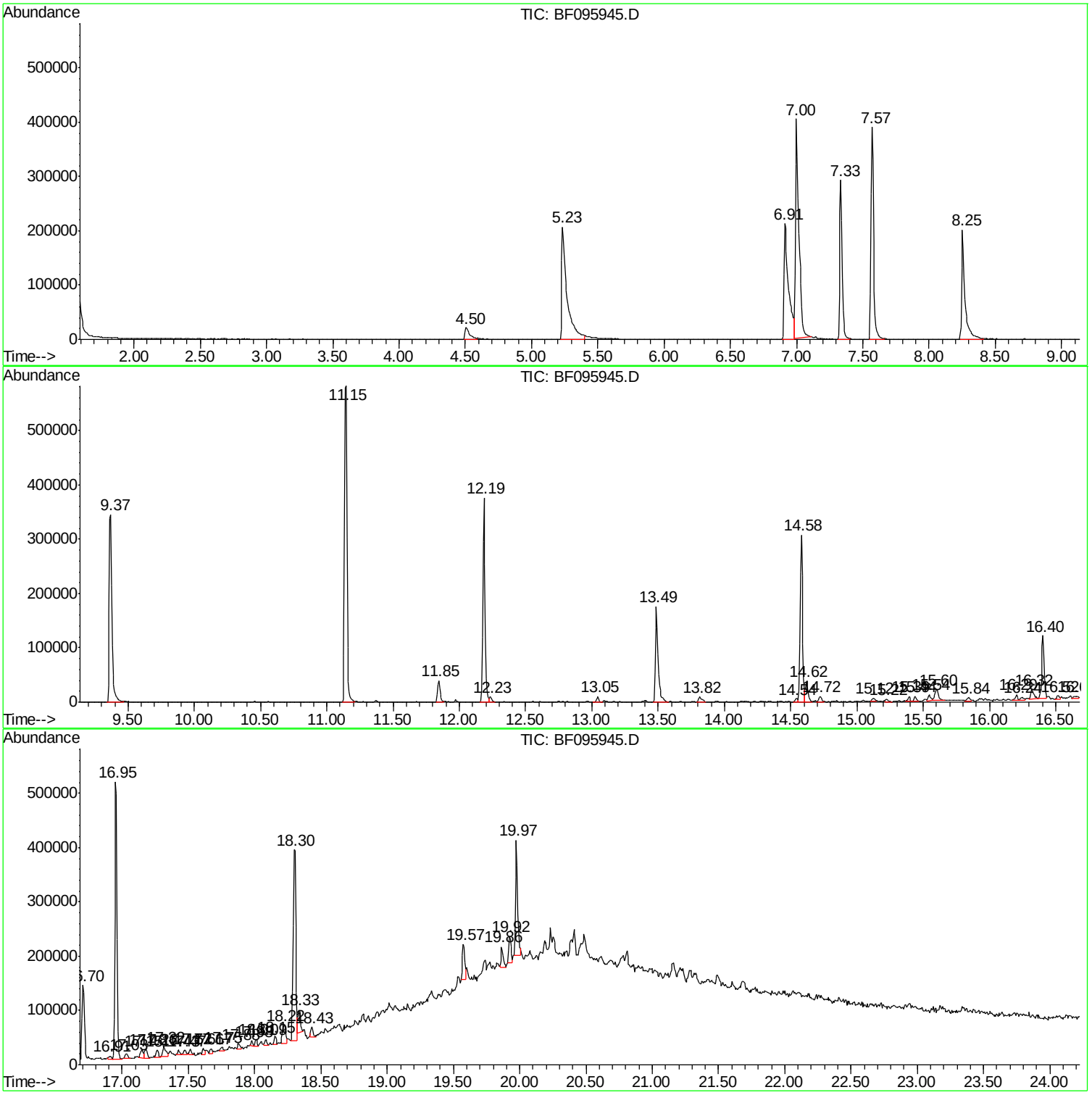
Data File : BF095945.D
Acq On : 15 Jun 2017 3:17
Operator : SJ/MA
Sample : I3635-13 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-061217-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095945.D
Acq On : 15 Jun 2017 3:17
Operator : SJ/MA
Sample : I3635-13 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-061217-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

