

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
 Data File : BF107716.D
 Acq On : 26 Jul 2018 22:43
 Operator : JU/SJ
 Sample : J4109-07
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-10(3-5)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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	5.201	482	487	498	rBV	348268	541571	13.29%	1.408%
2	5.595	551	554	578	rBV	2015981	3372558	82.75%	8.768%
3	6.595	720	724	744	rBV	2098846	3637973	89.26%	9.458%
4	6.737	744	748	772	rVB	2986907	3993215	97.97%	10.381%
5	6.960	783	786	803	rBV	634121	1051987	25.81%	2.735%
6	7.113	808	812	837	rBV	2413212	3061117	75.11%	7.958%
7	7.525	878	882	906	rBV	1671686	2470889	60.62%	6.424%
8	8.242	1000	1004	1027	rBV	1134844	1547646	37.97%	4.023%
9	9.313	1182	1186	1202	rBV	3682117	4075756	100.00%	10.596%
10	9.654	1241	1244	1247	rBV2	37182	45538	1.12%	0.118%
11	9.707	1250	1253	1262	rVB	294020	307725	7.55%	0.800%
12	9.860	1274	1279	1284	rBV2	42650	52314	1.28%	0.136%
13	10.001	1295	1303	1318	rBV	1467156	1577655	38.71%	4.101%
14	10.554	1393	1397	1403	rVB3	33189	47293	1.16%	0.123%
15	10.795	1434	1438	1451	rBV	2155574	2654468	65.13%	6.901%
16	10.883	1451	1453	1467	rVB4	43954	100685	2.47%	0.262%
17	11.101	1484	1490	1493	rBV4	23801	46408	1.14%	0.121%
18	11.395	1536	1540	1550	rVB	57202	79277	1.95%	0.206%
19	11.495	1553	1557	1560	rBV	1251209	1312048	32.19%	3.411%
20	11.519	1560	1561	1568	rVB	326448	271826	6.67%	0.707%
21	11.824	1611	1613	1617	rBV	44974	53903	1.32%	0.140%
22	11.913	1623	1628	1632	rBV	37347	54203	1.33%	0.141%
23	12.001	1639	1643	1646	rBV2	343651	377393	9.26%	0.981%
24	12.024	1646	1647	1653	rVB2	98438	92371	2.27%	0.240%
25	12.107	1658	1661	1664	rVV2	91701	118549	2.91%	0.308%
26	12.130	1664	1665	1669	rVB	53483	41782	1.03%	0.109%
27	12.289	1689	1692	1694	rBV2	38986	44038	1.08%	0.114%
28	12.324	1695	1698	1703	rVB3	42401	54603	1.34%	0.142%
