LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
Data File : BF095862.D
Acq On : 10 Jun 2017 22:53
Operator : SJ/MA
Sample : I3598-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-204-COMP

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	4.569	503	507	529	rBV	44865	130417	8.09%	0.865%
2	5.257	621	624	659	rBV	695167	1387094	86.00%	9.198%
3	6.928	904	908	920	rBV	847826	1316639	81.63%	8.731%
4	7.022	920	924	940	rVB	1056796	1612901	100.00%	10.695%
5	7.369	979	983	996	rBV	257634	344561	21.36%	2.285%
6	7.604	1018	1023	1050	rVB	838517	1118694	69.36%	7.418%
7	8.281	1134	1138	1157	rBV	550011	840764	52.13%	5.575%
8	8.410	1157	1160	1170	rVB4	10248	20702	1.28%	0.137%
9	8.669	1200	1204	1214	rBV3	16711	34507	2.14%	0.229%
10	9.398	1324	1328	1340	rBV	363924	506351	31.39%	3.358%
11	9.910	1410	1415	1419	rBV3	10398	16778	1.04%	0.111%
12	10.010	1428	1432	1439	rVB5	7847	18381	1.14%	0.122%
13	10.186	1454	1462	1470	rBV6	23227	59206	3.67%	0.393%
14	11.180	1625	1631	1645	rVB	1202342	1544638	95.77%	10.242%
15	11.404	1663	1669	1676	rBV3	12991	19958	1.24%	0.132%
16	11.874	1743	1749	1755	rBV	145182	194148	12.04%	1.287%
17	12.221	1803	1808	1813	rBV2	405551	512053	31.75%	3.395%
18	12.268	1813	1816	1824	rVB2	41817	64864	4.02%	0.430%
19	12.574	1865	1868	1875	rBV2	13270	20547	1.27%	0.136%
20	13.074	1946	1953	1957	rBV	24574	31602	1.96%	0.210%
21	13.121	1957	1961	1970	rVB	32807	49861	3.09%	0.331%
22	13.515	2023	2028	2044	rVB	529420	753921	46.74%	4.999%
23	13.745	2061	2067	2076	rBV5	12118	19706	1.22%	0.131%
24	13.845	2079	2084	2093	rBV2	20573	42225	2.62%	0.280%
25	14.615	2211	2215	2218	rVV	359539	445495	27.62%	2.954%
26	14.651	2218	2221	2230	rVB	144625	197042	12.22%	1.307%
27	14.745	2233	2237	2243	rVB	49553	65027	4.03%	0.431%
28	15.421	2348	2352	2356	rBV	27647	30655	1.90%	0.203%
29	15.462	2356	2359	2364	rVB	27841	36021	2.23%	0.239%
30	15.574	2374	2378	2383	rVV3	41795	63670	3.95%	0.422%
31	15.633	2383	2388	2397	rVB3	75311	115898	7.19%	0.769%
32	15.874	2425	2429	2434	rBV2	14814	20268	1.26%	0.134%
33	16.233	2487	2490	2493	rBV	21517	26068	1.62%	0.173%
34	16.268	2493	2496	2501	rVB6	11202	16209	1.00%	0.107%

LSC Area Percent Report

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Data File : BF095862.D
Acq On : 10 Jun 2017 22:53
Operator : SJ/MA
Sample : I3598-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-204-COMP

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	16.356	2507	2511	2517	rBV4	11589	20556	1.27%	0.136%
36	16.433	2520	2524	2530	rVB	220184	248051	15.38%	1.645%
37	16.533	2536	2541	2545	rBV7	10321	19995	1.24%	0.133%
38	16.733	2571	2575	2582	rBV	283042	352879	21.88%	2.340%
39	16.933	2605	2609	2611	rBV4	15580	19040	1.18%	0.126%
40	16.986	2614	2618	2624	rVB	970112	1096656	67.99%	7.272%
41	17.062	2624	2631	2637	rBV6	18407	38041	2.36%	0.252%
42	17.180	2648	2651	2653	rVV4	20041	30770	1.91%	0.204%
43	17.209	2653	2656	2662	rVB2	40615	54286	3.37%	0.360%
44	17.298	2667	2671	2675	rVB	32928	38422	2.38%	0.255%
45	17.339	2675	2678	2685	rBV4	24102	47247	2.93%	0.313%
46	17.456	2695	2698	2702	rBV2	19339	19983	1.24%	0.133%
47	17.980	2784	2787	2789	rBV3	31785	33680	2.09%	0.223%
48	18.039	2795	2797	2801	rVB2	16651	16498	1.02%	0.109%
49	18.245	2828	2832	2841	rBV4	72899	137167	8.50%	0.910%
50	18.333	2841	2847	2850	rBV2	423234	567366	35.18%	3.762%
51	18.368	2850	2853	2858	rVB2	69141	99133	6.15%	0.657%
52	18.809	2925	2928	2932	rVB4	23718	28879	1.79%	0.191%
53	19.603	3060	3063	3066	rBV	70633	99489	6.17%	0.660%
54	19.950	3120	3122	3126	rVB	59917	70038	4.34%	0.464%
55	20.003	3128	3131	3141	rVB	260465	365825	22.68%	2.426%