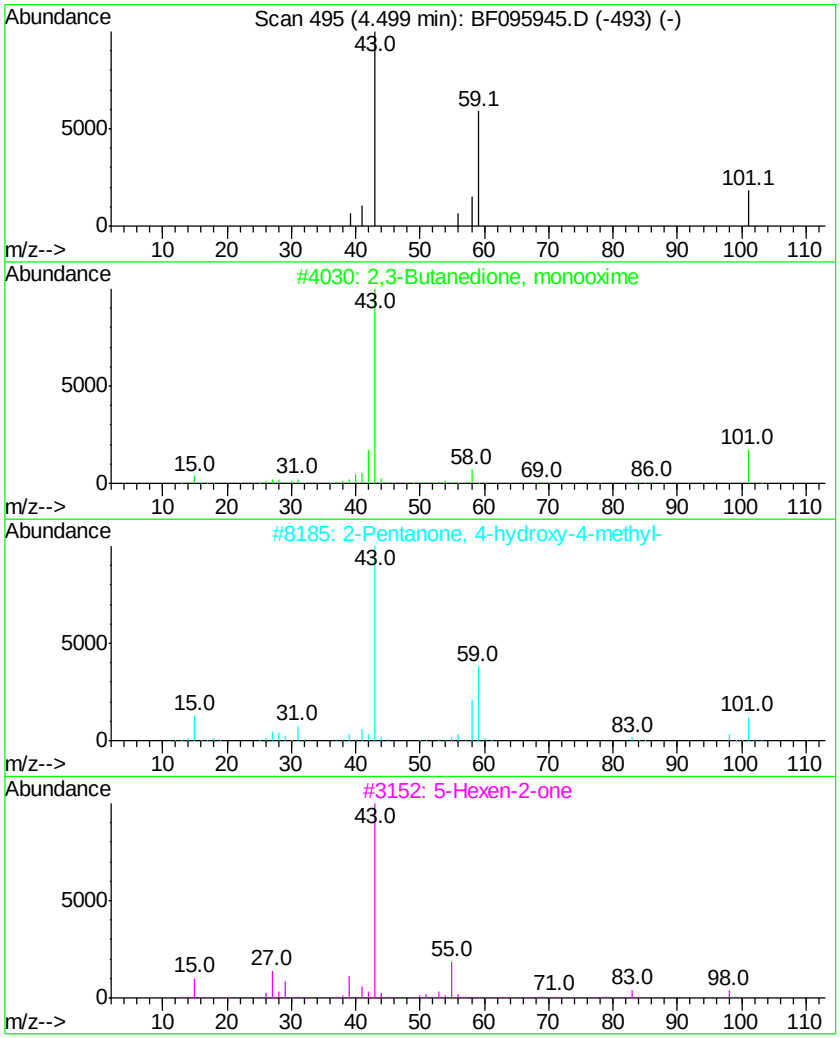
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

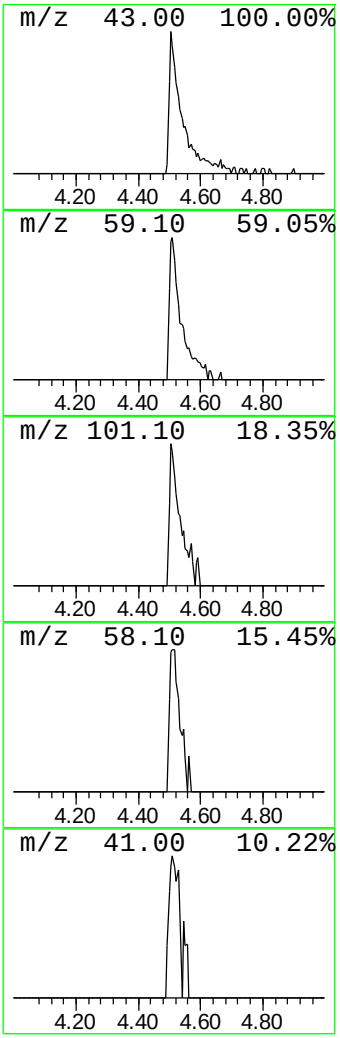
****

Peak Number 1 unknown4.50 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	2.71 ng	50941	1,4-Dichlorobenzene-d4	7.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
3	5-Hexen-2-one	98	C6H10O	000109-49-9	7
4	Propylamine	59	C3H9N	000107-10-8	5
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	5





