LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095277.D
Acq On : 19 May 2017 22:43
Operator : SJ/MA
Sample : I3202-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11COMP

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-BF050217.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	5.119	537	541	567	rBV	223462	642123	21.30%	2.420%
2	5.731	641	645	680	rBV	1019069	2221186	73.69%	8.371%
3	6.319	740	745	754	rBV2	14687	34670	1.15%	0.131%
4	7.307	908	913	929	rBV	1319971	2138764	70.95%	8.060%
5	7.431	929	934	955	rVB	1554968	2588087	85.86%	9.754%
6	7.766	987	991	1002	rBV	419676	523565	17.37%	1.973%
7	8.001	1026	1031	1050	rBV	1484438	1839844	61.03%	6.934%
8	8.666	1139	1144	1177	rBV	843114	1503864	49.89%	5.668%
9	9.784	1330	1334	1359	rBV	453527	788396	26.15%	2.971%
10	11.554	1629	1635	1656	rBV	2156910	3014409	100.00%	11.360%
11	12.101	1721	1728	1733	rBV2	22288	41378	1.37%	0.156%
12	12.248	1749	1753	1770	rBV	270864	480371	15.94%	1.810%
13	12.613	1810	1815	1823	rBV2	605598	928313	30.80%	3.498%
14	12.666	1823	1824	1836	rVB2	36221	49829	1.65%	0.188%
15	12.995	1871	1880	1887	rBV6	21098	45885	1.52%	0.173%
16	13.448	1953	1957	1961	rVB	43746	49433	1.64%	0.186%
17	13.524	1966	1970	1978	rVB2	53232	80785	2.68%	0.304%
18	13.801	2011	2017	2022	rBV5	19804	39513	1.31%	0.149%
19	13.907	2030	2035	2055	rBV	1089915	1857921	61.63%	7.002%
20	14.219	2084	2088	2091	rBV	55809	64689	2.15%	0.244%
21	14.430	2117	2124	2128	rBV2	17400	32021	1.06%	0.121%
22	14.948	2208	2212	2217	rBV	43084	50979	1.69%	0.192%
23	15.018	2217	2224	2228	rVV	644327	919740	30.51%	3.466%
24	15.054	2228	2230	2240	rVV	241103	386610	12.83%	1.457%
