

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
 Data File : BF096701.D
 Acq On : 12 Jul 2017 19:39
 Operator : SJ/JU
 Sample : I4144-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP3-0-3

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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	2.210	11	21	27	rVB	129049	199523	7.78%	0.634%
2	2.669	94	99	104	rVB5	19979	37731	1.47%	0.120%
3	3.010	154	157	172	rBV	27597	83838	3.27%	0.266%
4	4.857	466	471	486	rVB	348235	524925	20.46%	1.667%
5	5.239	533	536	539	rBV2	33824	37462	1.46%	0.119%
6	5.287	539	544	554	rVV	2301104	2463430	96.03%	7.822%
7	5.504	578	581	591	rVB2	37412	48738	1.90%	0.155%
8	5.981	659	662	666	rBV	35229	36212	1.41%	0.115%
9	6.198	697	699	706	rVB4	21277	37010	1.44%	0.118%
10	6.316	713	719	728	rVB	2402927	2565326	100.00%	8.146%
11	6.439	736	740	743	rBV	2660421	2494214	97.23%	7.920%
12	6.498	746	750	752	rBV	36273	35370	1.38%	0.112%
13	6.669	775	779	782	rBV	820365	724305	28.23%	2.300%
14	6.822	801	805	809	rBV	2092305	2121217	82.69%	6.735%
15	7.228	869	874	877	rBV	1553702	1595368	62.19%	5.066%
16	7.281	880	883	886	rVB	50125	42705	1.66%	0.136%
17	7.351	886	895	899	rBV2	76191	116656	4.55%	0.370%
