

Data Path : Z:\HPCHEM1\BNA_F\Data\BF051518\
 Data File : BF105416.D
 Acq On : 15 May 2018 14:44
 Operator : JU/SJ
 Sample : J2873-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

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-BF051018.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	4.987	488	493	502	rVB	223559	282390	8.71%	0.691%
2	5.398	558	563	579	rBV	2629635	2873267	88.59%	7.034%
3	6.422	732	737	755	rBV	2588786	3031166	93.45%	7.420%
4	6.557	755	760	768	rBV	2758758	2932190	90.40%	7.178%
5	6.787	795	799	806	rBV	831199	833933	25.71%	2.041%
6	6.840	806	808	814	rVB	47797	53352	1.64%	0.131%
7	6.940	821	825	841	rVB	2586137	2303701	71.03%	5.639%
8	7.351	890	895	905	rBV	1766964	1914794	59.04%	4.687%
9	7.422	905	907	917	rVB4	31999	52602	1.62%	0.129%
10	8.063	1013	1016	1030	rBV	1107286	1138322	35.10%	2.787%
11	9.139	1195	1199	1210	rBV	3312332	3243465	100.00%	7.940%
12	9.533	1262	1266	1276	rBV	531724	440912	13.59%	1.079%
13	9.745	1299	1302	1306	rVB3	27947	38030	1.17%	0.093%
14	9.816	1311	1314	1331	rVB	1232104	1252613	38.62%	3.066%
15	10.492	1426	1429	1432	rBV	60140	49578	1.53%	0.121%