25	15.154	2243	2247	2257	rVB	49801	84483	2.80%	0.318%
26	15.607	2321	2324	2331	rVB	33793	39495	1.31%	0.149%
27	15.807	2354	2358	2362	rBV	73699	89951	2.98%	0.339%
28	15.848	2362	2365	2374	rVB	79677	114376	3.79%	0.431%
29	15.971	2380	2386	2389	rBV3	112241	220454	7.31%	0.831%
30	16.248	2429	2433	2443	rVB4	22754	46514	1.54%	0.175%
31	16.601	2489	2493	2497	rBV	61861	81513	2.70%	0.307%
32	16.642	2497	2500	2504	rVB3	24336	34272	1.14%	0.129%
33	16.718	2510	2513	2516	rBV2	22995	30895	1.02%	0.116%
34	16.801	2523	2527	2538	rBV	168926	242692	8.05%	0.915%

LSC Area Percent Report

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Operator : SJ/MA
Sample : I3202-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11COMP

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.107	2575	2579	2587	rVV	243332	364207	12.08%	1.373%
36	17.277	2606	2608	2613	rBV3	20023	30404	1.01%	0.115%
37	17.336	2613	2618	2628	rVV2	2243889	2747169	91.13%	10.353%
38	17.430	2628	2634	2642	rVB5	29099	55609	1.84%	0.210%
39	17.536	2649	2652	2655	rBV3	17615	30292	1.00%	0.114%
40	17.571	2655	2658	2664	rVB2	41539	57138	1.90%	0.215%
41	17.659	2669	2673	2677	rBV	34123	41146	1.36%	0.155%
42	17.701	2677	2680	2686	rBV2	49024	74374	2.47%	0.280%
43	17.818	2697	2700	2705	rBV2	34780	41990	1.39%	0.158%
44	17.865	2705	2708	2715	rVB3	27467	38174	1.27%	0.144%
45	18.577	2825	2829	2843	rBV4	56215	140765	4.67%	0.530%
46	18.689	2843	2848	2852	rBV2	561705	810593	26.89%	3.055%
47	19.806	3035	3038	3043	rBV	34400	35669	1.18%	0.134%
48	19.971	3062	3066	3069	rBV	55737	76074	2.52%	0.287%
49	20.259	3111	3115	3122	rBV	43351	56916	1.89%	0.214%
