

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
 Data File : BF104378.D
 Acq On : 9 Apr 2018 17:56
 Operator : JU/SJ
 Sample : J2157-01 5X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-01-040618-A

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-BF040618.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	4.992	490	494	498	rVB	27874	28542	2.61%	0.265%
2	5.398	559	563	566	rBV	752835	633368	57.93%	5.874%
3	6.028	667	670	679	rBV	36940	39516	3.61%	0.366%
4	6.416	733	736	740	rBV	732773	633592	57.96%	5.876%
5	6.563	757	761	765	rBV	825844	678090	62.03%	6.289%
6	6.804	798	802	805	rBV	991936	788951	72.17%	7.317%
7	6.957	824	828	831	rBV	678755	512911	46.92%	4.757%
8	7.363	893	897	900	rVB	468096	375501	34.35%	3.483%
9	8.086	1016	1020	1023	rVB	1357454	1042888	95.39%	9.672%
10	9.163	1199	1203	1206	rBV	896219	748848	68.50%	6.945%
11	9.239	1213	1216	1219	rBV	21962	21105	1.93%	0.196%
12	9.557	1266	1270	1273	rBV	80316	78567	7.19%	0.729%
13	9.775	1304	1307	1311	rVB	29695	27117	2.48%	0.251%
14	9.839	1315	1318	1322	rVV	1165504	1093246	100.00%	10.139%
15	10.274	1389	1392	1394	rVB	40611	33480	3.06%	0.311%
16	10.492	1424	1429	1432	rBV3	16341	18819	1.72%	0.175%
17	10.627	1448	1452	1455	rBV	457648	378343	34.61%	3.509%
18	10.745	1469	1472	1481	rVB	46370	59416	5.43%	0.551%
19	11.192	1546	1548	1551	rBV2	27231	25499	2.33%	0.236%
20	11.221	1551	1553	1559	rVB	24059	26009	2.38%	0.241%
21	11.327	1567	1571	1574	rBV	1111398	932583	85.30%	8.649%
22	11.351	1574	1575	1577	rVB	45849	22630	2.07%	0.210%
23	11.621	1619	1621	1624	rBV	23525	16851	1.54%	0.156%
24	11.857	1658	1661	1664	rVB2	33109	33431	3.06%	0.310%
25	11.939	1672	1675	1677	rBV2	16160	16118	1.47%	0.149%
26	11.963	1677	1679	1683	rVB2	12205	12978	1.19%	0.120%
27	12.027	1688	1690	1694	rVB	20569	17488	1.60%	0.162%
28	12.257	1726	1729	1731	rBV4	14713	14400	1.32%	0.134%
29	12.380	1747	1750	1752	rBV	25166	23098	2.11%	0.214%
30	12.421	1752	1757	1761	rVB5	30148	44446	4.07%	0.412%
31	12.539	1774	1777	1780	rBV	81358	62595	5.73%	0.581%
32	12.586	1783	1785	1790	rVB6	15856	19725	1.80%	0.183%
33	12.633	1790	1793	1796	rBV5	16809	22277	2.04%	0.207%
34	12.698	1801	1804	1806	rBV2	12866	16125	1.47%	0.150%

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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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.768	1811	1816	1818	rBV	84553	80274	7.34%	0.745%
36	12.792	1818	1820	1823	rVB2	39170	32562	2.98%	0.302%
37	12.916	1837	1841	1849	rVB	615797	525139	48.03%	4.870%
38	13.098	1870	1872	1876	rVB2	31532	27483	2.51%	0.255%
39	13.151	1879	1881	1887	rVB3	36461	44359	4.06%	0.411%
40	13.363	1915	1917	1921	rVB5	27236	25093	2.30%	0.233%
41	13.498	1938	1940	1943	rBV2	31166	27327	2.50%	0.253%
42	13.833	1994	1997	2001	rBV3	72646	89418	8.18%	0.829%
43	13.992	2020	2024	2027	rBV	795972	791266	72.38%	7.339%
44	15.504	2277	2281	2285	rBV	528592	640723	58.61%	5.942%

