

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102017\
 Data File : BF099706.D
 Acq On : 20 Oct 2017 17:42
 Operator : SJ/JU
 Sample : I5981-01 5X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-01-101817-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-BF092317.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	5.022	496	499	514	rBV	44571	59877	8.45%	0.664%
2	5.434	566	569	583	rBV	354441	416830	58.81%	4.623%
3	6.451	739	742	761	rBV	388299	438786	61.91%	4.867%
4	6.581	761	764	771	rBV	523600	468010	66.03%	5.191%
5	6.810	800	803	812	rBB	614873	521868	73.63%	5.788%
6	6.969	826	830	842	rBB	389237	362726	51.18%	4.023%
7	7.375	896	899	918	rBV	276365	256535	36.20%	2.845%
8	8.092	1018	1021	1028	rBV	866997	708757	100.00%	7.861%
9	8.892	1154	1157	1166	rBV	27708	45820	6.46%	0.508%
10	9.163	1200	1203	1207	rBV	674020	510865	72.08%	5.666%
11	9.563	1263	1271	1277	rBB2	8879	10286	1.45%	0.114%
12	9.845	1316	1319	1323	rBV	806405	680221	95.97%	7.544%
13	9.880	1323	1325	1328	rVB	26467	20327	2.87%	0.225%
14	10.398	1410	1413	1418	rBV	18640	15922	2.25%	0.177%