50	20.318	3122	3125	3129	rBV	54756	66717	2.21%	0.251%
51	20.365	3129	3133	3144	rBV	294880	486955	16.15%	1.835%
52	21.747	3362	3368	3372	rBV2	18225	37758	1.25%	0.142%
53	22.130	3428	3433	3440	rBV3	16102	35758	1.19%	0.135%

Sum of corrected areas: 26534728

LSC Report - Integrated Chromatogram

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Data File : BF095277.D
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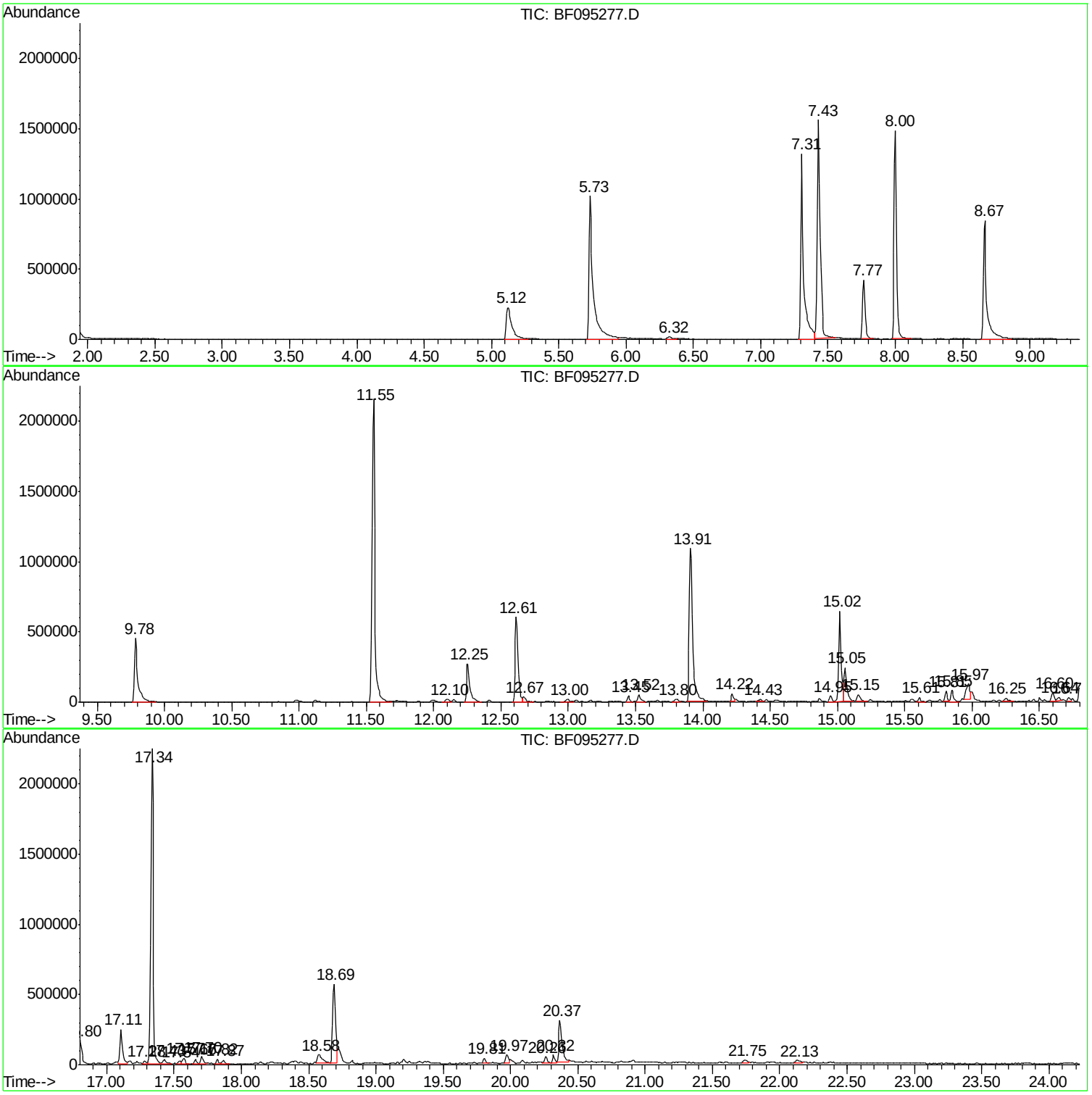
Operator : SJ/MA
Sample : I3202-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-11COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF051917\
Data File : BF095277.D
Acq On : 19 May 2017 22:43
Operator : SJ/MA
Sample : I3202-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

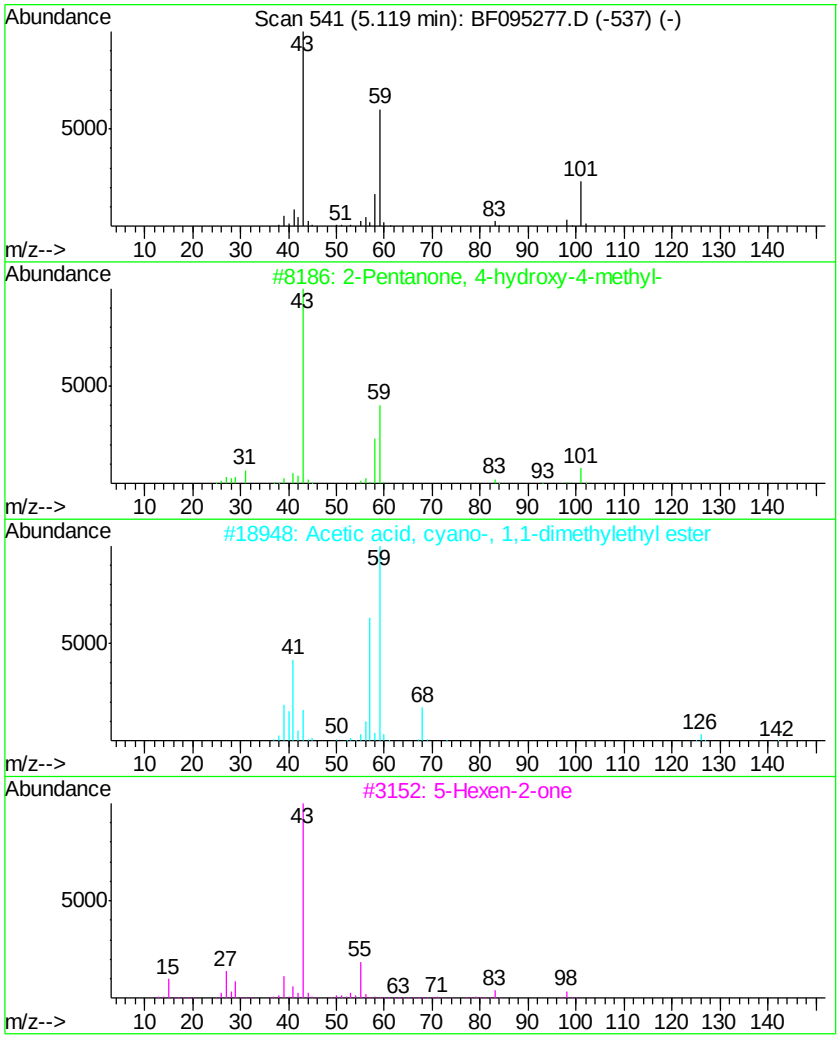