Sum of corrected areas: 15080872

LSC Report - Integrated Chromatogram

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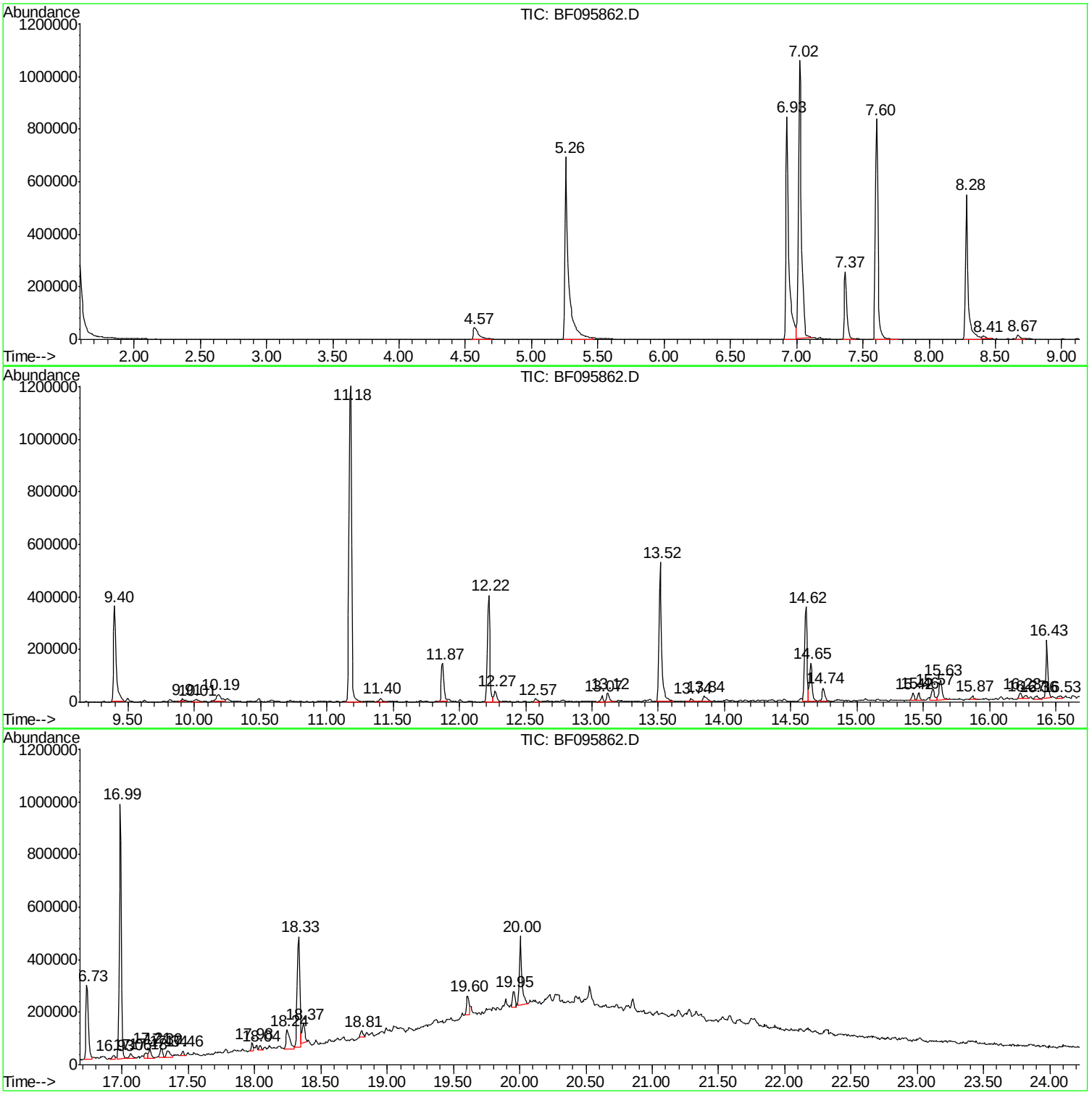
Data File : BF095862.D
Acq On : 10 Jun 2017 22:53
Operator : SJ/MA
Sample : I3598-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-204-COMP