18	7.863	978	982	985	rBV	50638	50055	1.95%	0.159%
19	7.951	993	997	999	rBV	1001487	929657	36.24%	2.952%
20	8.386	1069	1071	1074	rVB	63107	52780	2.06%	0.168%
21	8.557	1097	1100	1103	rVB	75690	55811	2.18%	0.177%
22	8.663	1114	1118	1121	rVB	147482	136645	5.33%	0.434%
23	8.757	1131	1134	1138	rVB	119324	99726	3.89%	0.317%
24	9.027	1175	1180	1183	rBV	2677415	2438670	95.06%	7.743%
25	9.122	1189	1196	1199	rBV	104452	104165	4.06%	0.331%
26	9.286	1217	1224	1229	rBV3	44300	59923	2.34%	0.190%
27	9.363	1234	1237	1239	rVV	64472	63293	2.47%	0.201%
28	9.386	1239	1241	1243	rVV	57552	41625	1.62%	0.132%
29	9.422	1243	1247	1249	rVV	789124	634734	24.74%	2.015%
30	9.439	1249	1250	1252	rVV	65740	38565	1.50%	0.122%
31	9.557	1266	1270	1274	rVB	165829	141477	5.51%	0.449%
32	9.651	1283	1286	1289	rVB	76167	66505	2.59%	0.211%
33	9.698	1289	1294	1298	rBV2	916224	840416	32.76%	2.669%
34	9.904	1325	1329	1333	rBV	78312	77460	3.02%	0.246%

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35	10.016	1343	1348	1351	rBV2	27082	39133	1.53%	0.124%
36	10.110	1359	1364	1368	rBV3	56733	75177	2.93%	0.239%
37	10.145	1368	1370	1373	rVB	127440	93388	3.64%	0.297%
38	10.239	1384	1386	1389	rBV2	48989	40124	1.56%	0.127%