29	12.548	1732	1736	1739	rBV2	51384	65439	1.61%	0.170%
30	12.642	1748	1752	1760	rVB7	27043	54074	1.33%	0.141%
31	12.713	1760	1764	1768	rBV	233439	243929	5.98%	0.634%
32	12.807	1778	1780	1785	rVB	47809	48099	1.18%	0.125%
33	12.866	1787	1790	1797	rVB3	33067	52708	1.29%	0.137%
34	12.942	1797	1803	1809	rBV	291727	355547	8.72%	0.924%

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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

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35	13.077	1822	1826	1836	rBV	2698191	2708877	66.46%	7.042%
36	13.154	1836	1839	1845	rVB5	28125	52836	1.30%	0.137%
37	13.265	1855	1858	1864	rVB4	49937	86243	2.12%	0.224%
38	13.624	1915	1919	1922	rBV3	36150	45690	1.12%	0.119%
39	13.954	1971	1975	1985	rVV3	309970	391042	9.59%	1.017%
40	14.142	2002	2007	2011	rBV	1056338	1332151	32.68%	3.463%
41	14.895	2132	2135	2139	rVB2	57691	59434	1.46%	0.155%
42	15.218	2186	2190	2192	rBV	89270	136232	3.34%	0.354%
43	15.248	2193	2195	2205	rVV3	110867	147495	3.62%	0.383%
44	15.536	2241	2244	2250	rBV	69367	103354	2.54%	0.269%
45	15.607	2252	2256	2260	rBV	97830	151424	3.72%	0.394%
46	15.677	2261	2268	2277	rVB	746344	1266685	31.08%	3.293%
47	16.112	2338	2342	2348	rVB	54048	79730	1.96%	0.207%

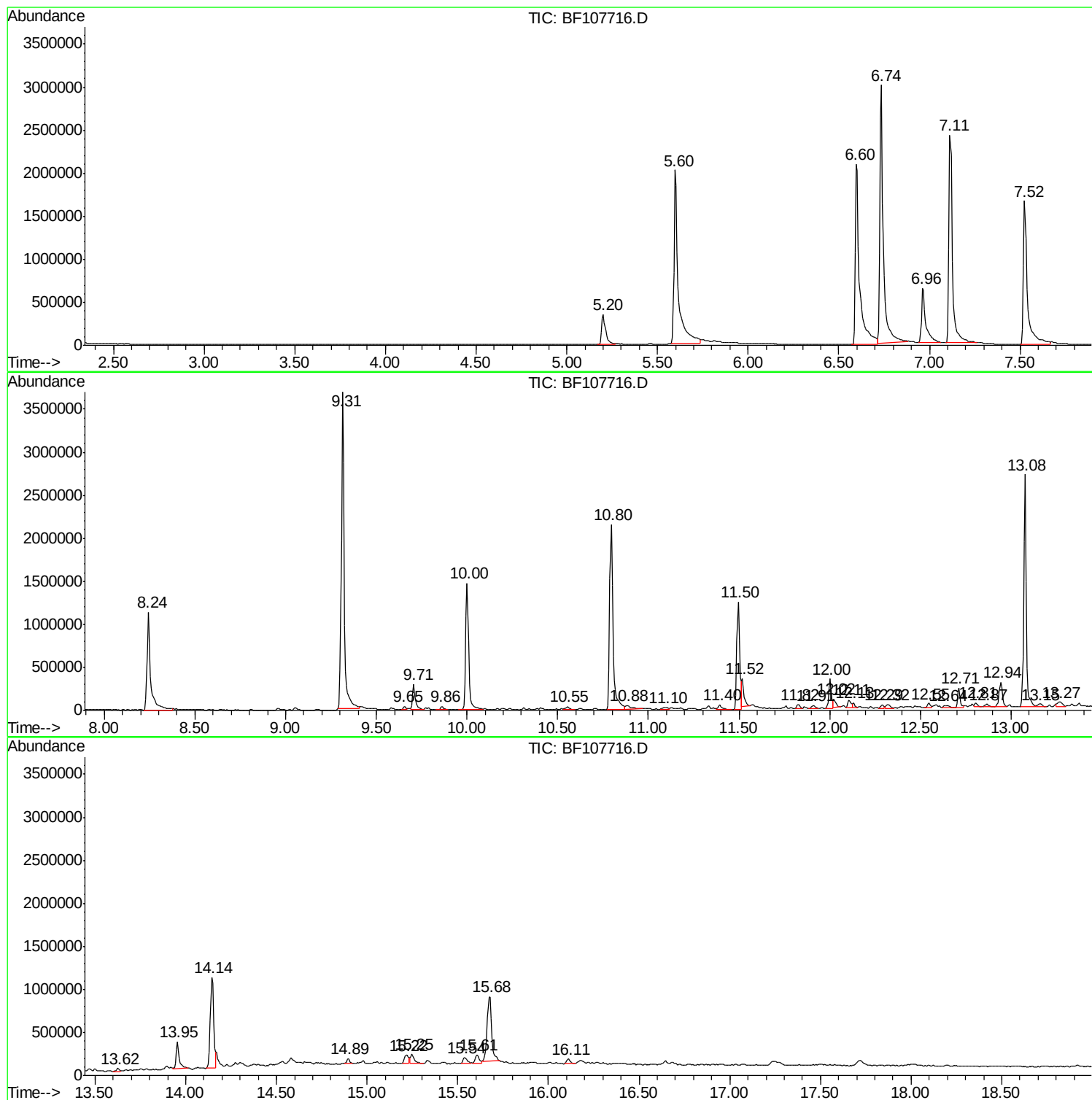
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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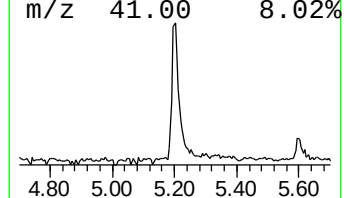
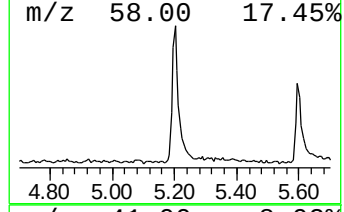
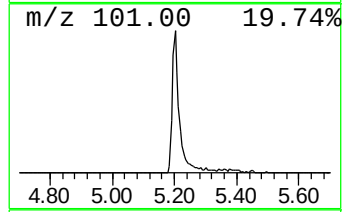
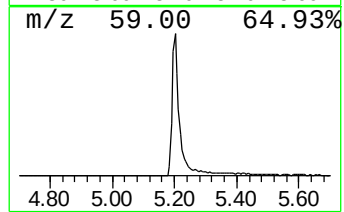
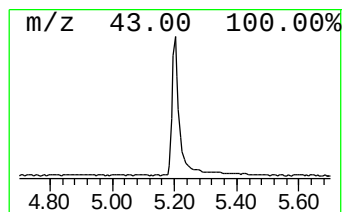
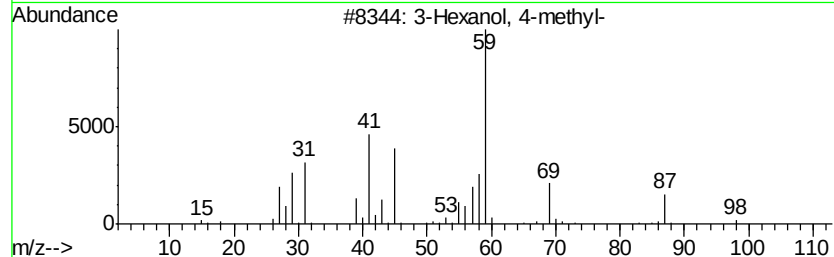
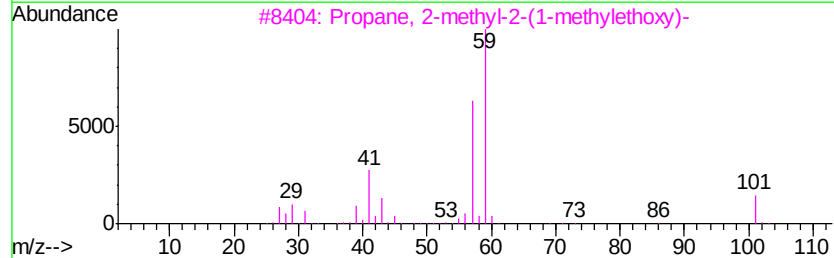
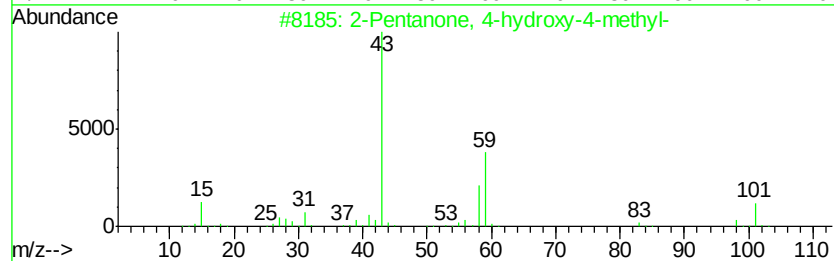
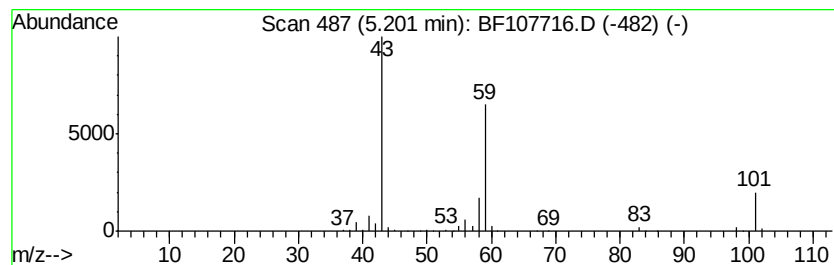
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.20	10.30 ng	541571	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			Acetone	58	C3H6O	000067-64-1	9