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\BF061017\
Data File : BF095862.D
Acq On : 10 Jun 2017 22:53
Operator : SJ/MA
Sample : I3598-01
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

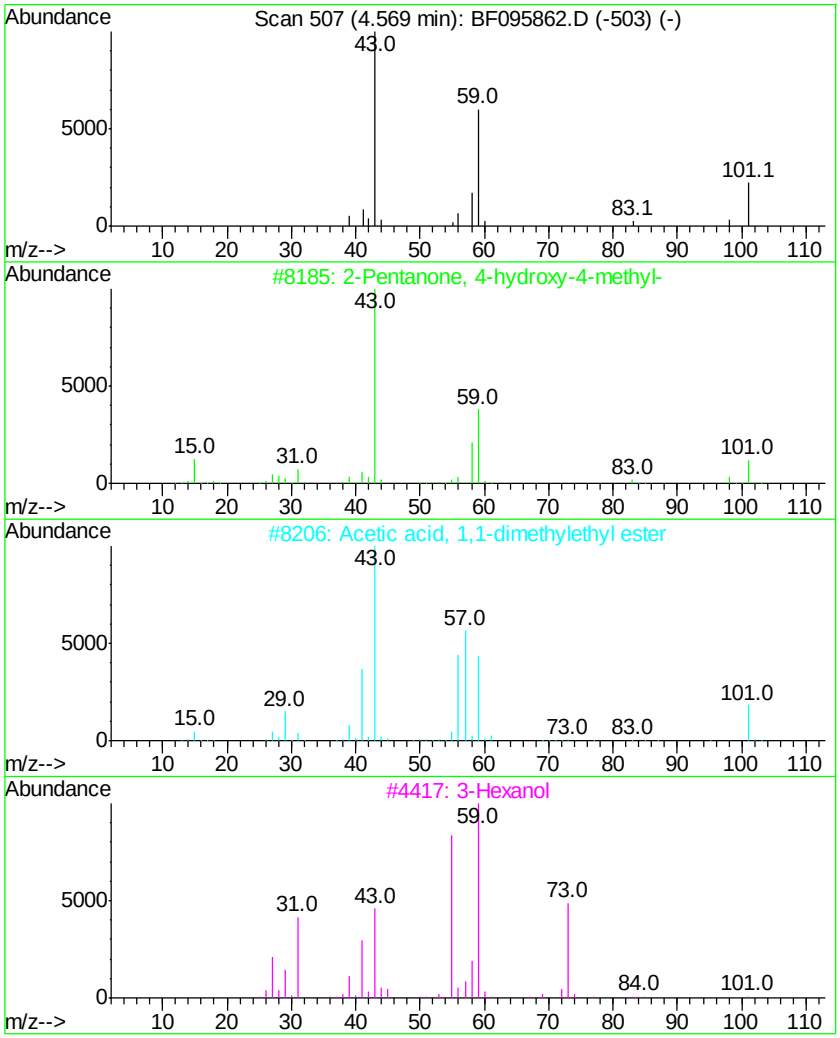
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

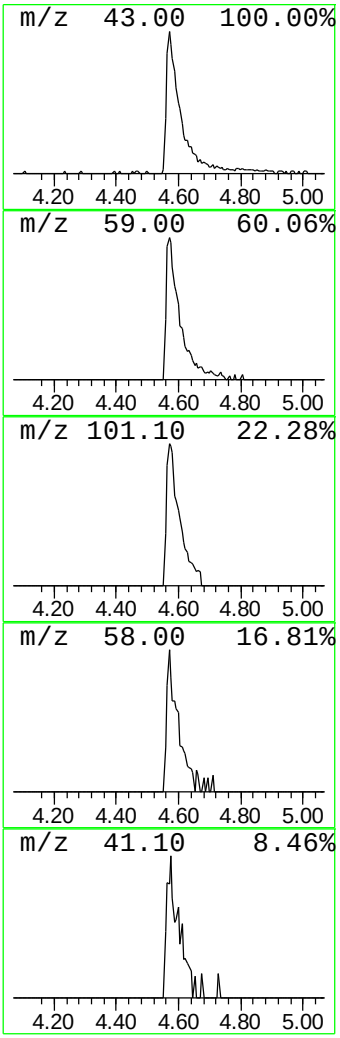
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	7.57 ng	130417	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
Data File : BF095862.D
Acq On : 10 Jun 2017 22:53
Operator : SJ/MA
Sample : I3598-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-204-COMP