15	10.639	1450	1454	1461	rVB	202317	191672	27.04%	2.126%
16	11.333	1569	1572	1575	rBV	611966	544476	76.82%	6.039%
17	11.357	1575	1576	1580	rVV	180510	119192	16.82%	1.322%
18	11.410	1583	1585	1590	rVB	33368	32493	4.58%	0.360%
19	11.575	1609	1613	1617	rBV	19635	18998	2.68%	0.211%
20	11.616	1617	1620	1627	rVB2	6787	10550	1.49%	0.117%
21	11.839	1655	1658	1660	rBV	11736	13877	1.96%	0.154%
22	11.869	1660	1663	1665	rVB	15261	13566	1.91%	0.150%
23	11.951	1674	1677	1680	rBV	27191	29618	4.18%	0.328%
24	12.398	1748	1753	1755	rBV4	17182	18756	2.65%	0.208%
25	12.416	1755	1756	1759	rVB3	15105	11840	1.67%	0.131%
26	12.551	1775	1779	1783	rVB	264598	228057	32.18%	2.529%
27	12.780	1811	1818	1823	rBV	217256	240726	33.96%	2.670%
28	12.910	1837	1840	1844	rVB	387951	323146	45.59%	3.584%
29	12.945	1844	1846	1850	rVB	10112	9732	1.37%	0.108%
30	12.998	1850	1855	1859	rVB4	8620	13336	1.88%	0.148%
31	13.110	1870	1874	1877	rVB	24606	25588	3.61%	0.284%
32	13.169	1882	1884	1887	rVB	22480	20731	2.92%	0.230%
33	13.210	1887	1891	1893	rBV2	13725	15122	2.13%	0.168%