39	10.363	1403	1407	1410	rBV2	59256	67294	2.62%	0.214%
40	10.404	1410	1414	1416	rBV	35957	35498	1.38%	0.113%
41	10.486	1423	1428	1431	rBV	1194381	1156995	45.10%	3.674%
42	10.616	1446	1450	1452	rBV2	163371	179749	7.01%	0.571%
43	10.633	1452	1453	1457	rVB	145215	86769	3.38%	0.276%
44	10.921	1497	1502	1504	rBV3	43039	65794	2.56%	0.209%
45	10.980	1510	1512	1517	rVB2	57715	55847	2.18%	0.177%
46	11.063	1523	1526	1529	rVV2	155390	126477	4.93%	0.402%
47	11.092	1529	1531	1535	rVB	45242	45076	1.76%	0.143%
48	11.174	1542	1545	1548	rBV	714164	671593	26.18%	2.132%
49	11.198	1548	1549	1553	rVV	308677	190413	7.42%	0.605%
50	11.251	1555	1558	1561	rVB	168445	136208	5.31%	0.432%
51	11.416	1580	1586	1595	rBV2	293542	324327	12.64%	1.030%
52	11.492	1596	1599	1605	rVB2	91808	94133	3.67%	0.299%
53	11.721	1633	1638	1640	rBV2	168057	196140	7.65%	0.623%
54	11.751	1640	1643	1646	rVB2	65422	59372	2.31%	0.189%
55	11.786	1646	1649	1652	rBV	75499	90139	3.51%	0.286%
56	11.898	1663	1668	1672	rVB	73439	87696	3.42%	0.278%
57	11.974	1678	1681	1683	rBV	75296	65046	2.54%	0.207%
58	11.992	1683	1684	1688	rVB2	45673	36171	1.41%	0.115%
59	12.233	1721	1725	1731	rBV2	382308	389394	15.18%	1.236%
60	12.280	1731	1733	1736	rVV	82313	80963	3.16%	0.257%