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

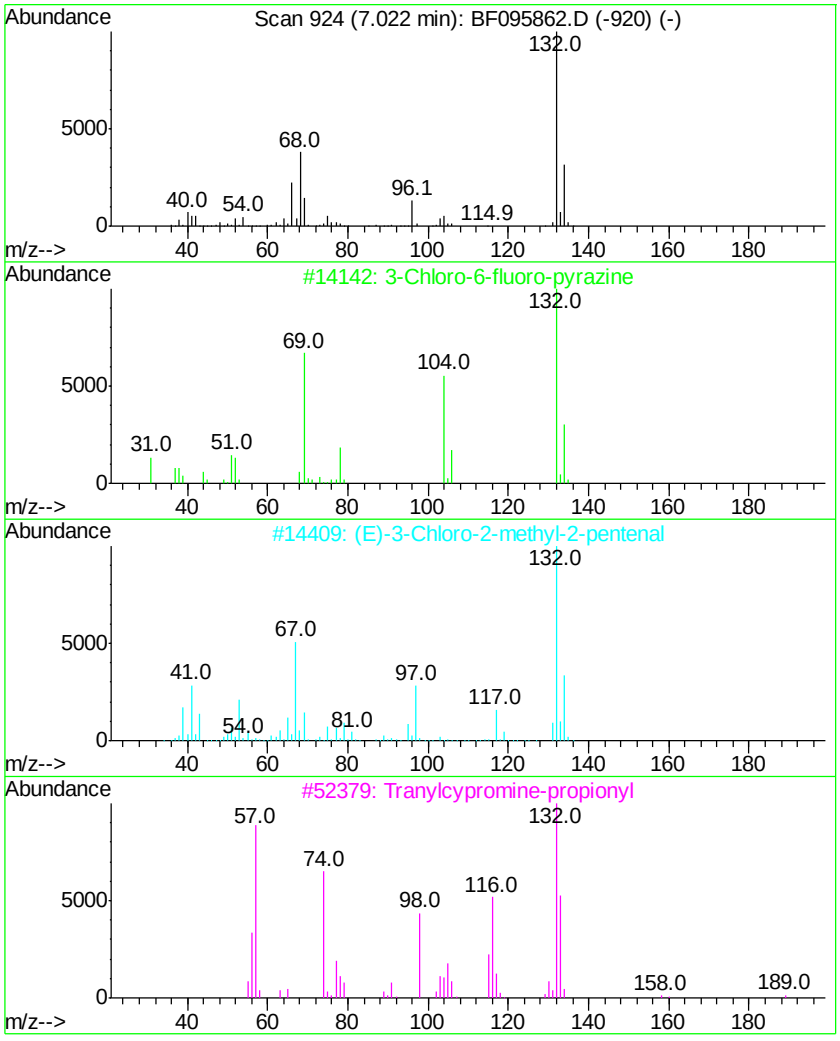
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

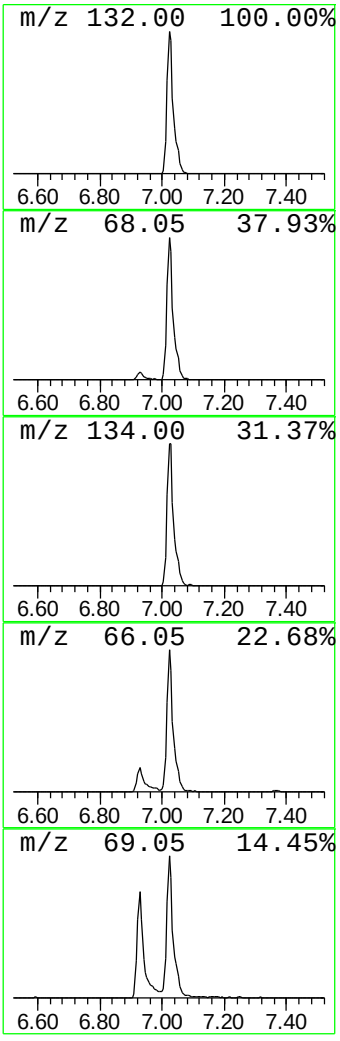
****

Peak Number 2 unknown7.02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	93.62 ng	1612900	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
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Operator : SJ/MA
Sample : I3598-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-204-COMP