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

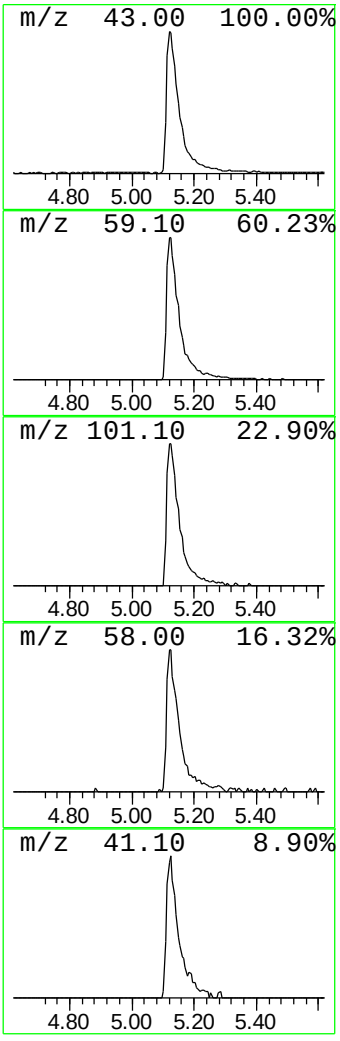
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	24.53 ng	642123	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : SJ/MA
Sample : I3202-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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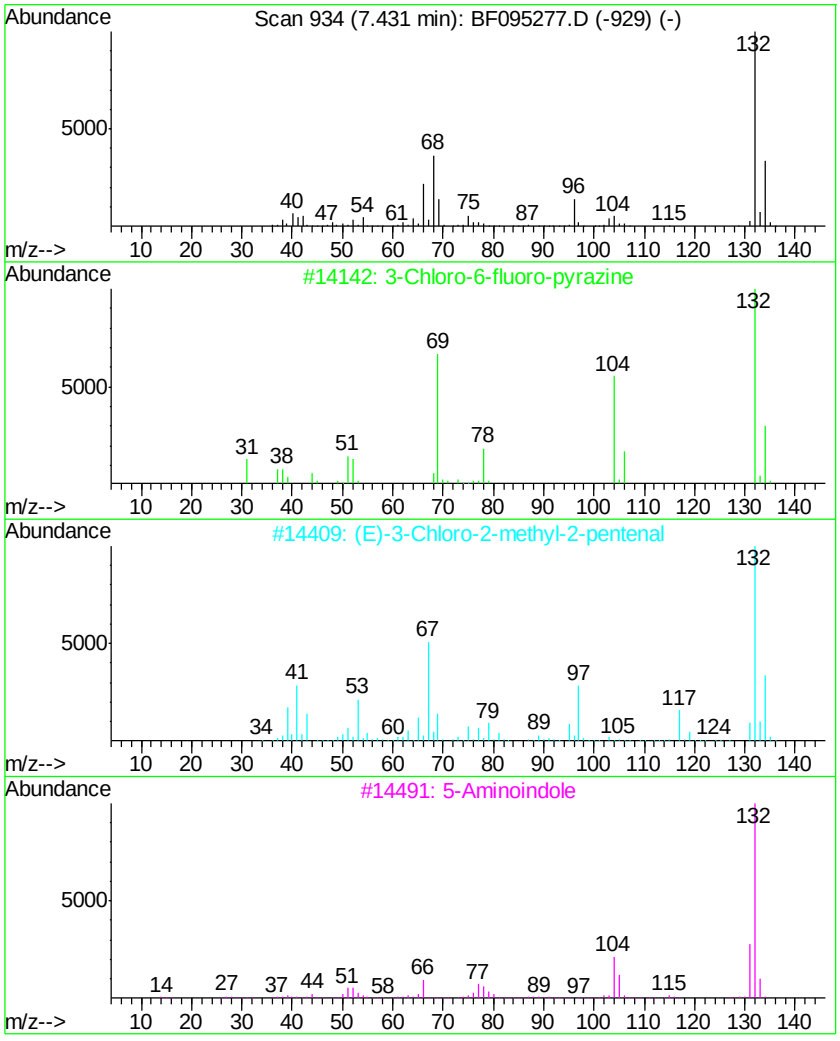
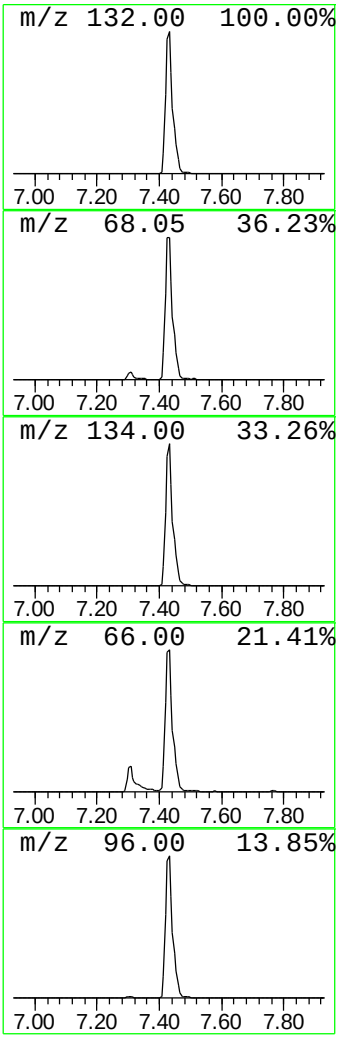
Peak Number 2 unknown7.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.43	98.86 ng	2588090	1,4-Dichlorobenzene-d4	7.77

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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Instrument : BNA_F
ClientSampleId : SB-11COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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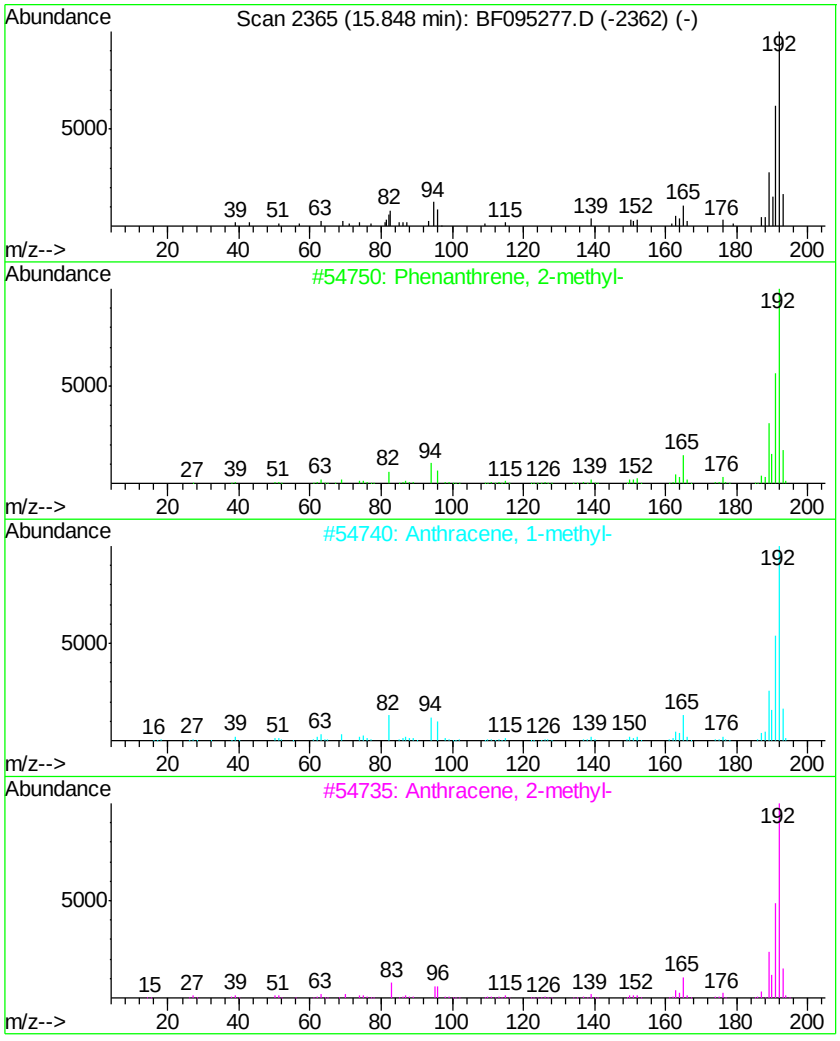