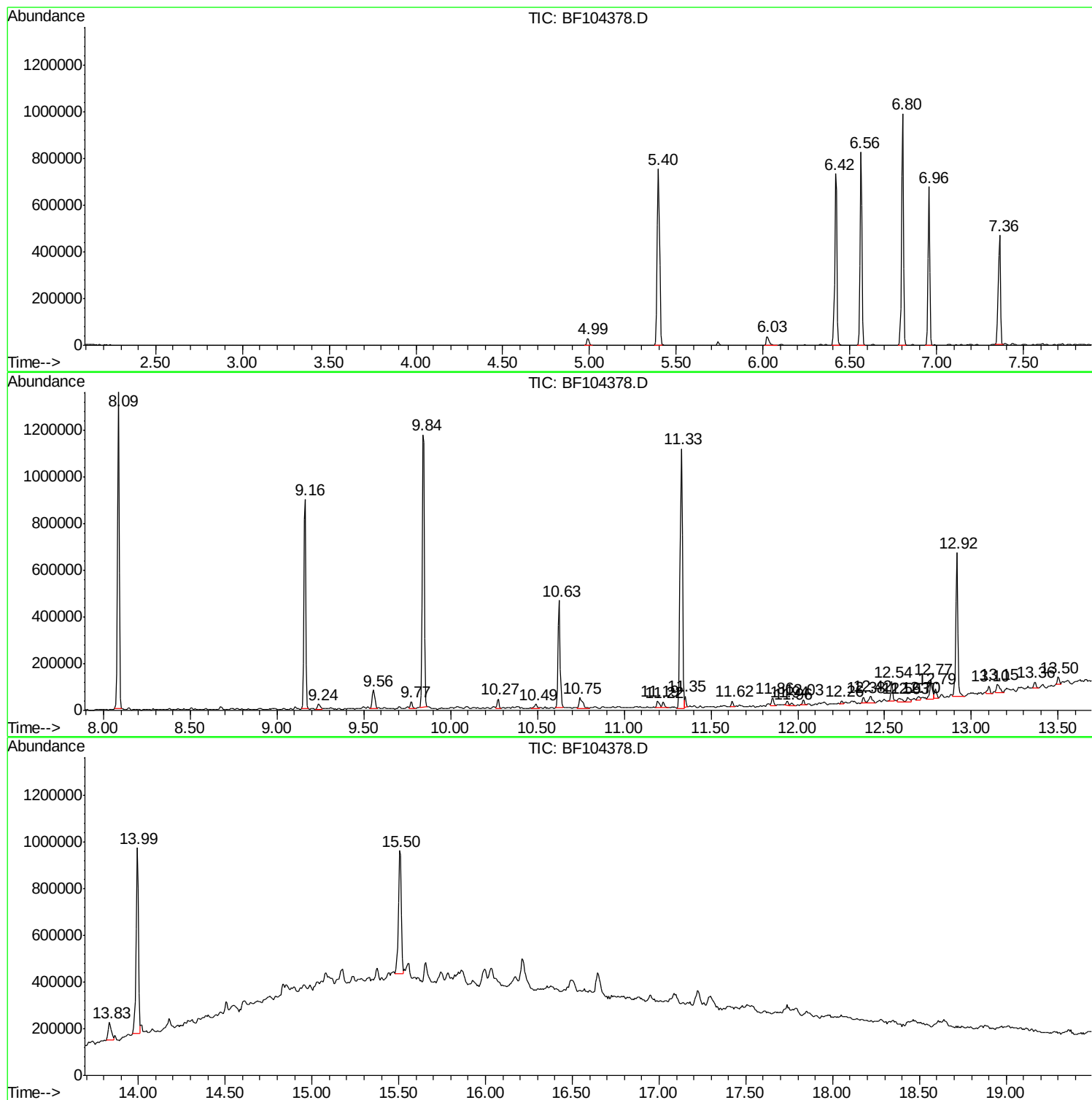
Sum of corrected areas: 10782197

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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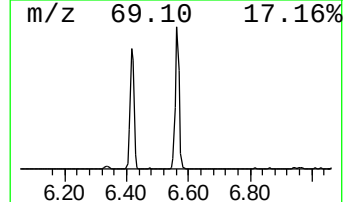
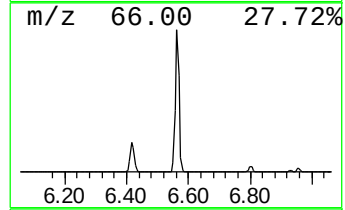
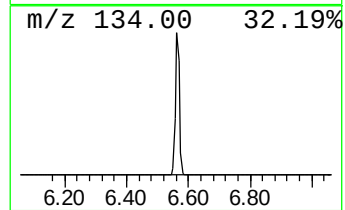
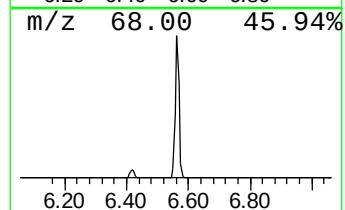