34	13.333	1910	1912	1918	rVB2	9414	11558	1.63%	0.128%

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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-BF092317.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.592	1953	1956	1959	rBV4	8380	9114	1.29%	0.101%
36	13.627	1959	1962	1966	rVB	9144	10320	1.46%	0.114%
37	13.727	1976	1979	1981	rBV	18967	15704	2.22%	0.174%
38	13.751	1981	1983	1985	rVV	18256	18337	2.59%	0.203%
39	13.798	1989	1991	1995	rVV2	30929	33644	4.75%	0.373%
40	13.833	1995	1997	2003	rVB2	21244	21583	3.05%	0.239%
41	13.898	2003	2008	2011	rBV3	9207	13556	1.91%	0.150%
42	13.974	2011	2021	2024	rBV2	613920	687629	97.02%	7.626%
43	14.004	2024	2026	2029	rVB	111582	91912	12.97%	1.019%
44	14.080	2037	2039	2043	rVB	28614	28839	4.07%	0.320%
45	14.180	2053	2056	2057	rBV	10127	9002	1.27%	0.100%
46	14.210	2060	2061	2064	rVB	11898	9328	1.32%	0.103%
47	14.363	2083	2087	2089	rBV2	19062	21768	3.07%	0.241%
48	14.398	2091	2093	2095	rBV	10193	9985	1.41%	0.111%
49	14.421	2095	2097	2098	rBV2	15181	13026	1.84%	0.144%
50	14.510	2110	2112	2134	rVB4	43859	169346	23.89%	1.878%