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

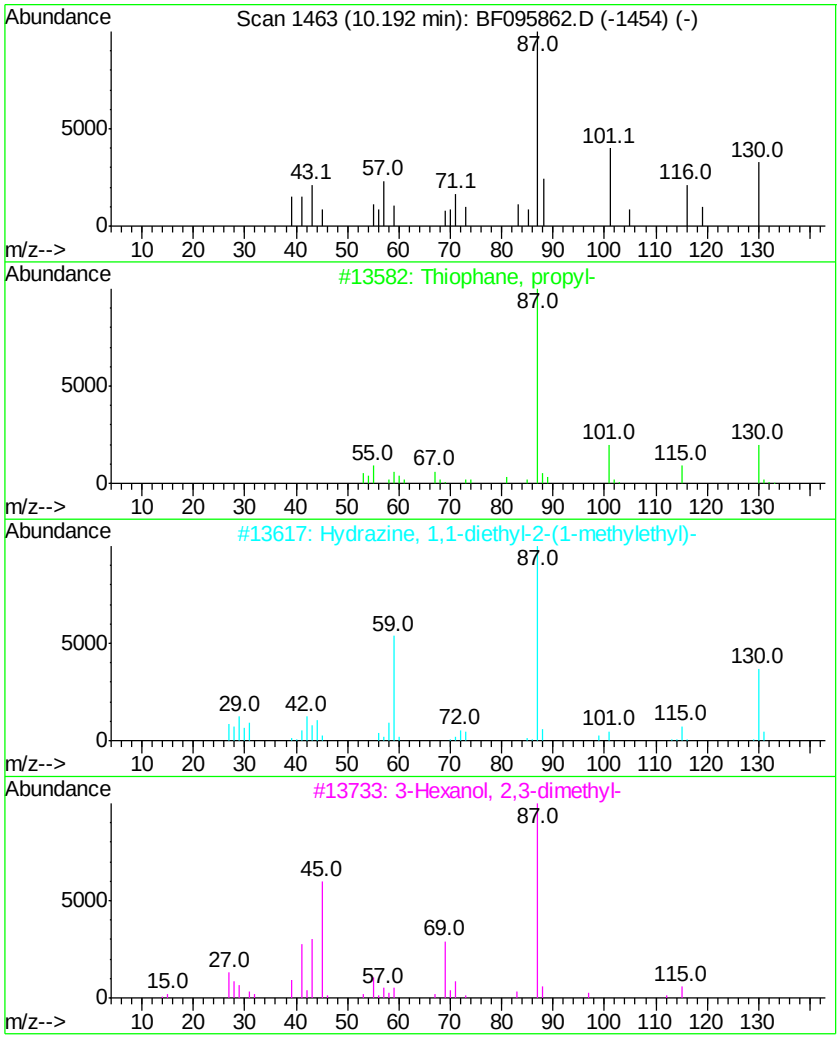
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

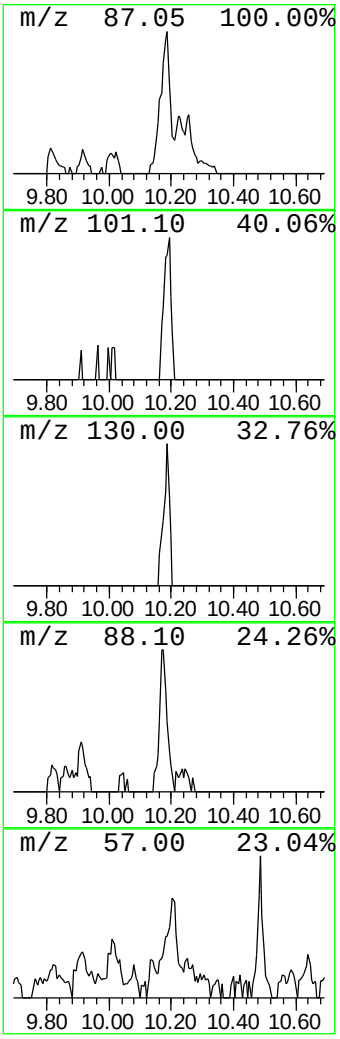
****

Peak Number 4 Thiophane, propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	2.34 ng	59206	Naphthalene-d8	9.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophane, propyl-	130	C7H14S	001551-34-4	59
2	Hydrazine, 1,1-diethyl-2-(1-meth...	130	C7H18N2	067398-39-4	47
3	3-Hexanol, 2,3-dimethyl-	130	C8H18O	004166-46-5	32
4	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	16
5	Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	9





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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-204-COMP