16	10.610	1444	1449	1465	rBV	2189364	2269439	69.97%	5.555%
17	10.969	1507	1510	1518	rVB3	41688	46941	1.45%	0.115%
18	11.310	1564	1568	1570	rBV	1286734	1198965	36.97%	2.935%
19	11.327	1570	1571	1575	rVB	127993	104309	3.22%	0.255%
20	11.533	1600	1606	1611	rBV5	20883	37479	1.16%	0.092%
21	11.845	1654	1659	1670	rVB	724077	763967	23.55%	1.870%
22	12.374	1744	1749	1754	rBV7	54391	90159	2.78%	0.221%
23	12.416	1754	1756	1762	rVV3	48882	73940	2.28%	0.181%
24	12.469	1762	1765	1768	rVB3	41688	41876	1.29%	0.103%
25	12.545	1775	1778	1781	rBV	164329	173773	5.36%	0.425%
26	12.610	1786	1789	1792	rVB3	37152	43550	1.34%	0.107%
27	12.663	1792	1798	1803	rBV2	249492	292859	9.03%	0.717%
28	12.763	1811	1815	1817	rBV3	91368	88615	2.73%	0.217%
29	12.792	1817	1820	1823	rVB	144269	122361	3.77%	0.300%
30	12.886	1833	1836	1840	rBV	135994	122752	3.78%	0.300%
31	12.957	1843	1848	1857	rBV	2913731	3084906	95.11%	7.552%
32	13.186	1884	1887	1889	rBV2	70807	67836	2.09%	0.166%
33	13.216	1889	1892	1896	rVB3	111881	119388	3.68%	0.292%
34	13.263	1897	1900	1902	rBV2	40670	45295	1.40%	0.111%