51	14.692	2140	2143	2144	rBV3	10130	10375	1.46%	0.115%
52	14.721	2145	2148	2151	rBV5	22327	32228	4.55%	0.357%
53	14.863	2169	2172	2177	rBV4	22130	29141	4.11%	0.323%
54	15.015	2194	2198	2201	rBV	113105	172818	24.38%	1.917%
55	15.045	2201	2203	2207	rVB2	65058	70399	9.93%	0.781%
56	15.121	2213	2216	2220	rBV	22484	28973	4.09%	0.321%
57	15.210	2229	2231	2235	rBV4	8797	9373	1.32%	0.104%
58	15.315	2245	2249	2255	rVB	73421	91614	12.93%	1.016%
59	15.374	2255	2259	2263	rBV	90538	118800	16.76%	1.318%
60	15.439	2263	2270	2274	rBV	445663	543499	76.68%	6.028%
61	15.615	2297	2300	2305	rBV5	12888	15798	2.23%	0.175%
62	15.839	2334	2338	2343	rBV2	44520	60793	8.58%	0.674%
63	16.086	2377	2380	2382	rBV4	9919	13060	1.84%	0.145%
64	16.333	2417	2422	2428	rVB3	19424	39694	5.60%	0.440%
65	16.904	2513	2519	2526	rBV2	54424	104257	14.71%	1.156%
66	17.080	2546	2549	2553	rVV6	10517	13518	1.91%	0.150%
67	17.145	2556	2560	2569	rVB9	11886	25871	3.65%	0.287%
68	17.351	2590	2595	2603	rBV	31029	63240	8.92%	0.701%

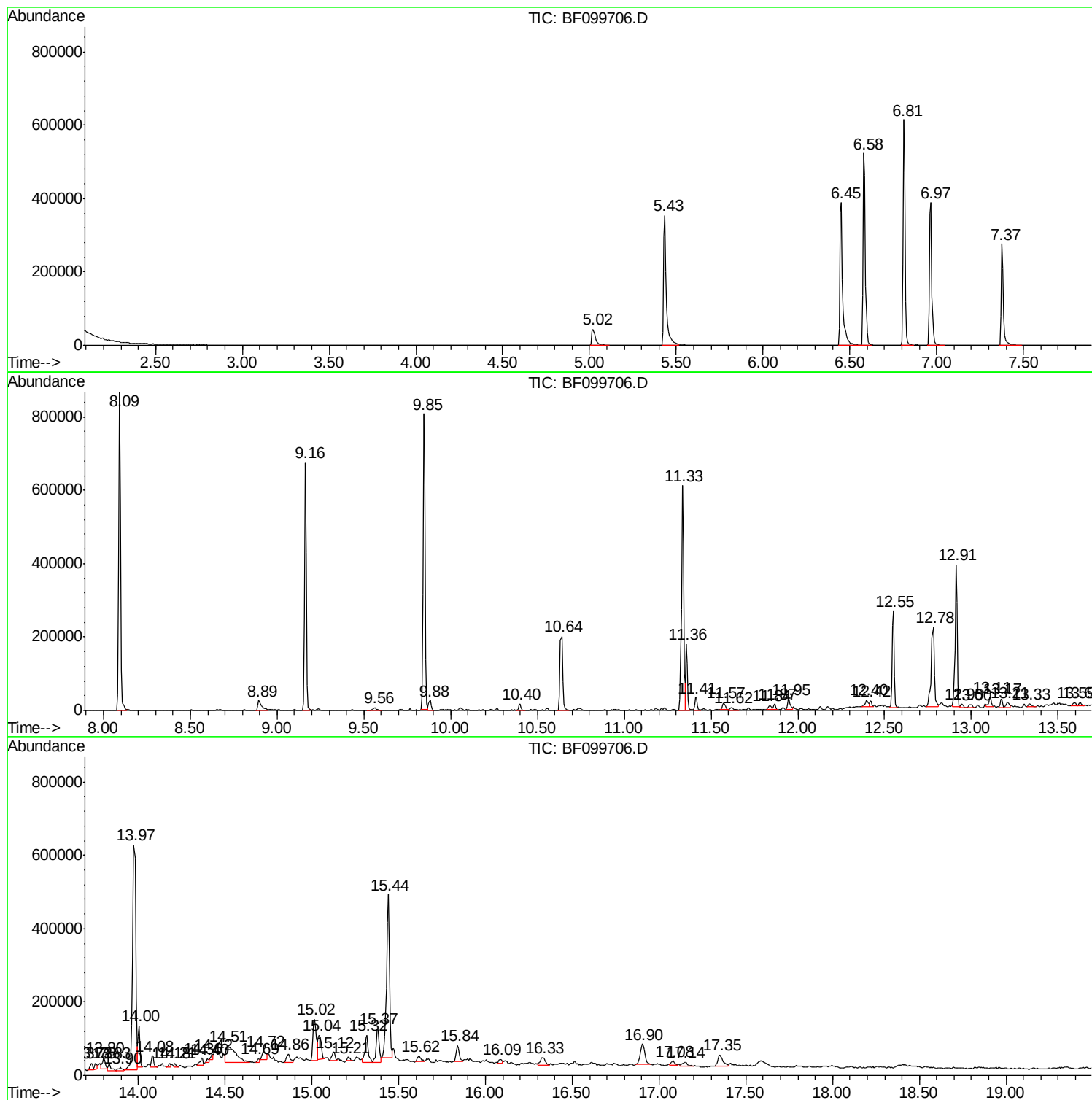