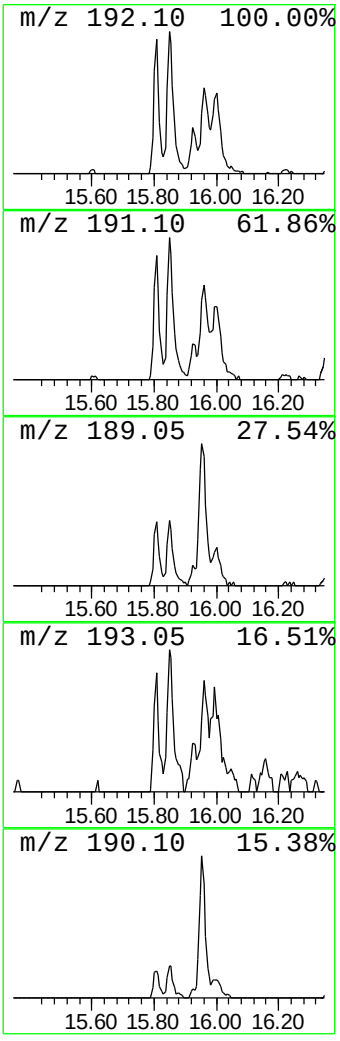
Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	2.49 ng	114376	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	97
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90





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Instrument : BNA_F
ClientSampleId : SB-11COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
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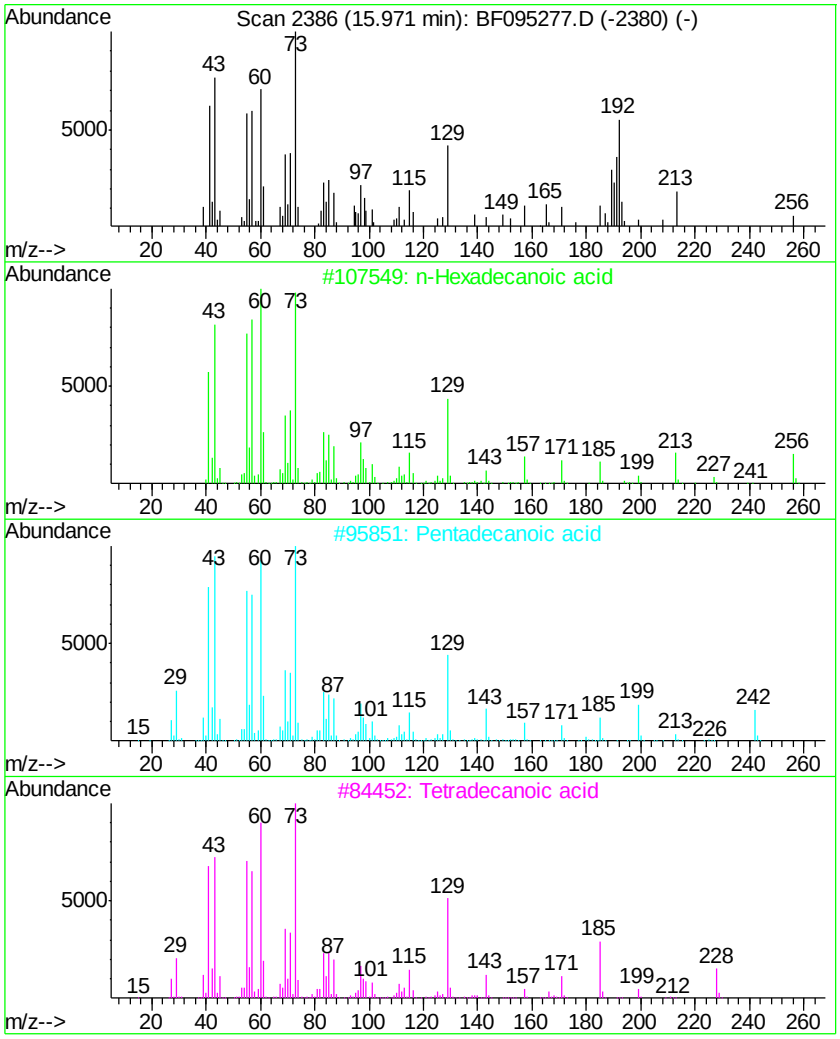
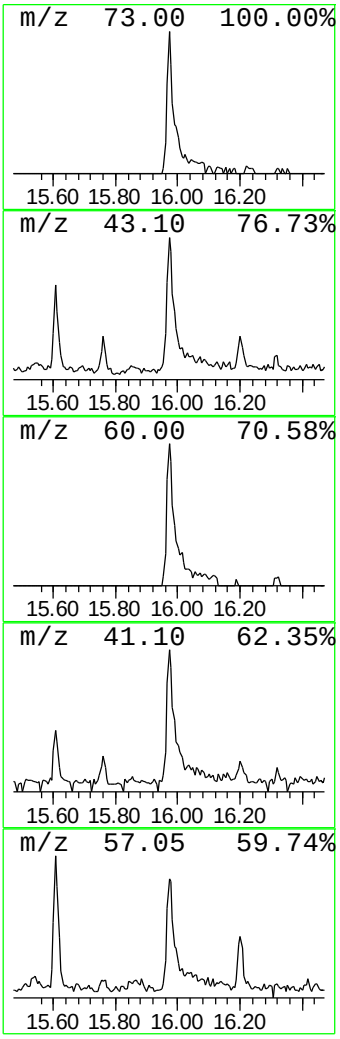
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	4.79 ng	220454	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4	Tridecanoic acid	214	C13H26O2	000638-53-9	38
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	25