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Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
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Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
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35	13.292	1902	1905	1912	rVB2	130988	156362	4.82%	0.383%
36	13.369	1915	1918	1922	rVB	94478	101624	3.13%	0.249%
37	13.433	1925	1929	1932	rBV2	169754	164519	5.07%	0.403%
38	13.469	1932	1935	1940	rBV2	111641	134964	4.16%	0.330%
39	13.557	1947	1950	1953	rBV	56911	59287	1.83%	0.145%
40	13.598	1953	1957	1962	rVV	674603	688916	21.24%	1.686%
41	13.745	1977	1982	1988	rVB3	122205	155818	4.80%	0.381%
42	13.868	1999	2003	2006	rVB4	35253	48041	1.48%	0.118%
43	13.992	2020	2024	2033	rVV	596316	783355	24.15%	1.918%
44	14.063	2033	2036	2042	rVB2	41876	61894	1.91%	0.152%
45	14.163	2048	2053	2057	rBV	837882	973269	30.01%	2.382%
46	14.392	2089	2092	2101	rBV2	88382	143968	4.44%	0.352%
47	14.551	2115	2119	2123	rBV	125532	136556	4.21%	0.334%
48	14.680	2137	2141	2144	rBV6	23248	36502	1.13%	0.089%
49	14.798	2156	2161	2169	rBV	939620	1353460	41.73%	3.313%
50	14.863	2169	2172	2175	rVB2	46560	54529	1.68%	0.133%