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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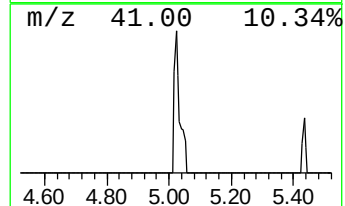
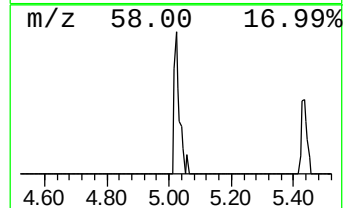
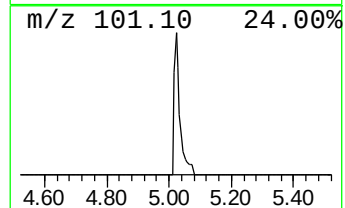
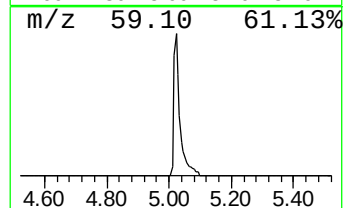
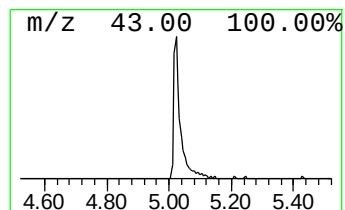
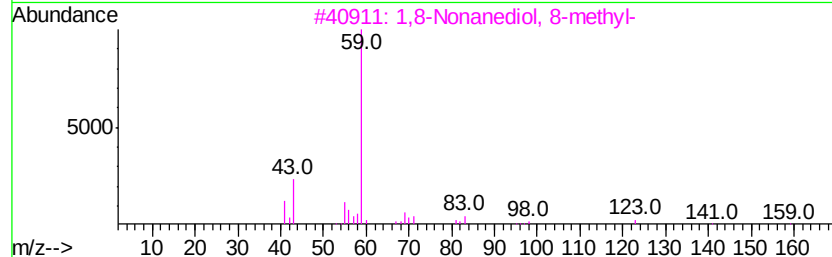
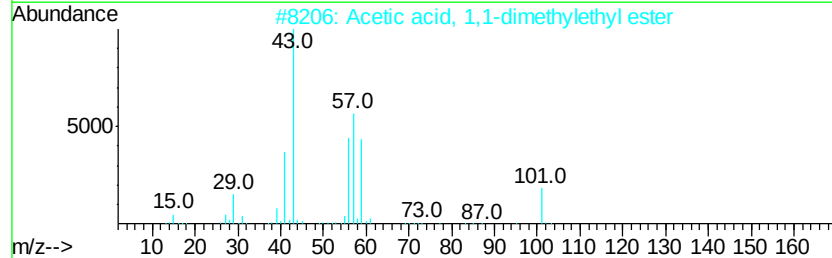
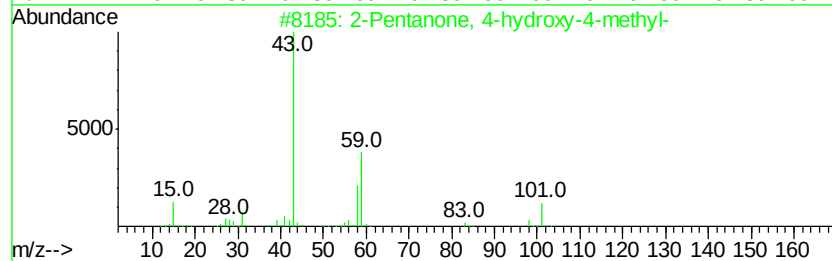
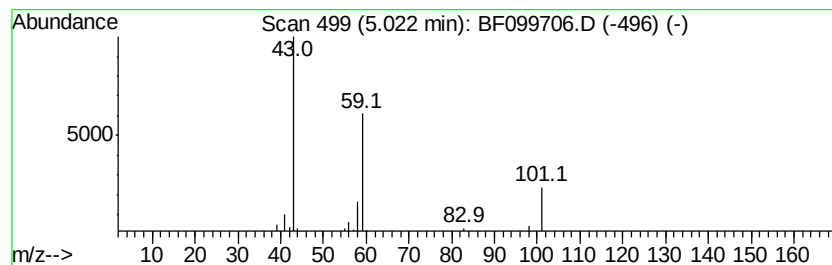
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.29 ng	59877	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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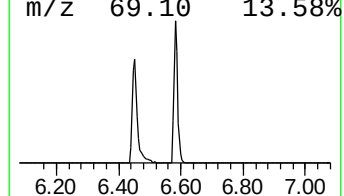
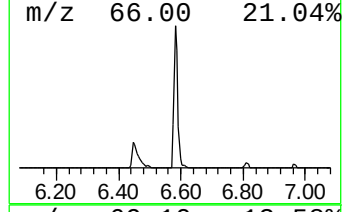
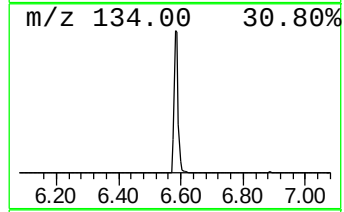
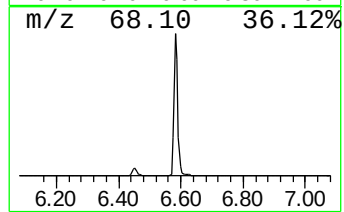
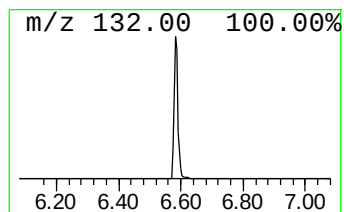
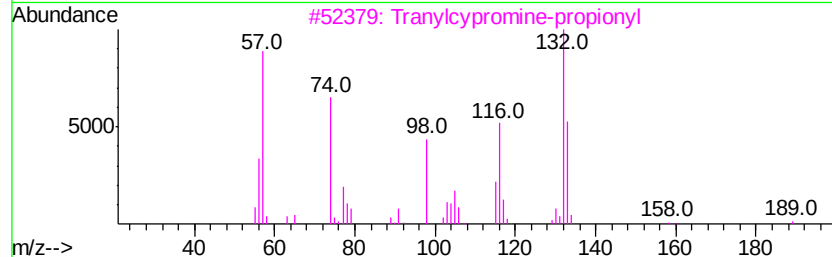
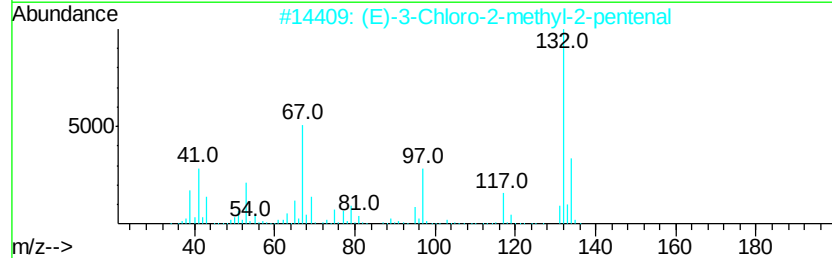
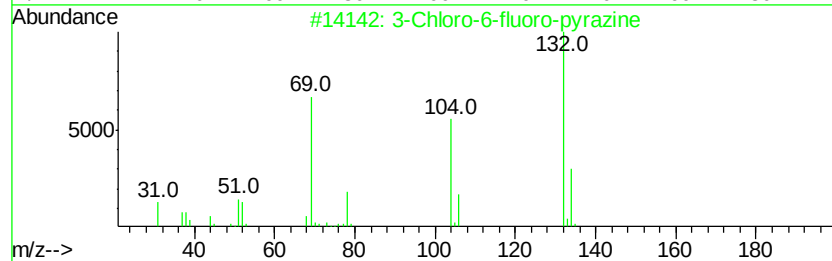
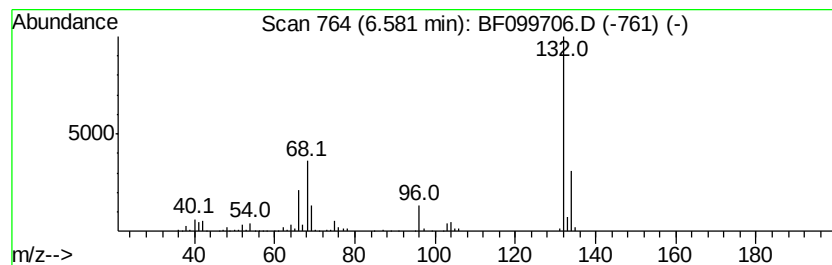