61	12.310	1736	1738	1742	rVB3	49435	49221	1.92%	0.156%
62	12.386	1747	1751	1754	rBV	479457	427806	16.68%	1.358%
63	12.433	1754	1759	1764	rBV9	20028	44369	1.73%	0.141%
64	12.504	1769	1771	1778	rBV4	47213	68383	2.67%	0.217%
65	12.610	1784	1789	1792	rBV	470214	479127	18.68%	1.521%
66	12.657	1794	1797	1803	rVB3	66151	95588	3.73%	0.304%
67	12.762	1811	1815	1818	rVV	1366033	1288278	50.22%	4.091%
68	12.833	1821	1827	1830	rBV4	50888	85289	3.32%	0.271%
69	12.915	1838	1841	1843	rBV3	49061	58178	2.27%	0.185%
70	12.939	1843	1845	1848	rVB	67838	60312	2.35%	0.192%
71	12.980	1848	1852	1854	rBV4	29791	39855	1.55%	0.127%

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72	13.010	1854	1857	1859	rBV	64849	52259	2.04%	0.166%
73	13.045	1859	1863	1865	rBV	76836	79747	3.11%	0.253%
74	13.133	1875	1878	1881	rVB	49014	42546	1.66%	0.135%
75	13.162	1881	1883	1888	rBV2	37877	48719	1.90%	0.155%
76	13.215	1890	1892	1894	rVV2	51027	54281	2.12%	0.172%
77	13.245	1895	1897	1904	rVV	125128	143389	5.59%	0.455%
78	13.327	1907	1911	1913	rVV5	35264	61211	2.39%	0.194%
79	13.351	1913	1915	1920	rVB5	61686	72850	2.84%	0.231%
80	13.445	1928	1931	1936	rVB	80580	78454	3.06%	0.249%