51	15.186	2222	2227	2234	rBV4	53991	135774	4.19%	0.332%
52	15.257	2236	2239	2243	rVB	199337	212731	6.56%	0.521%
53	15.339	2250	2253	2261	rVB	242463	283566	8.74%	0.694%
54	15.415	2263	2266	2269	rBV	52468	78837	2.43%	0.193%
55	15.557	2285	2290	2292	rBV	430923	567275	17.49%	1.389%
56	15.574	2292	2293	2299	rVV	328553	332391	10.25%	0.814%
57	15.633	2301	2303	2308	rVB	72925	86610	2.67%	0.212%
58	15.727	2316	2319	2323	rBV2	65085	80216	2.47%	0.196%
59	15.862	2337	2342	2351	rBV	665732	862844	26.60%	2.112%
60	16.151	2387	2391	2399	rVB	282379	383116	11.81%	0.938%
61	16.392	2428	2432	2436	rBV	299710	413776	12.76%	1.013%
62	16.439	2436	2440	2447	rVB2	214007	328804	10.14%	0.805%
63	16.509	2448	2452	2459	rVB2	187776	306083	9.44%	0.749%
64	17.198	2563	2569	2575	rBV2	227140	440832	13.59%	1.079%
65	17.586	2632	2635	2643	rVB4	87907	149563	4.61%	0.366%
66	17.939	2689	2695	2701	rBV3	174741	415052	12.80%	1.016%
67	18.009	2702	2707	2718	rVB5	171845	433500	13.37%	1.061%
68	18.262	2743	2750	2758	rBV4	171110	431759	13.31%	1.057%
69	18.633	2806	2813	2824	rVB5	173026	515400	15.89%	1.262%