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	17.94 ng	468010	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10



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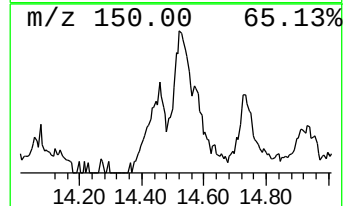
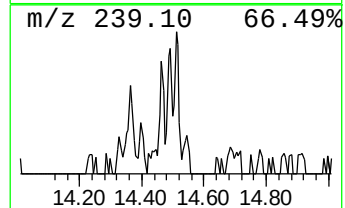
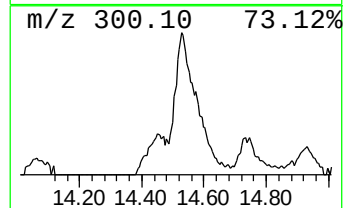
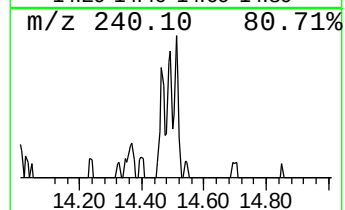
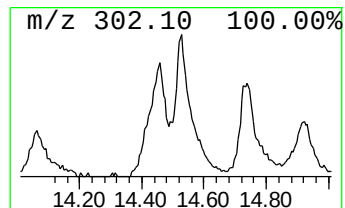
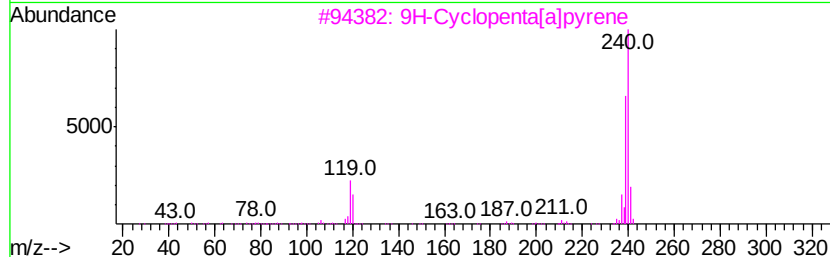
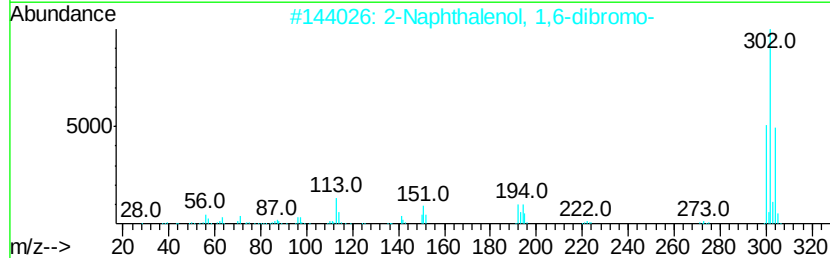
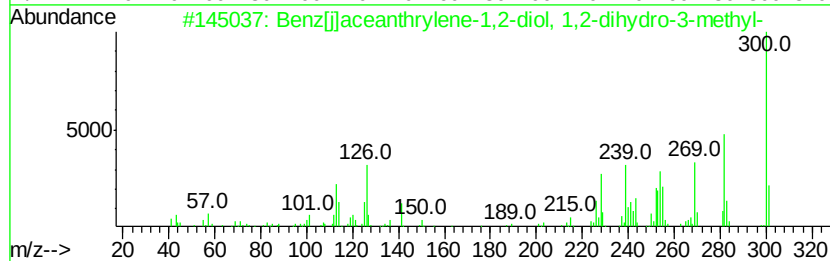
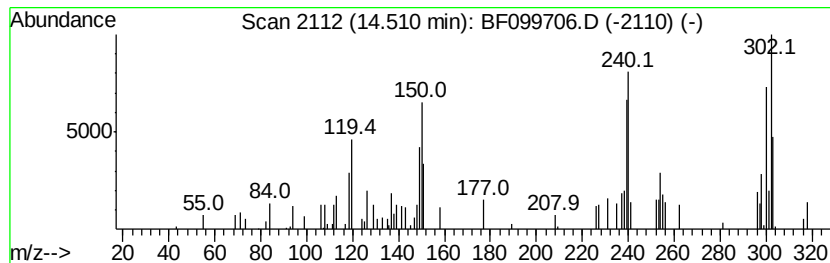
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown14.51 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.51	4.93 ng	169346	Chrysene-d12	13.98		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benz[il]aceanthrylene-1,2-diol, 1...	300	C21H16O2	015544-91-9	35
2		2-Naphthalenol, 1,6-dibromo-	300	C10H6Br2O	016239-18-2	27
3		9H-Cyclopenta[al]pyrene	240	C19H12	050861-05-7	14
4		Chrysene, 1,2,3,4,4a,7,8,9,10,11...	240	C18H24	001610-22-6	11
5		1,2,4-Oxadiazole, 3-(1,3-benzodi...	302	C15H8F2N2O3	1000350-01-7	10