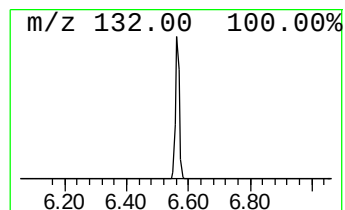
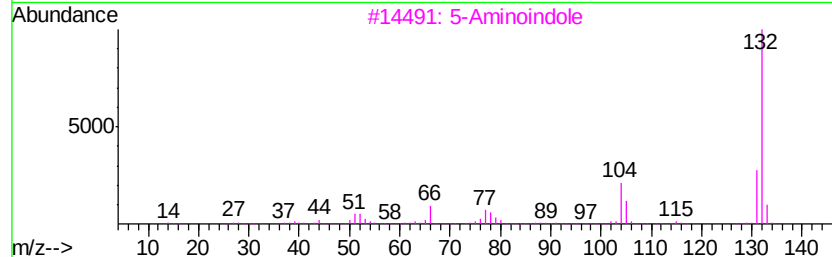
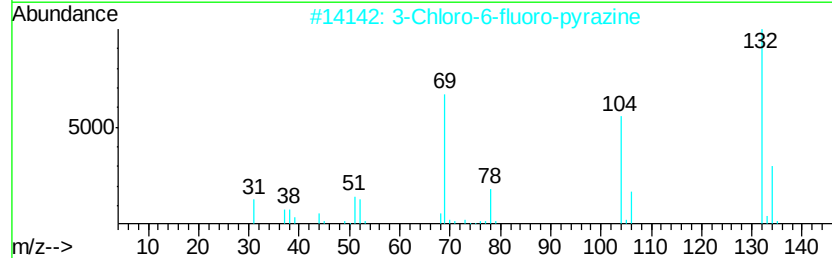
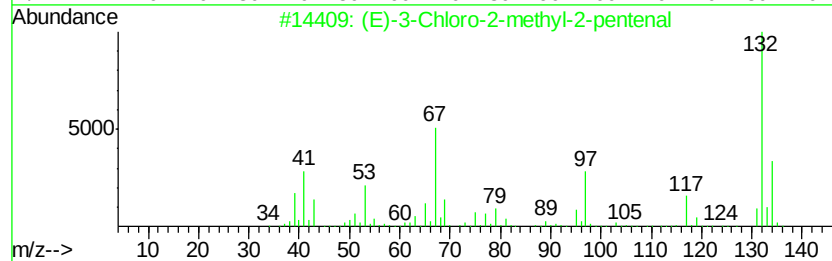
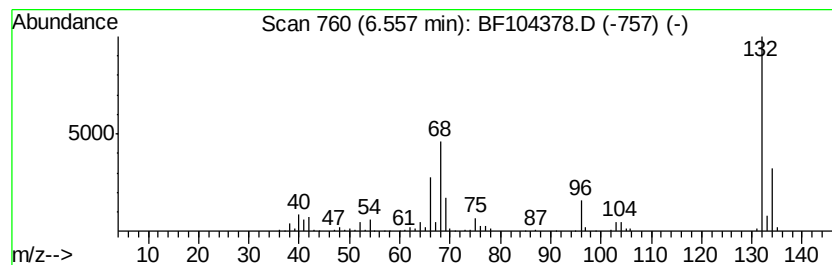
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	17.19 ng	678090	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	10