70	18.739	2826	2831	2833	rBV6	59821	111133	3.43%	0.272%

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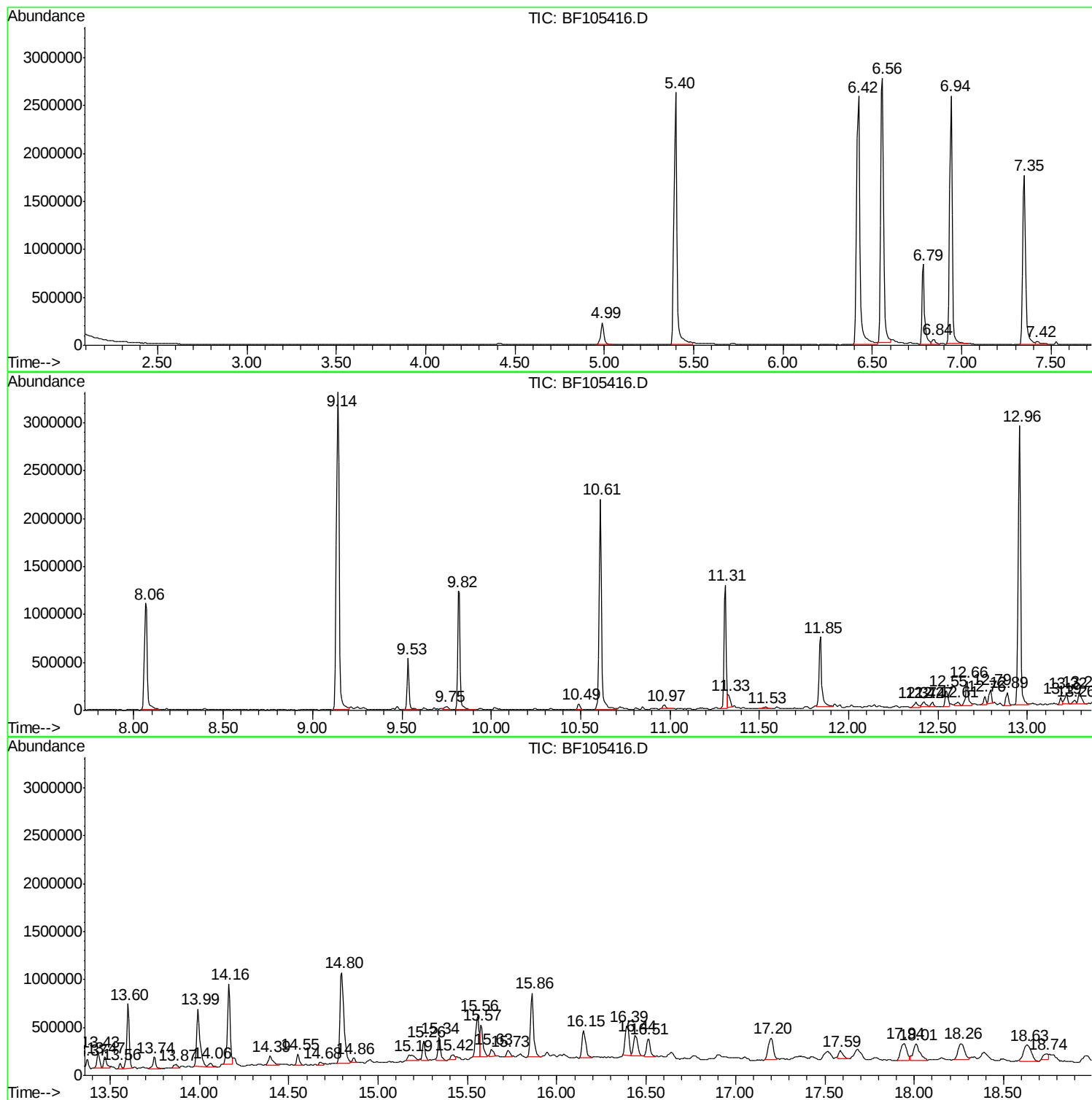
Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 40851051

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051018.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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ALS Vial : 4 Sample Multiplier: 1

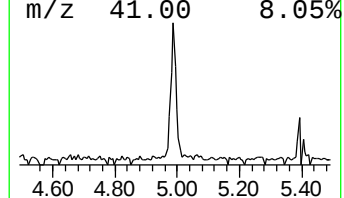
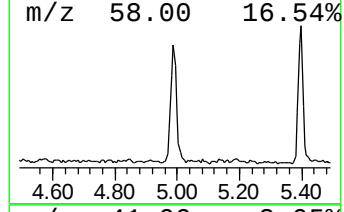
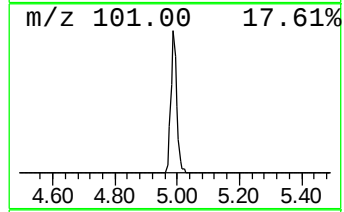
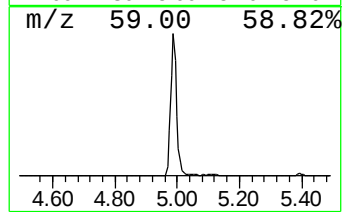
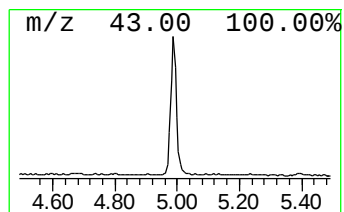
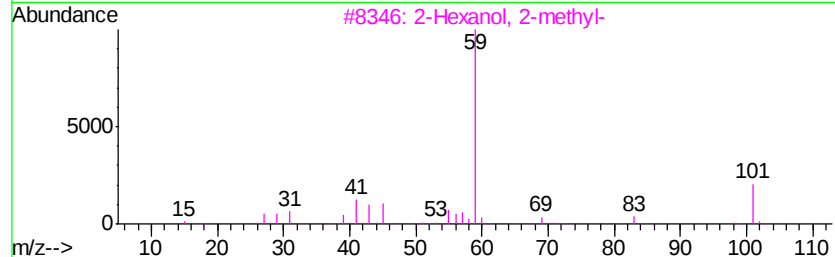
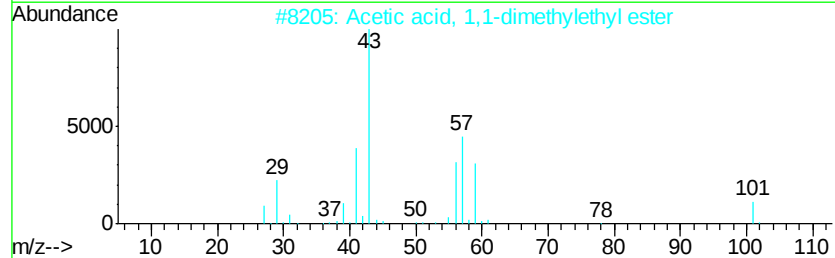
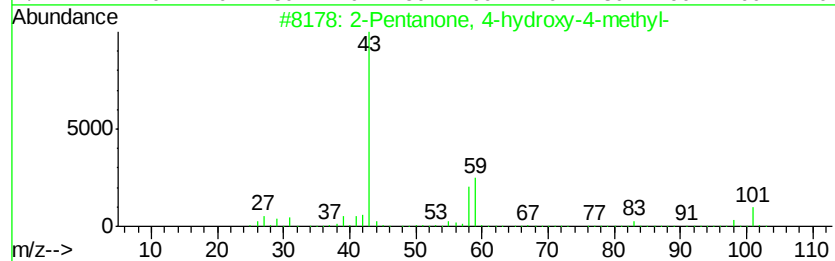
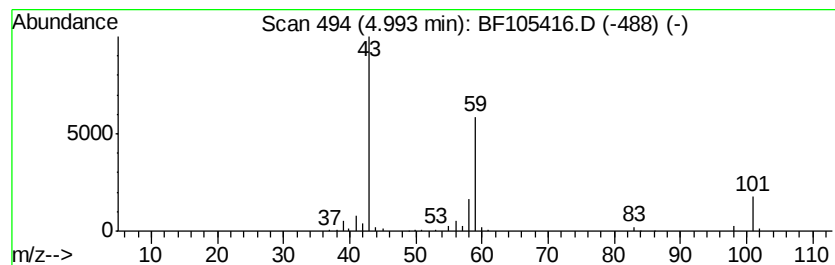
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	6.77 ng	282390	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	32
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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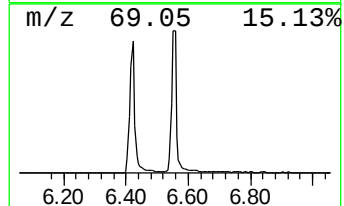
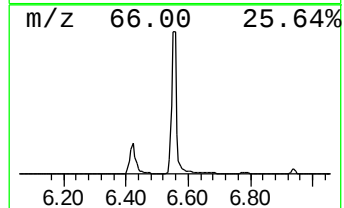
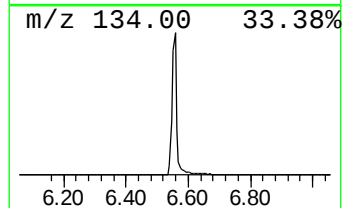