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

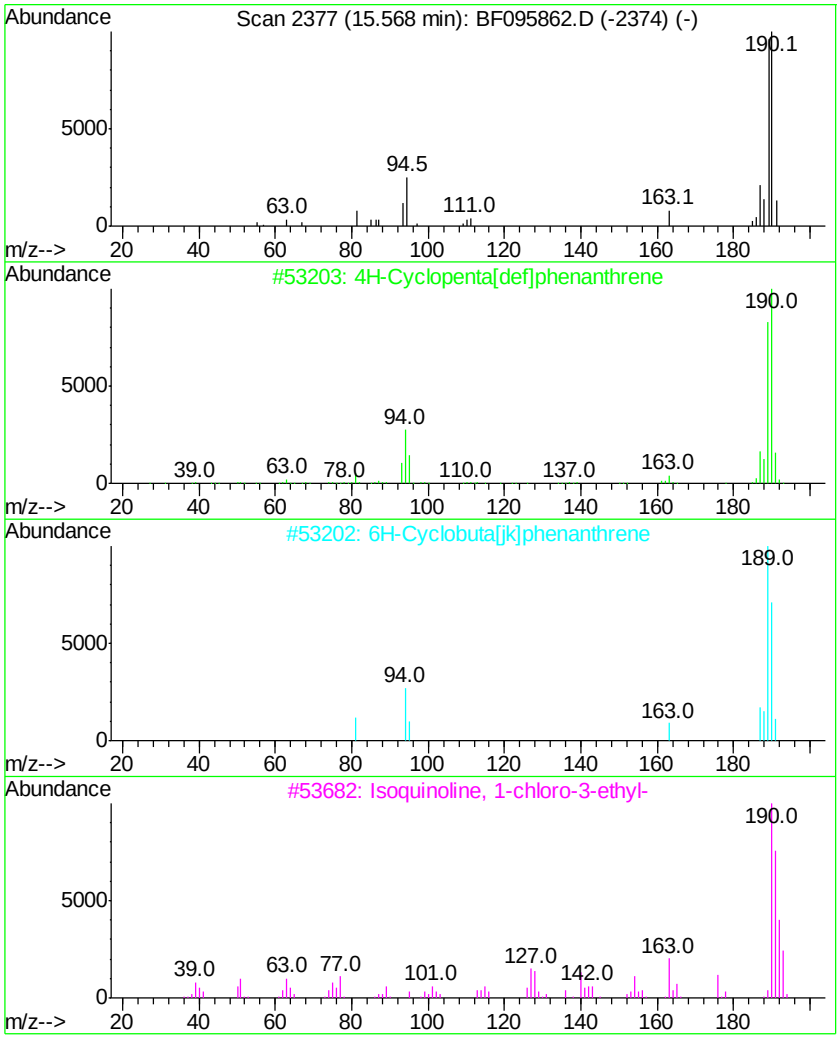
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

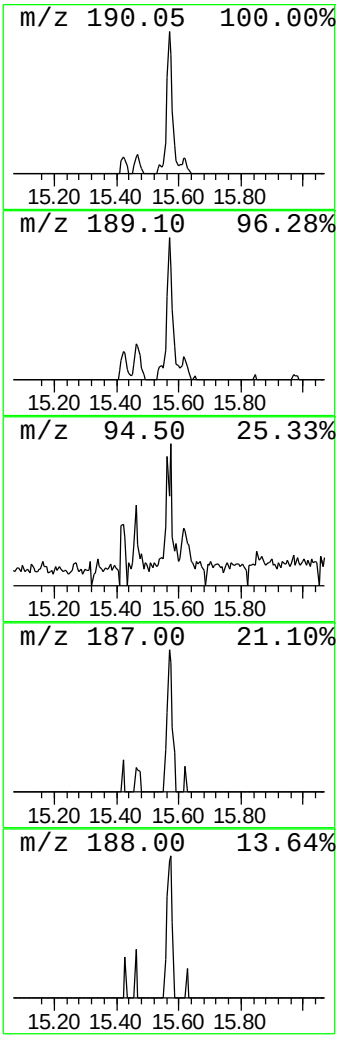
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	2.86 ng	63670	Phenanthrene-d10	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	42
3	Isoquinoline, 1-chloro-3-ethyl-	191	C11H10ClN	055150-52-2	14
4	2-Fluoro-4-(trifluoromethyl)benz...	189	C8H3F4N	146070-34-0	14
5	3-Fluoro-5-(trifluoromethyl)benz...	189	C8H3F4N	149793-69-1	12





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : VNJ-204-COMP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