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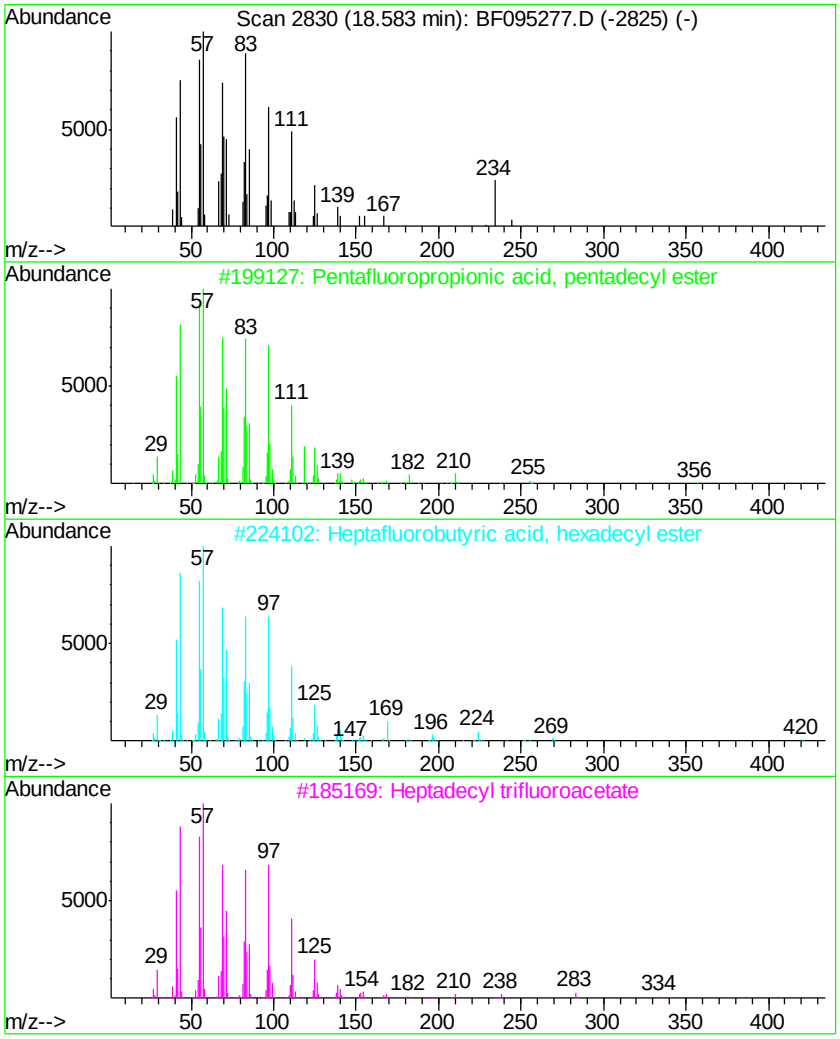
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

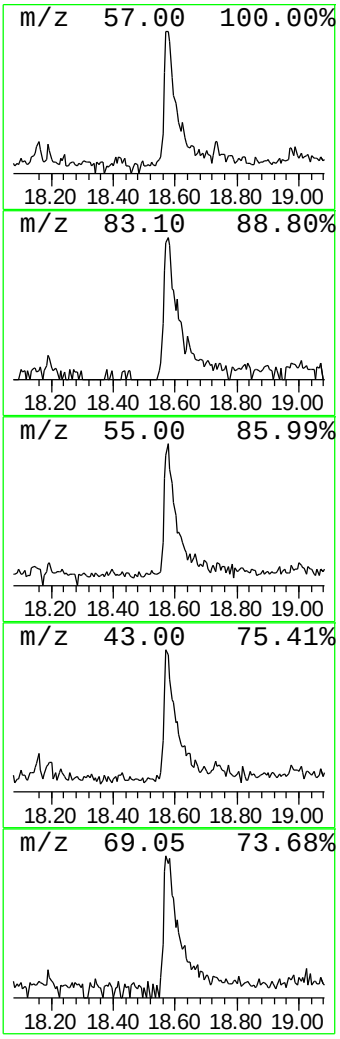
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	3.47 ng	140765	Chrysene-d12	18.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	95
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	95
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94





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
2-Pentanone, 4-hy...	5.12	24.5	ng	642123	1	7.77	523565	20.0
unknown7.43	7.43	98.9	ng	2588090	1	7.77	523565	20.0
Phenanthrene, 2-m...	15.85	2.5	ng	114376	4	15.02	919740	20.0
n-Hexadecanoic acid	15.97	4.8	ng	220454	4	15.02	919740	20.0
Pentafluoropropio...	18.58	3.5	ng	140765	5	18.69	810593	20.0