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Misc :
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Instrument : BNA_F
ClientSampleId : CL-02-061217-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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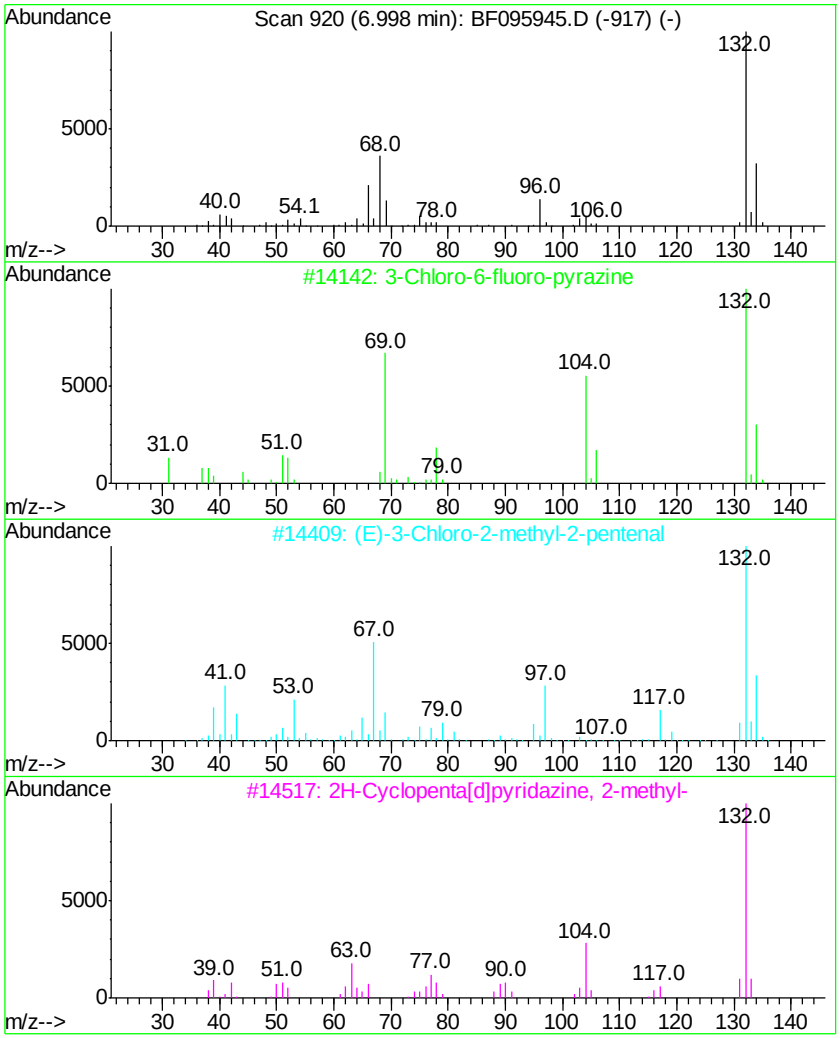
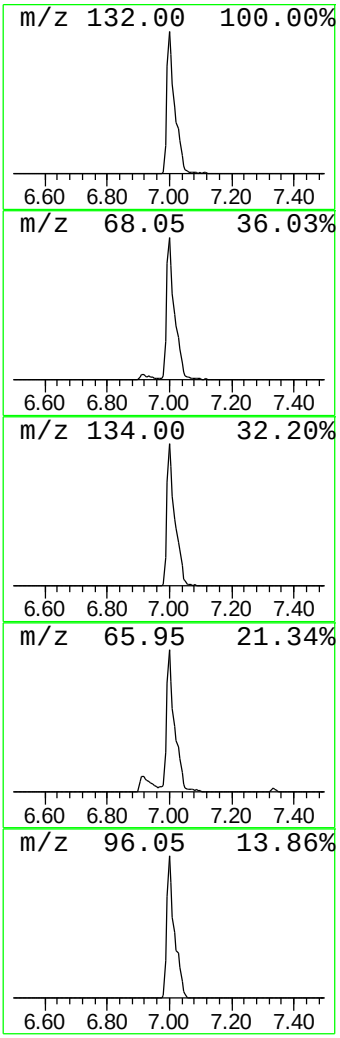
Peak Number 2 unknown7.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.00	40.18 ng	755537	1,4-Dichlorobenzene-d4	7.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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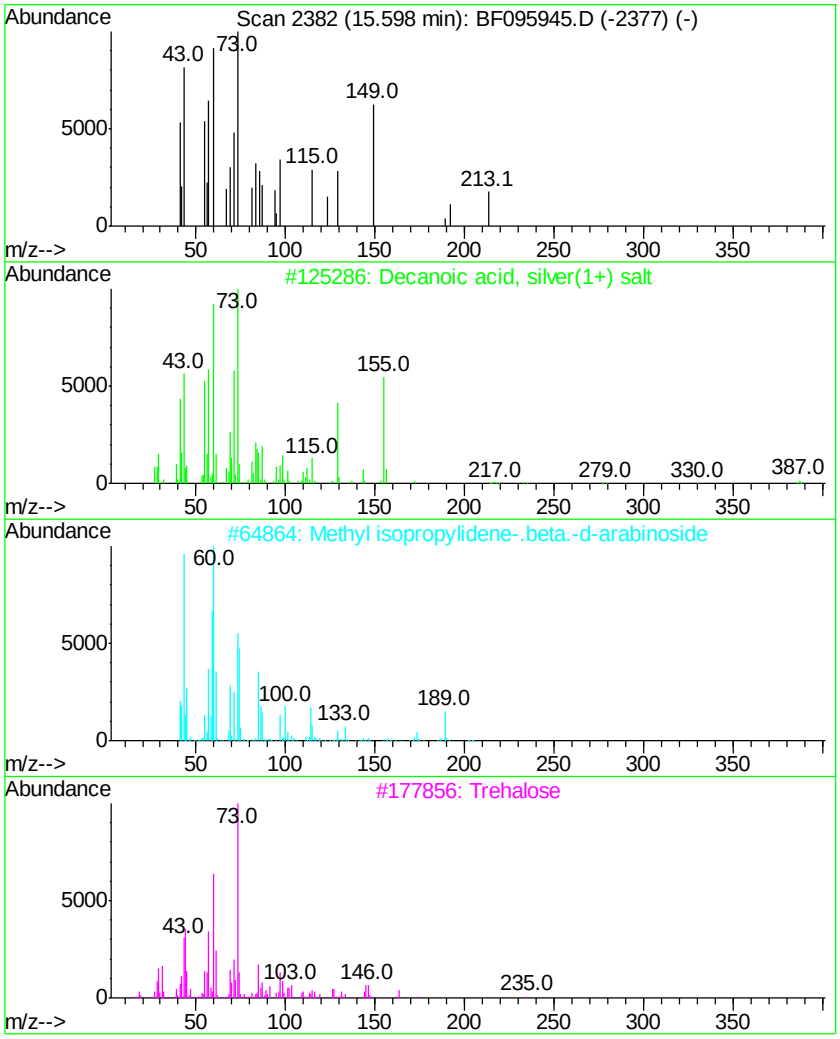
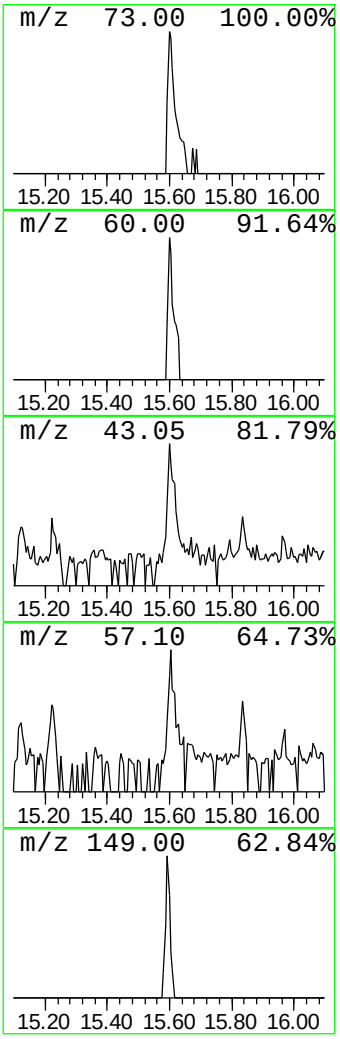
Peak Number 4 unknown15.60 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	2.09 ng	39505	Phenanthrene-d10	14.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	43
2	Methyl isopropylidene-.beta.-d-a...	204	C9H16O5	1000129-88-1	38
3	Trehalose	342	C12H22O11	000099-20-7	38
4	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	38
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : CL-02-061217-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