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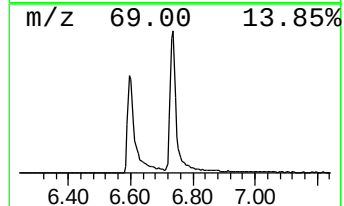
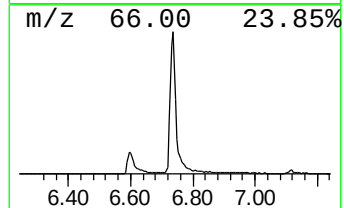
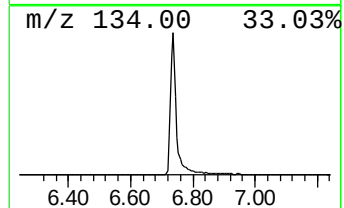
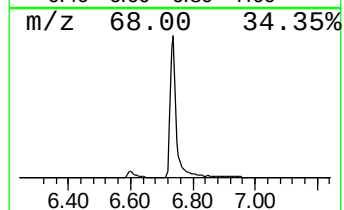
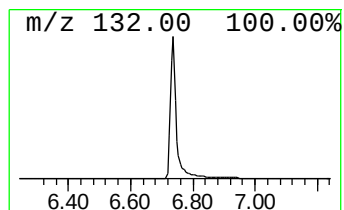
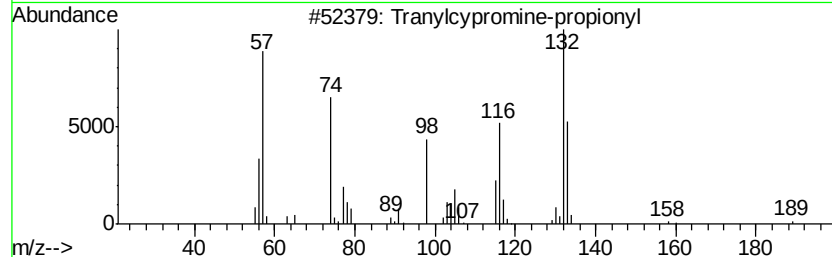
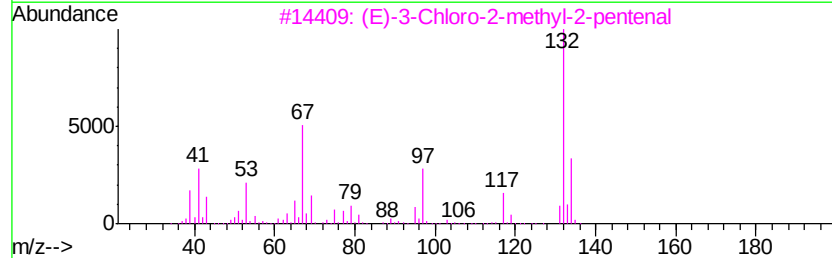
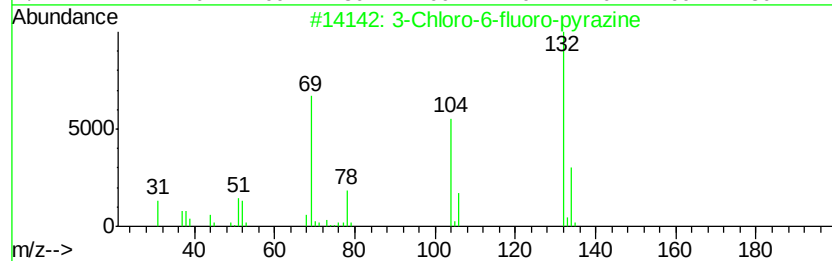
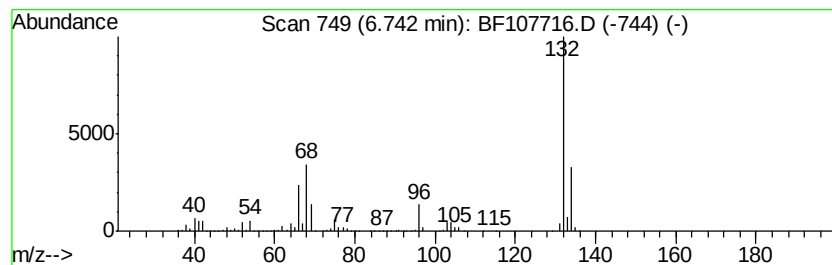
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	75.92 ng	3993220	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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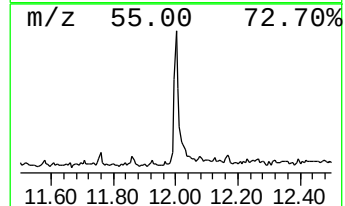
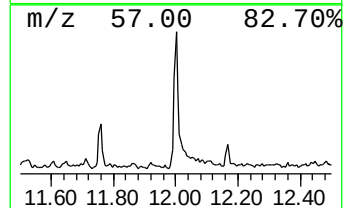
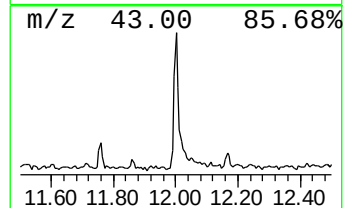
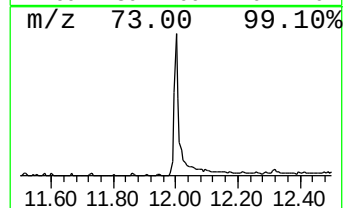
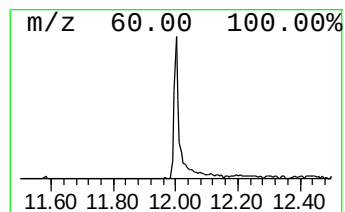
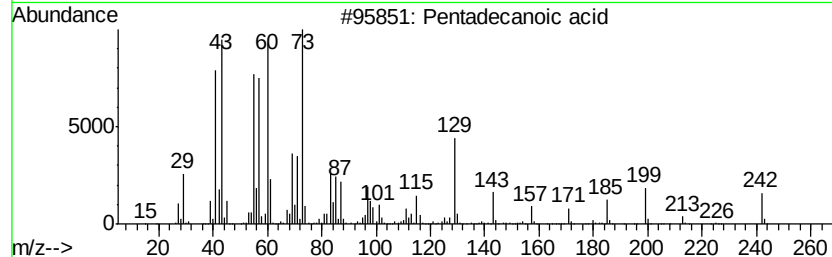
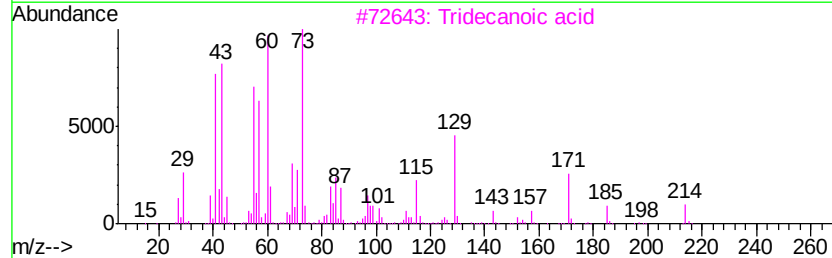
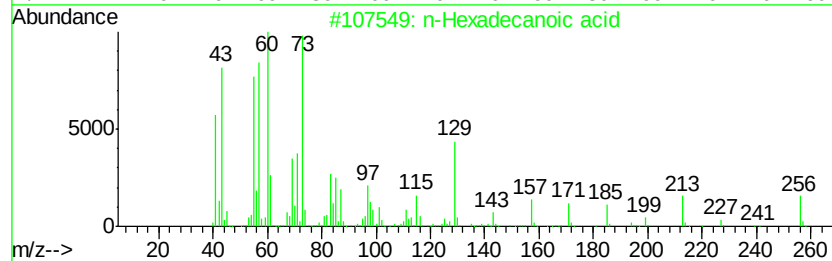