81	13.551	1946	1949	1953	rBV2	76764	111182	4.33%	0.353%
82	13.610	1956	1959	1964	rVB2	52298	71824	2.80%	0.228%
83	13.668	1964	1969	1973	rBV2	127983	192888	7.52%	0.612%
84	13.804	1987	1992	1995	rBV2	816981	1034905	40.34%	3.286%
85	13.833	1995	1997	1999	rVB	281619	222229	8.66%	0.706%
86	13.992	2022	2024	2026	rVB2	44714	35998	1.40%	0.114%
87	14.192	2056	2058	2061	rVB	74147	60862	2.37%	0.193%
88	14.227	2061	2064	2068	rVB3	55838	58238	2.27%	0.185%
89	14.592	2124	2126	2133	rBV5	46014	59894	2.33%	0.190%
90	14.656	2134	2137	2143	rVV4	71958	99453	3.88%	0.316%
91	14.727	2147	2149	2152	rVV2	43868	37783	1.47%	0.120%
92	14.815	2159	2164	2166	rBV	475871	645528	25.16%	2.050%
93	14.909	2177	2180	2184	rVB	124787	129725	5.06%	0.412%
94	15.086	2207	2210	2216	rVB	279272	350877	13.68%	1.114%
95	15.145	2216	2220	2225	rBV	259795	318813	12.43%	1.012%
96	15.204	2226	2230	2233	rBV	437564	504193	19.65%	1.601%
97	16.527	2450	2455	2466	rVB2	161573	344315	13.42%	1.093%
98	16.739	2488	2491	2494	rBV5	36620	49023	1.91%	0.156%
99	16.927	2518	2523	2531	rVB	133496	246336	9.60%	0.782%
100	18.956	2862	2868	2873	rVB5	38255	105052	4.10%	0.334%

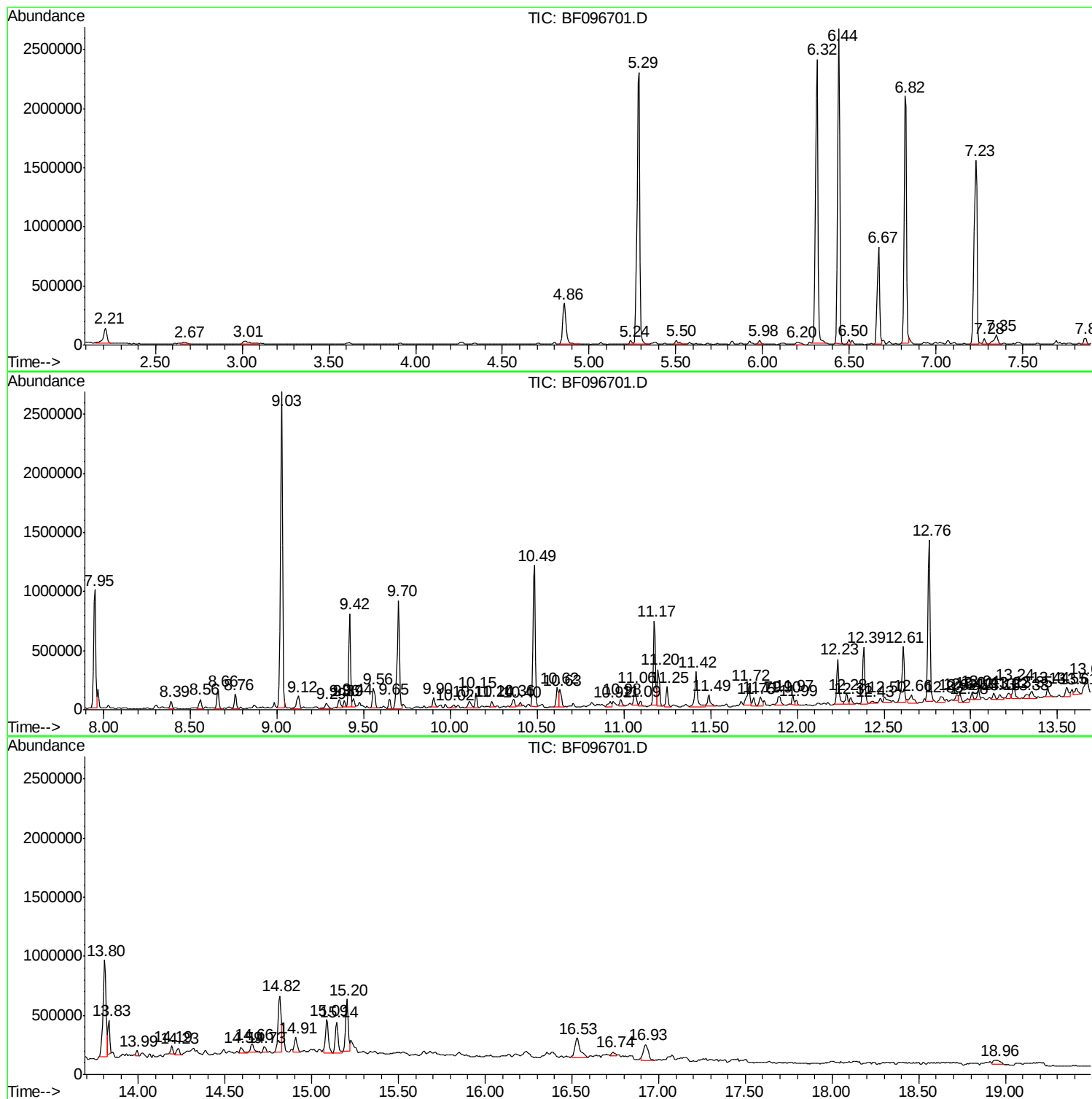
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BNA_F
ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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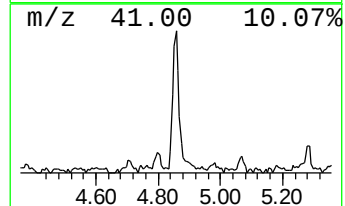
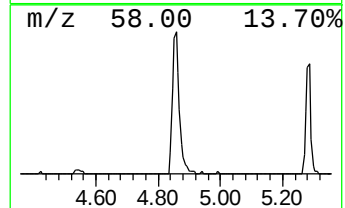
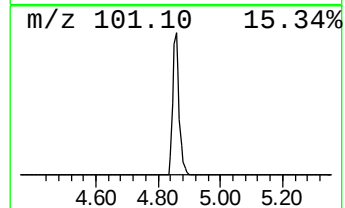
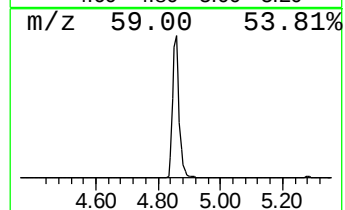
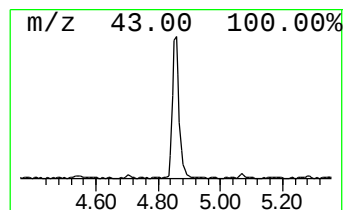
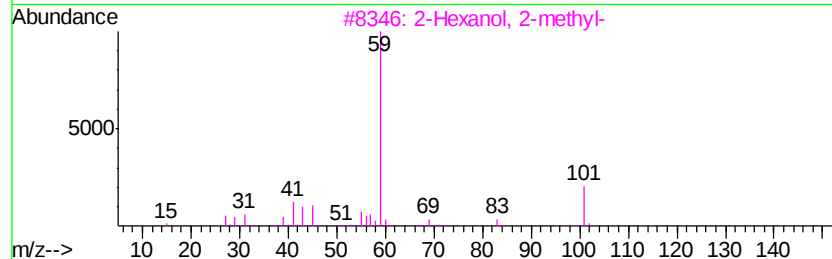
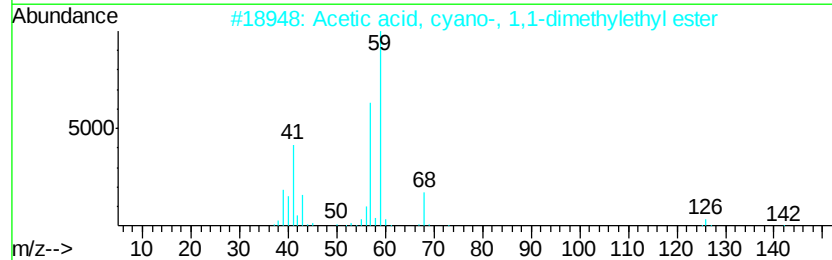
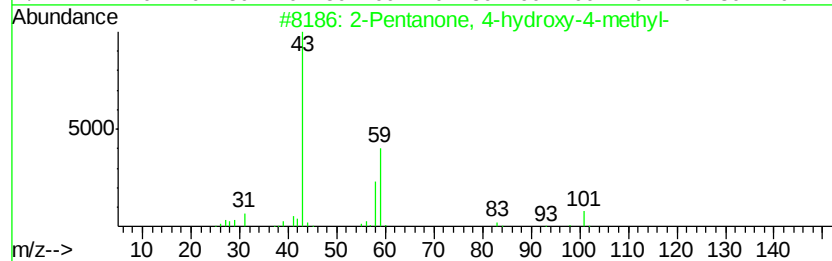
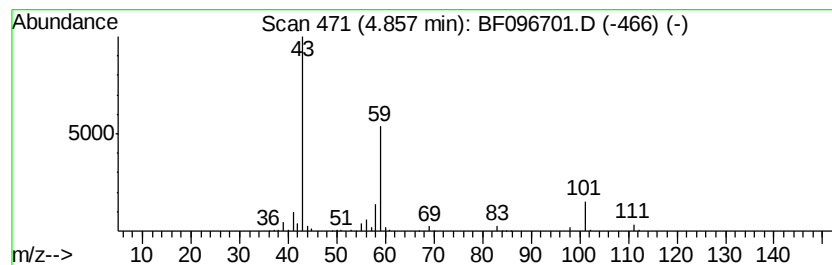
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	14.49 ng	524925	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33



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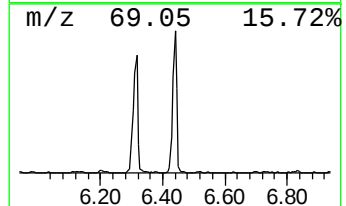
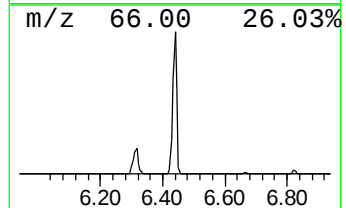
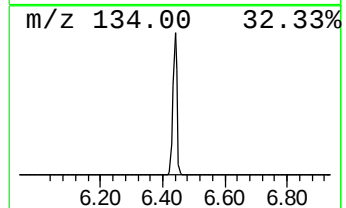
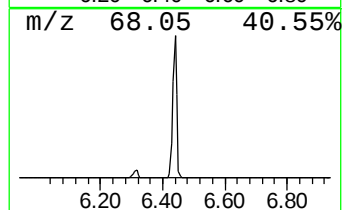
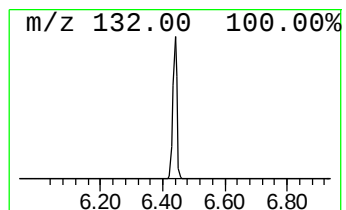
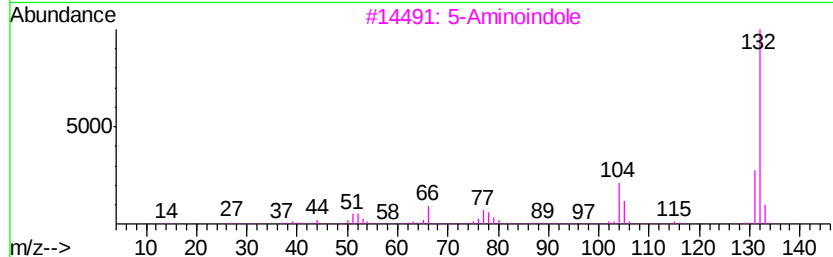
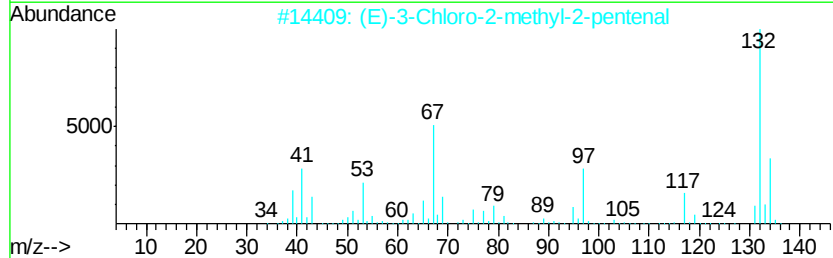
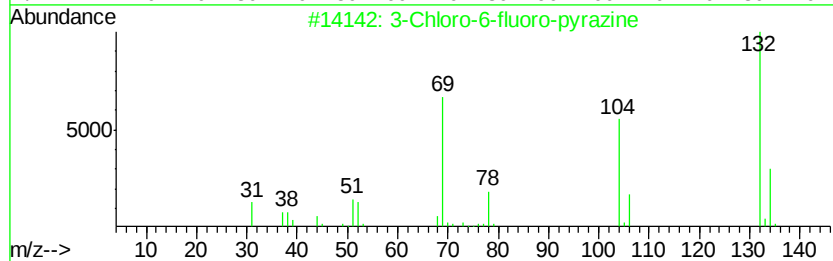
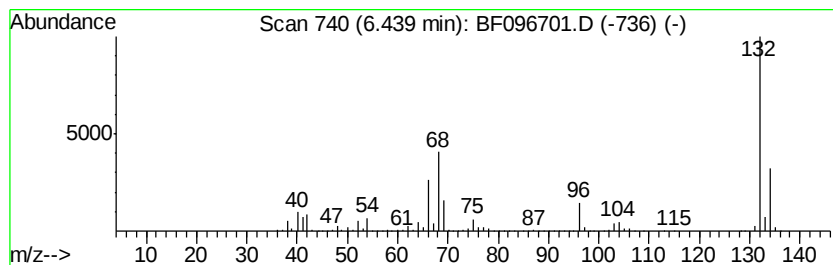
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	68.87 ng	2494210	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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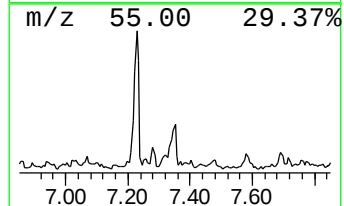