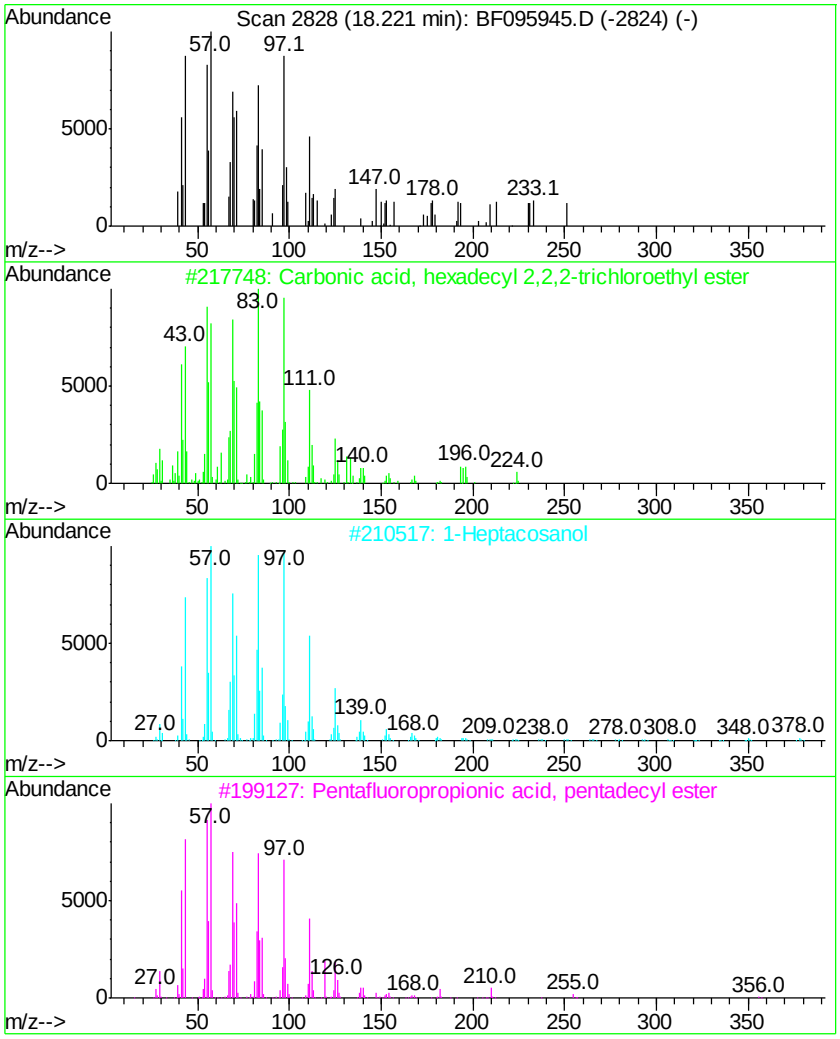
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