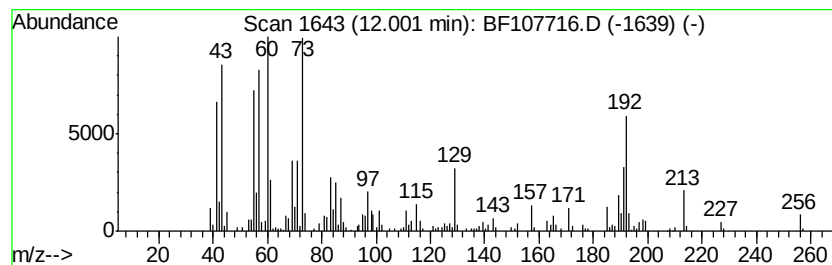
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.00	5.75 ng	377393	Phenanthrene-d10		11.49
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	56



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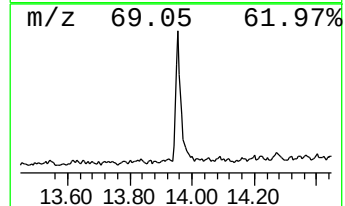
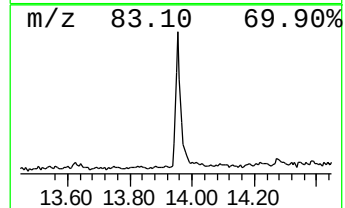
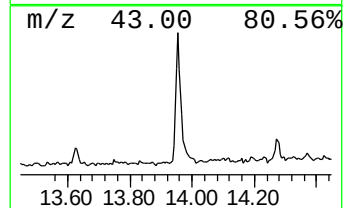
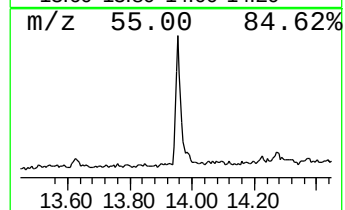
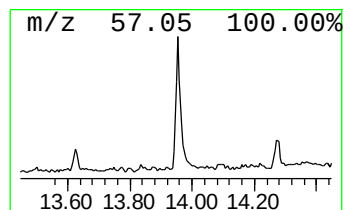
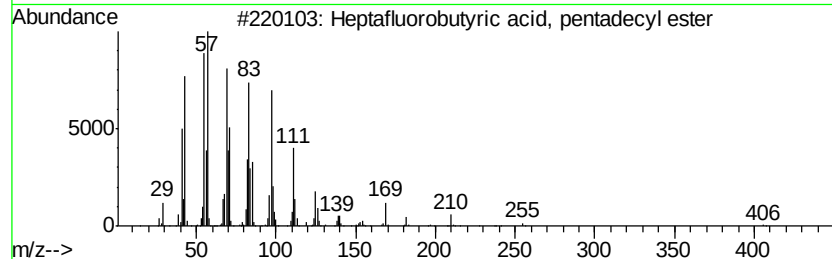
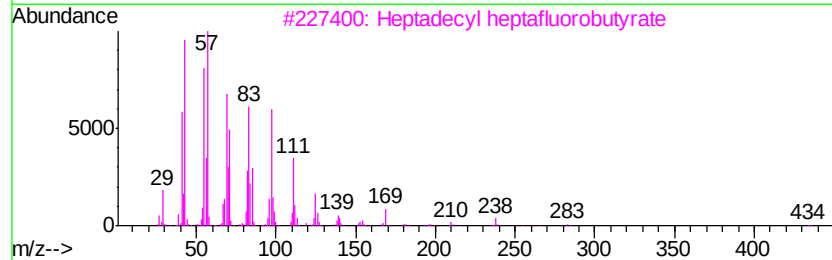
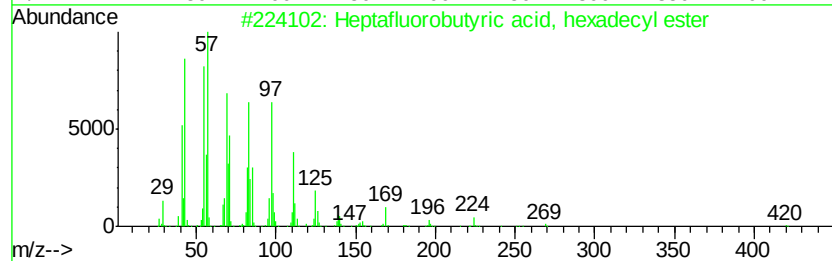
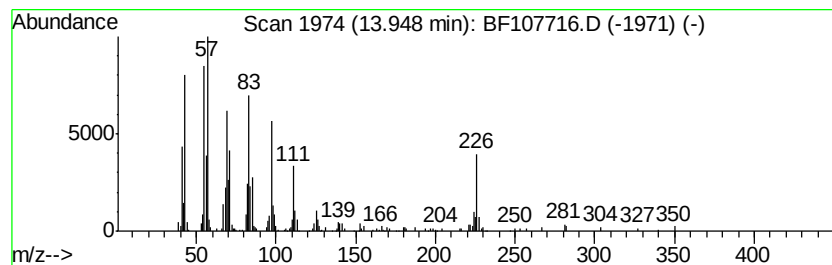
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	5.87 ng	391042	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	10.3	ng	541571	1	6.96	1051990	20.0
unknown6.74	6.74	75.9	ng	3993220	1	6.96	1051990	20.0
n-Hexadecanoic acid	12.00	5.8	ng	377393	4	11.49	1312050	20.0
Heptafluorobutyri...	13.95	5.9	ng	391042	5	14.14	1332150	20.0