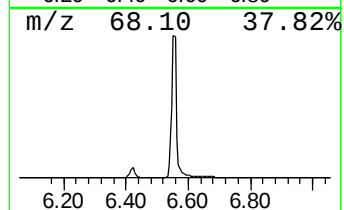
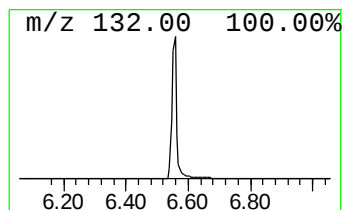
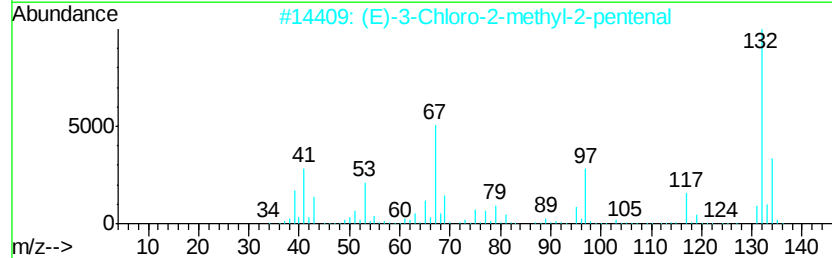
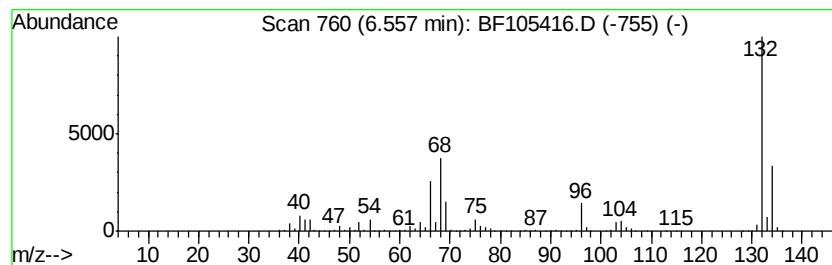
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	70.32 ng	2932190	1,4-Dichlorobenzene-d4	6.79

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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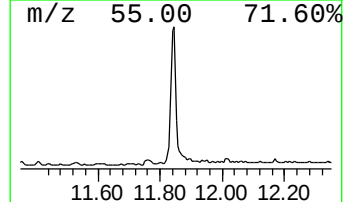
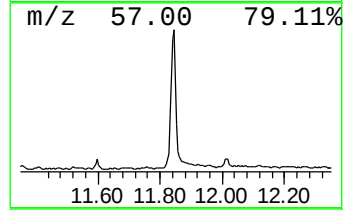
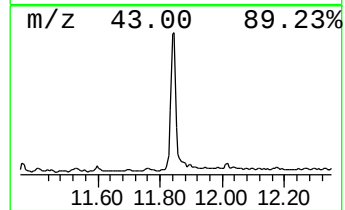
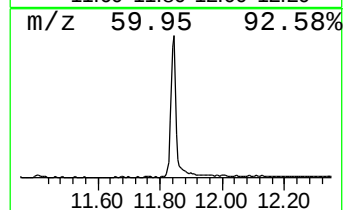
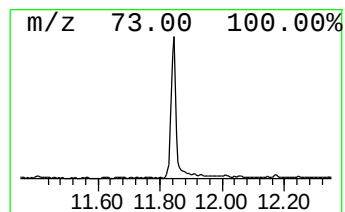
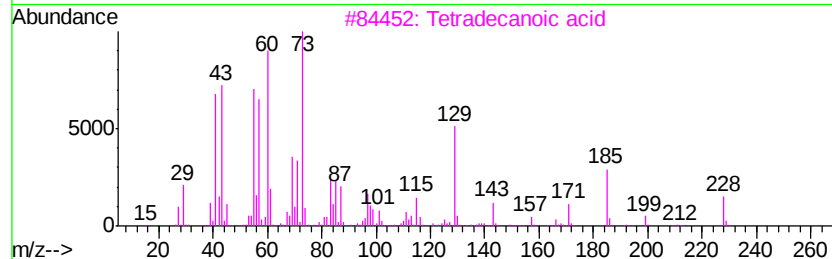
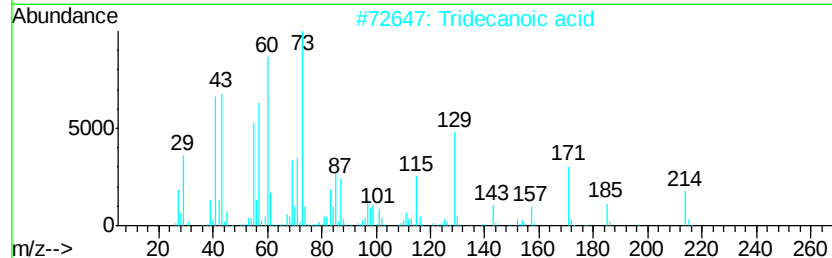
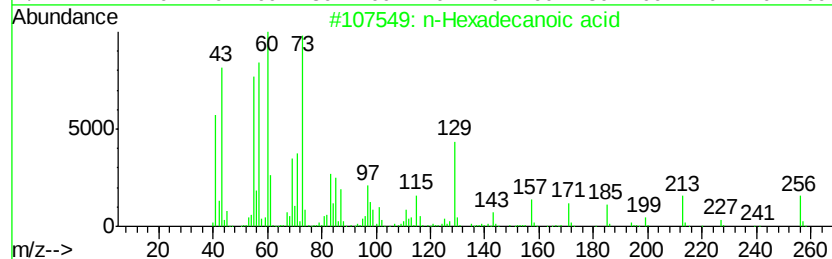
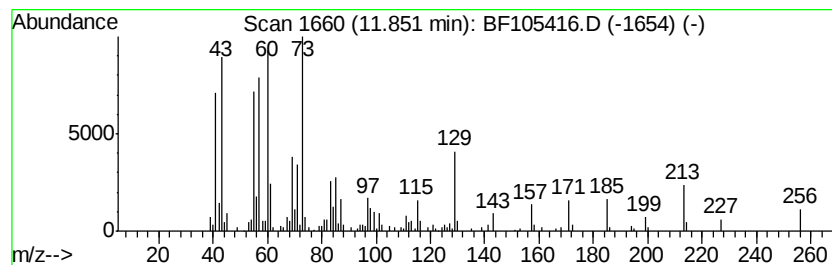
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	12.74 ng	763967	Phenanthrene-d10	11.31

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	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5		Dodecanoic acid	200	C12H24O2	000143-07-7	59



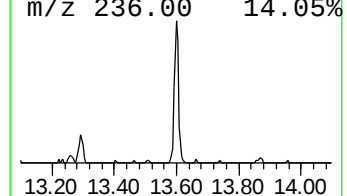
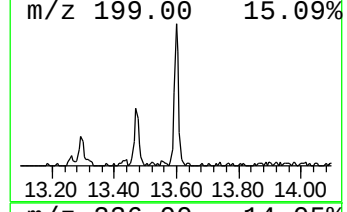
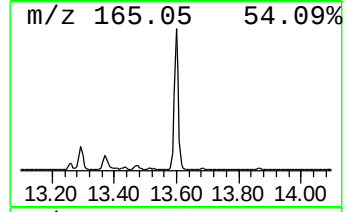