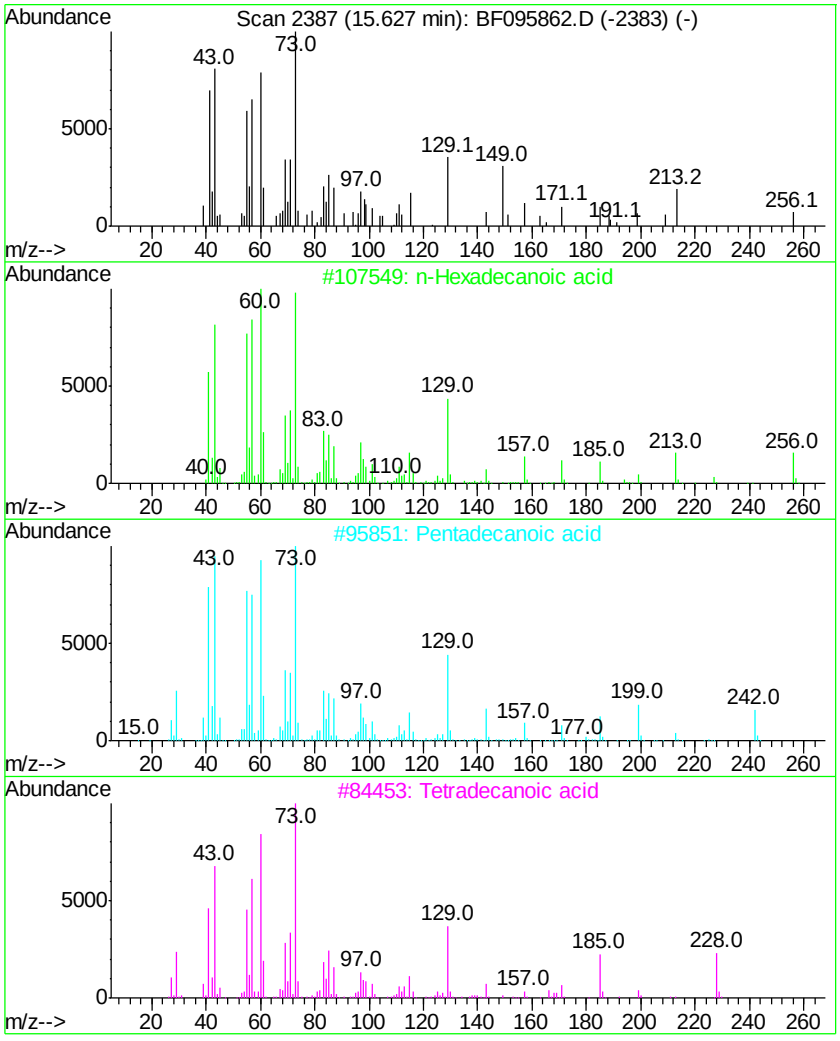
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

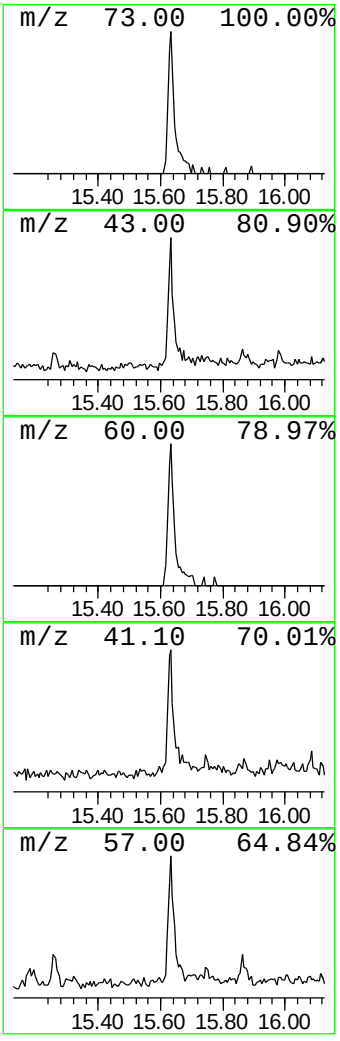
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	5.20 ng	115898	Phenanthrene-d10	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-204-COMP