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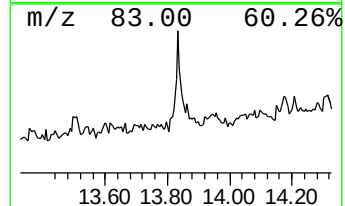
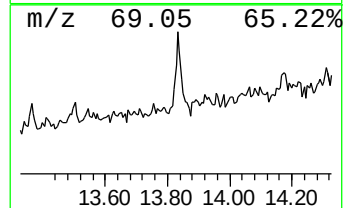
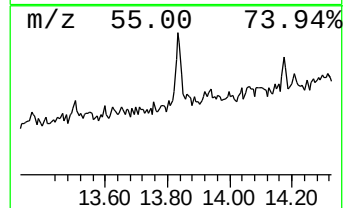
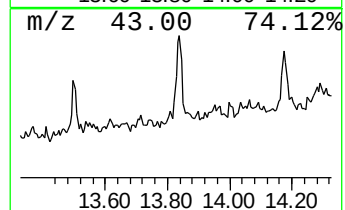
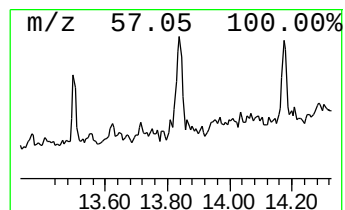
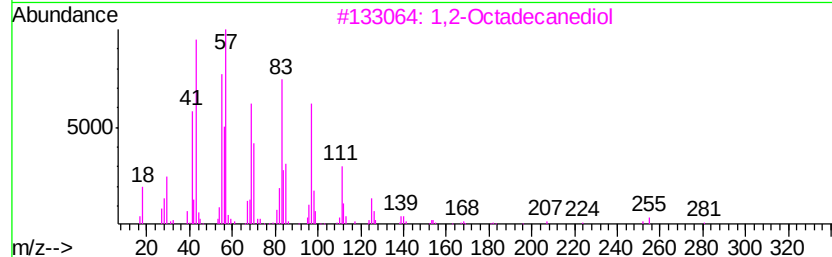
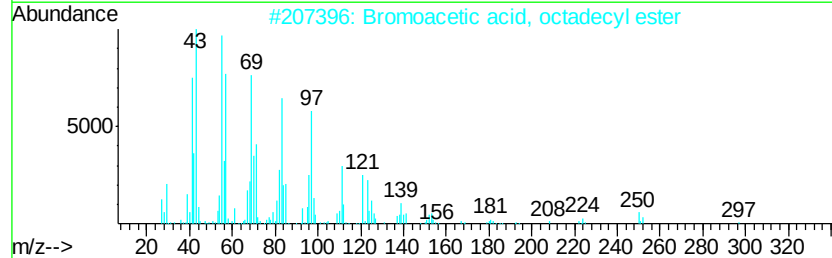
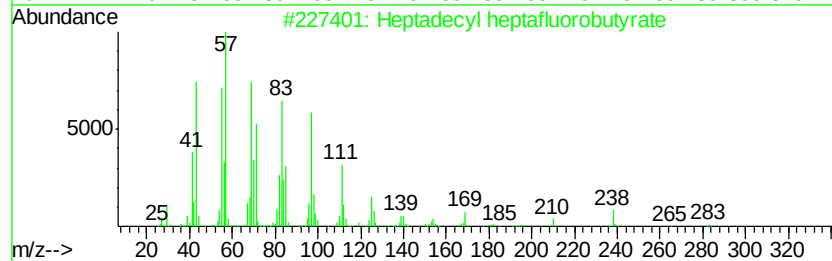
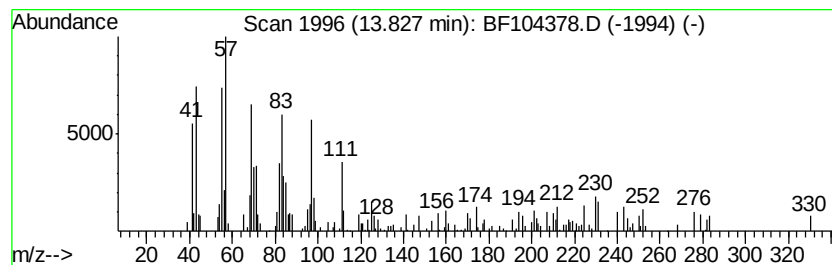
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.83	2.26 ng	89418	Chrysene-d12		13.99	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	83
3		1,2-Octadecanediol	286	C18H38O2	020294-76-2	76
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	68
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	68



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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.56	6.56	17.2	ng	678090	1	6.80	788951	20.0
Heptadecyl heptaf...	13.83	2.3	ng	89418	5	13.99	791266	20.0