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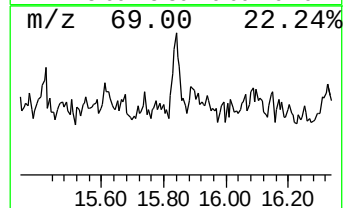
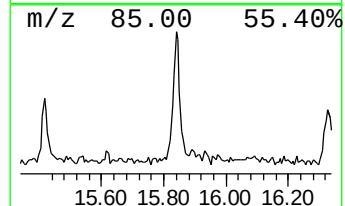
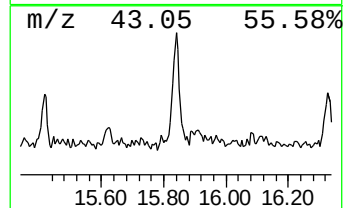
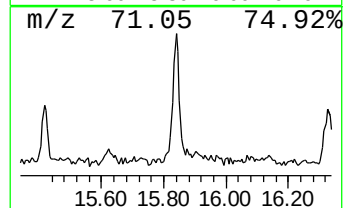
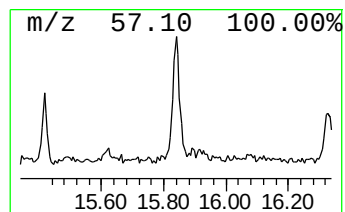
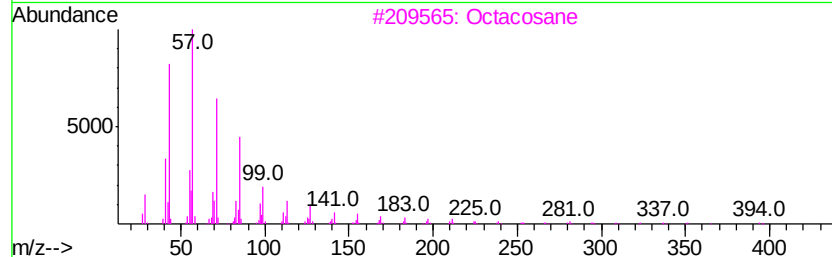
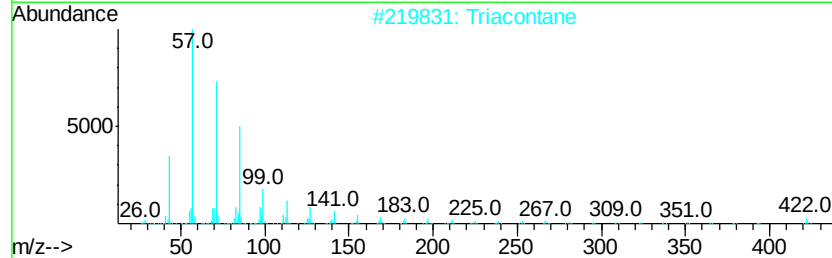
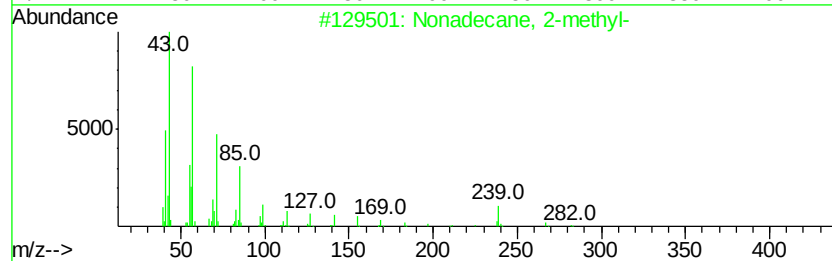
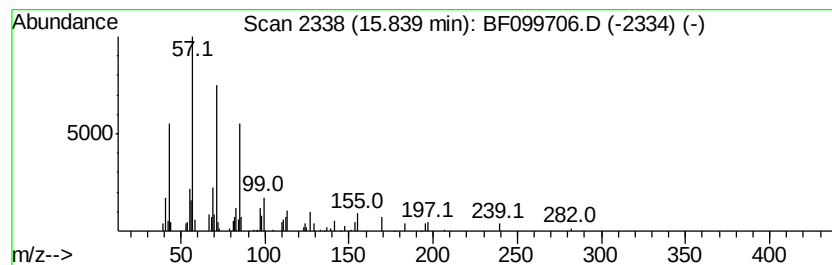
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Nonadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.24 ng	60793	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	94
2		Triacontane	422	C30H62	000638-68-6	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Hexacosane	366	C26H54	000630-01-3	87
5		Heneicosane	296	C21H44	000629-94-7	87



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NB-01-101817-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
unknown5.02	5.02	2.3	ng	59877	1	6.81	521868	20.0
unknown6.58	6.58	17.9	ng	468010	1	6.81	521868	20.0
unknown14.51	14.51	4.9	ng	169346	5	13.98	687629	20.0
Nonadecane, 2-met...	15.84	2.2	ng	60793	6	15.44	543499	20.0