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

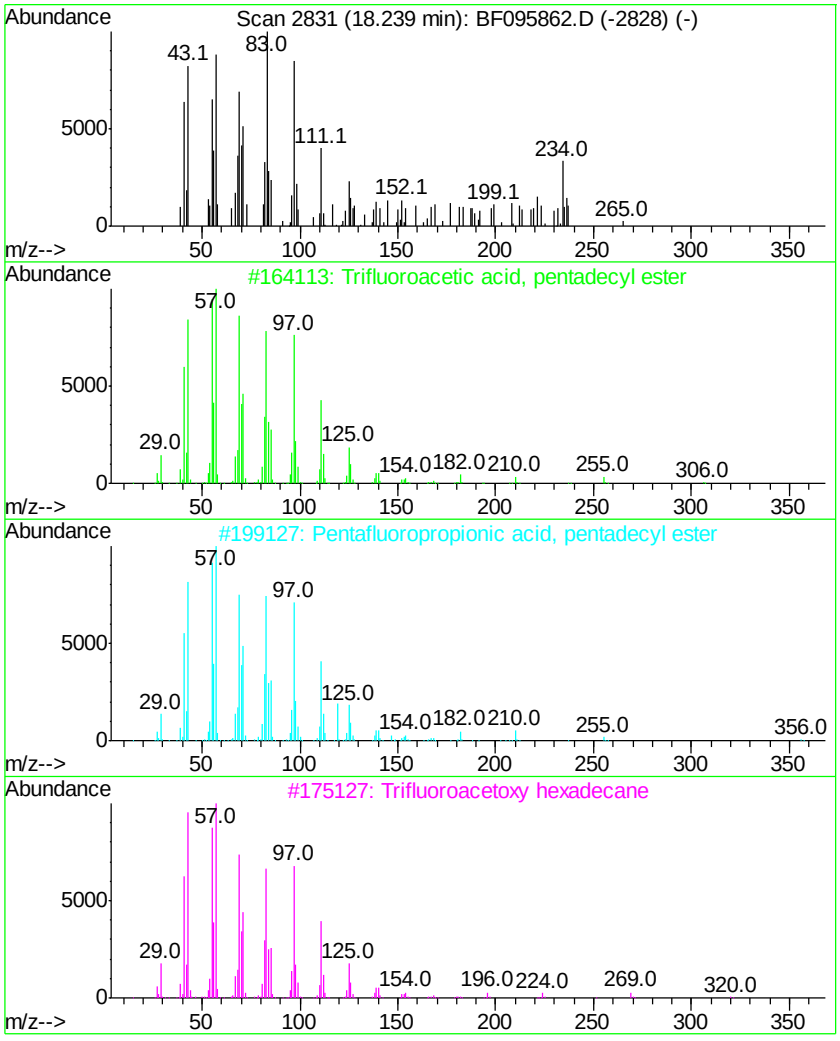
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

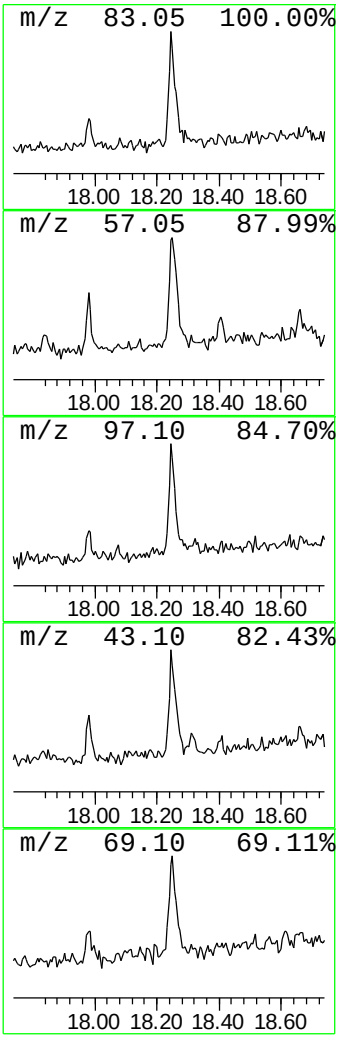
****

Peak Number 7 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	4.84 ng	137167	Chrysene-d12	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	9-Nonadecene	266	C19H38	031035-07-1	93
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061017\
Data File : BF095862.D
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Operator : SJ/MA
Sample : I3598-01
Misc :
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Instrument : BNA_F
ClientSampleId : VNJ-204-COMP

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.57	7.6	ng	130417	1	7.37	344561	20.0
unknown7.02	7.02	93.6	ng	1612900	1	7.37	344561	20.0
Thiophane, propyl-	10.19	2.3	ng	59206	2	9.40	506351	20.0
4H-Cyclopenta[def...	15.57	2.9	ng	63670	4	14.62	445495	20.0
n-Hexadecanoic acid	15.63	5.2	ng	115898	4	14.62	445495	20.0
Trifluoroacetic a...	18.24	4.8	ng	137167	5	18.33	567366	20.0