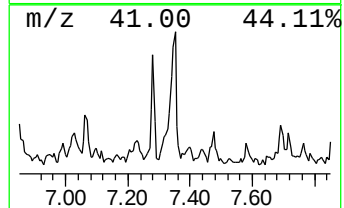
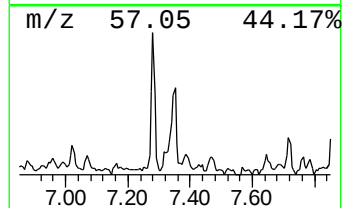
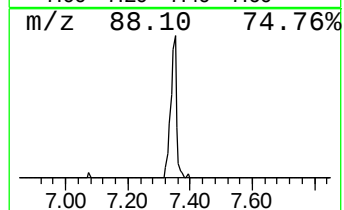
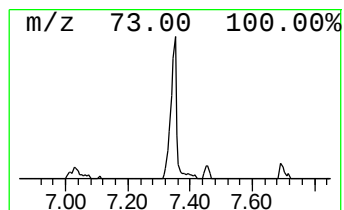
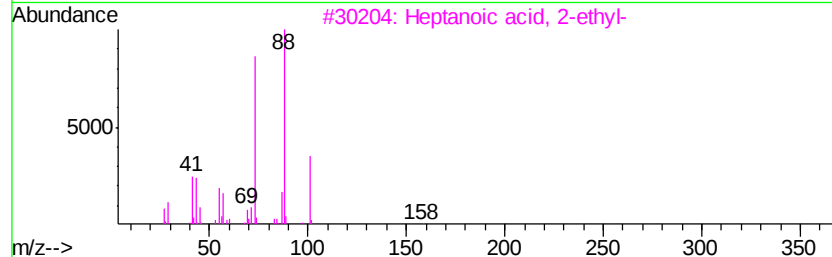
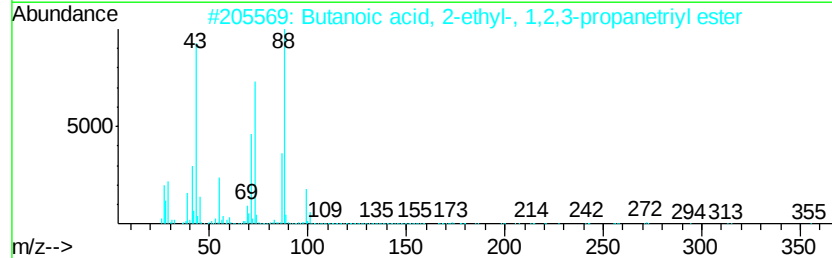
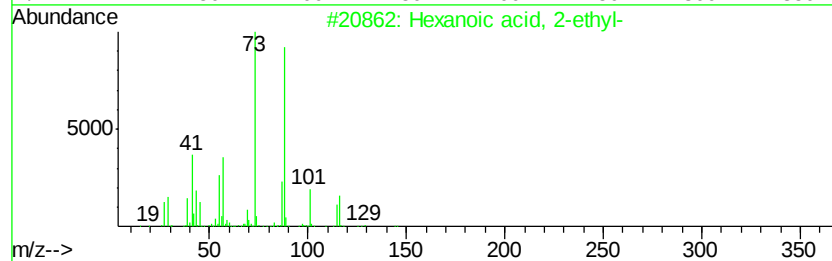
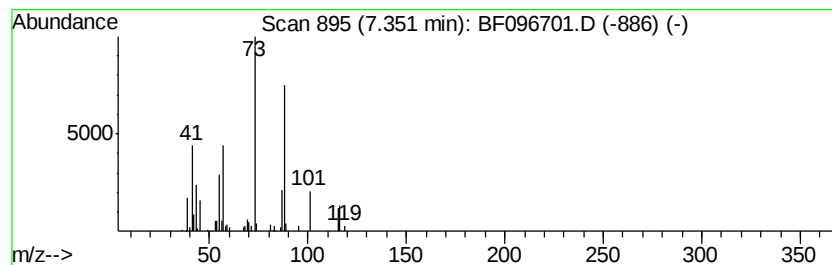
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Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.35	2.51 ng	116656	Naphthalene-d8	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50
3		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	45
4		Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	38
5		Pentanoic acid, ethyl ester	130	C7H14O2	000539-82-2	36



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Operator : SJ/JU
Sample : I4144-03
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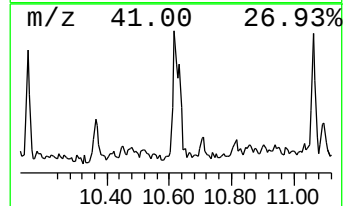
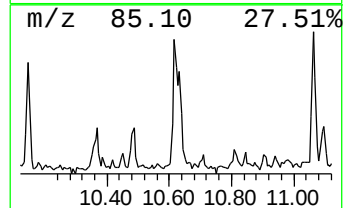
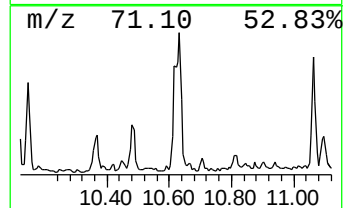
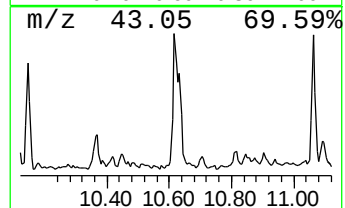
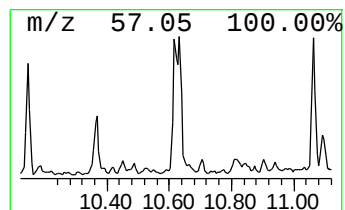
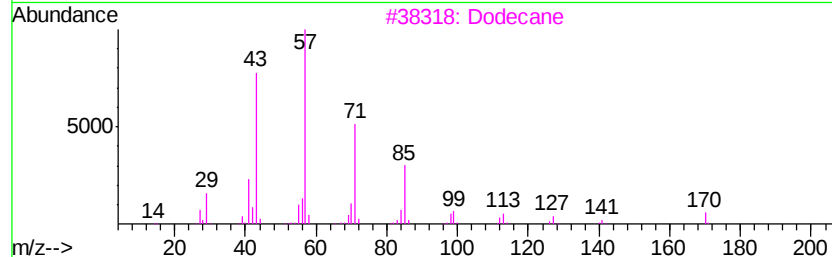
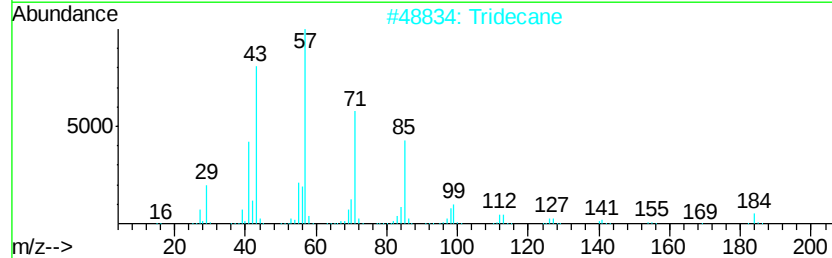