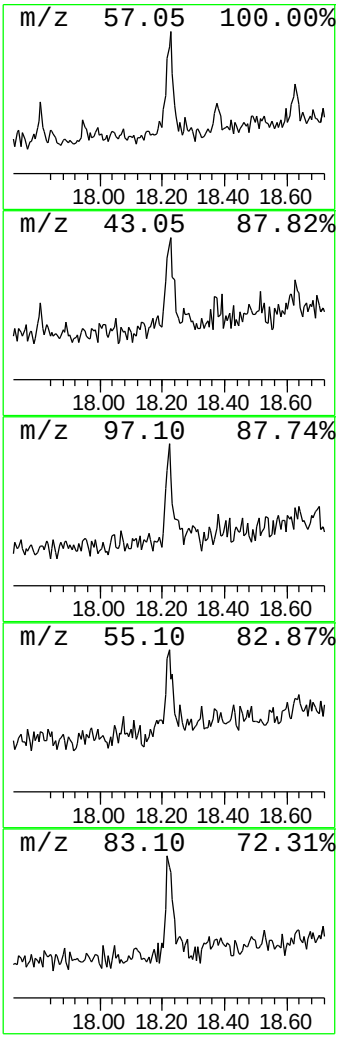
****

Peak Number 5 Carbonic acid, hexadecyl 2,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.22	2.38 ng	57680	Chrysene-d12	18.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	83
2	1-Heptacosanol	396	C27H56O	002004-39-9	81
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	80
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	74
5	Triacontyl acetate	480	C32H64O2	041755-58-2	74