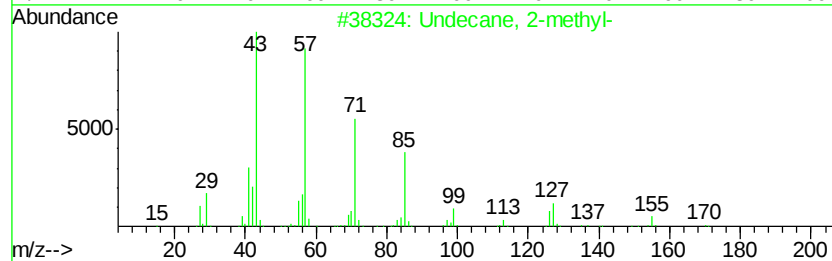
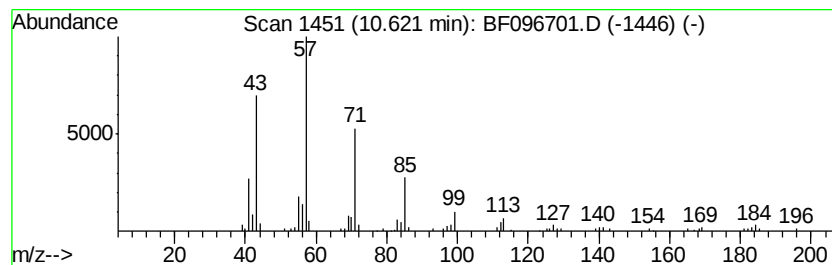
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ClientSampleId :
TP3-0-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Undecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.62	5.35 ng	179749	Phenanthrene-d10	11.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2-methyl-	170	C12H26	007045-71-8	87
2	Tridecane	184	C13H28	000629-50-5	87
3	Dodecane	170	C12H26	000112-40-3	83
4	Hexadecane	226	C16H34	000544-76-3	80
5	5-Ethyldecane	170	C12H26	017302-36-2	74



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
Data File : BF096701.D
Acq On : 12 Jul 2017 19:39
Operator : SJ/JU
Sample : I4144-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-0-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dodecane, 2,6,10-trimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.58 ng	86769	Phenanthrene-d10	11.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	59
2		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	59
3		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	59
4		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
5		Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	53