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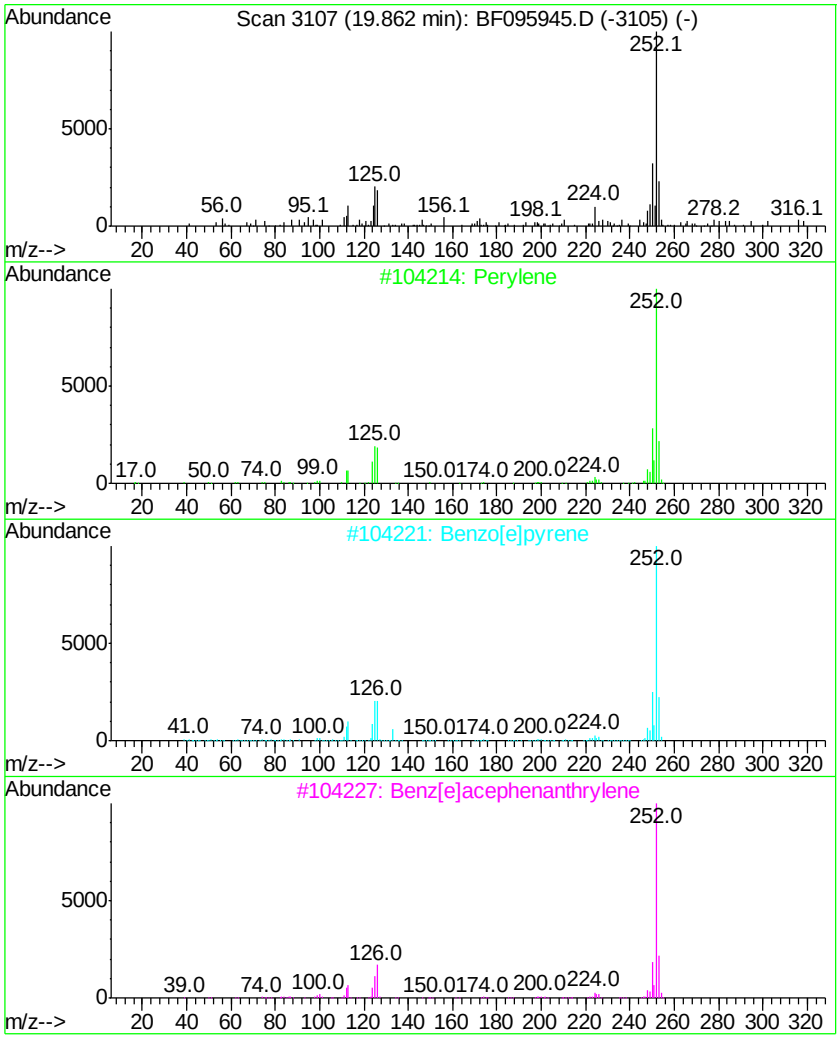
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

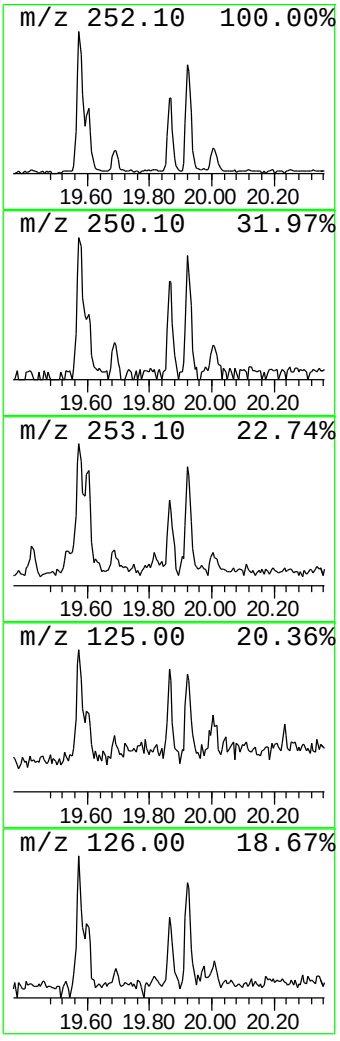
****

Peak Number 6 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.86	3.62 ng	44770	Perylene-d12	19.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	96
2	Benzo[e]pyrene	252	C20H12	000192-97-2	95
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	92
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	76
5	Benzo[a]pyrene	252	C20H12	000050-32-8	74





Tentatively Identified Compound (LSC) summary

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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
unknown4.50	4.50	2.7	ng	50941	1	7.33	376106	20.0
unknown7.00	7.00	40.2	ng	755537	1	7.33	376106	20.0
unknown15.60	15.60	2.1	ng	39505	4	14.58	378492	20.0
Carbonic acid, he...	18.22	2.4	ng	57680	5	18.30	483707	20.0
Perylene	19.86	3.6	ng	44770	6	19.97	247413	20.0