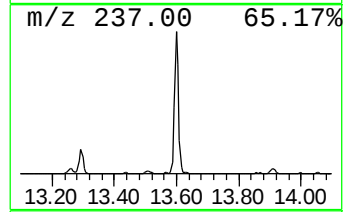
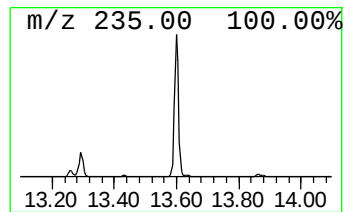
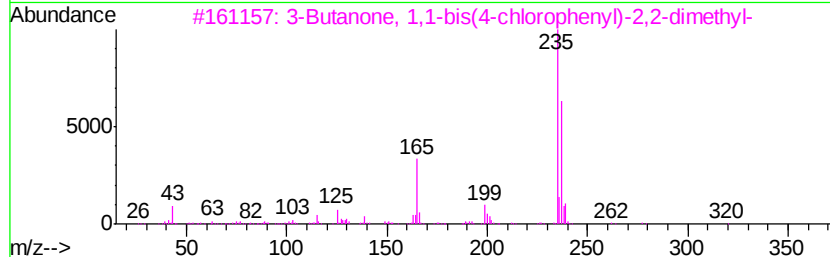
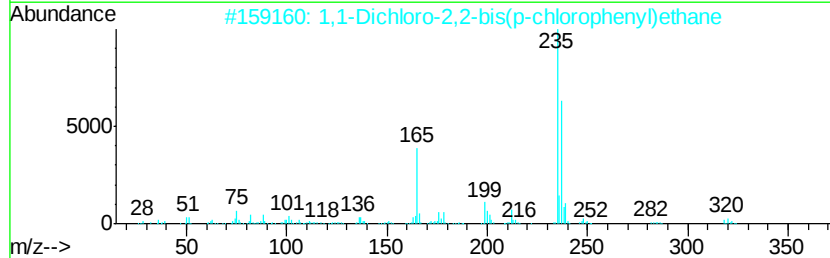
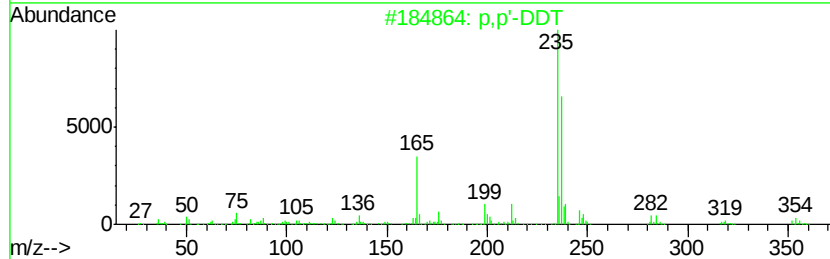
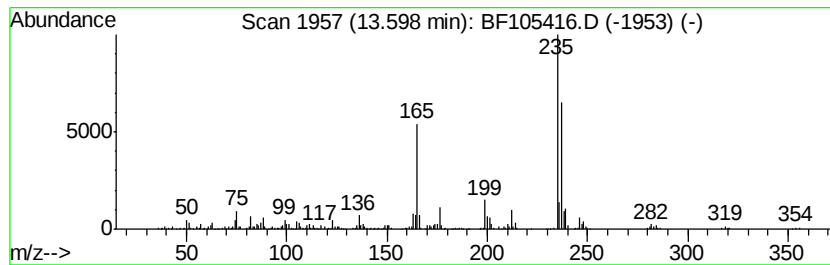
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Peak Number 5 p,p'-DDT Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	14.16 ng	688916	Chrysene-d12	14.16
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	p,p'-DDT		352 C14H9Cl5	000050-29-3 99
2	1,1-Dichloro-2,2-bis(p-chlorophe...		318 C14H10Cl4	000072-54-8 95
3	3-Butanone, 1,1-bis(4-chlorophen...		320 C18H18Cl2O	1000158-20-4 93
4	o,p'-DDT		352 C14H9Cl5	000789-02-6 90
5	m,p'-DDD		318 C14H10Cl4	004329-12-8 90



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Misc :
ALS Vial : 4 Sample Multiplier: 1

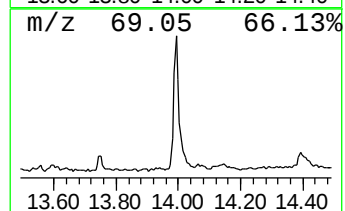
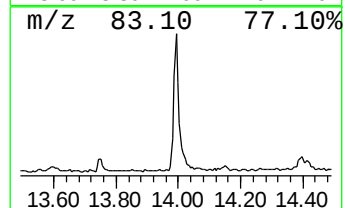
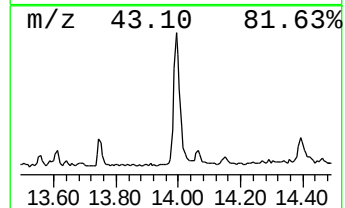
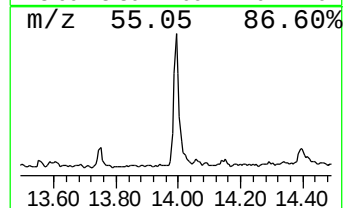
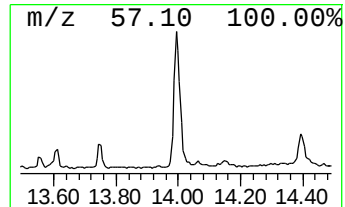
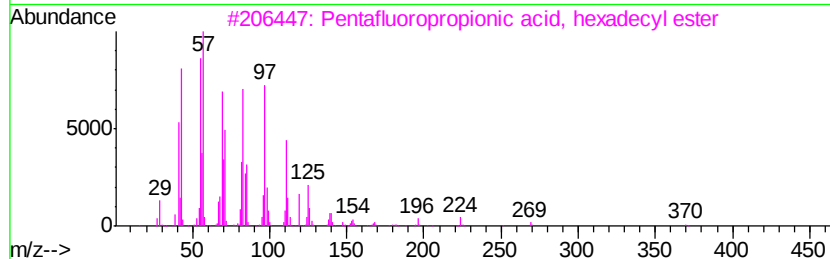
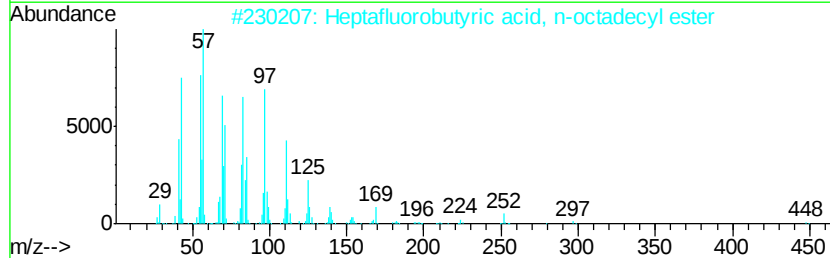
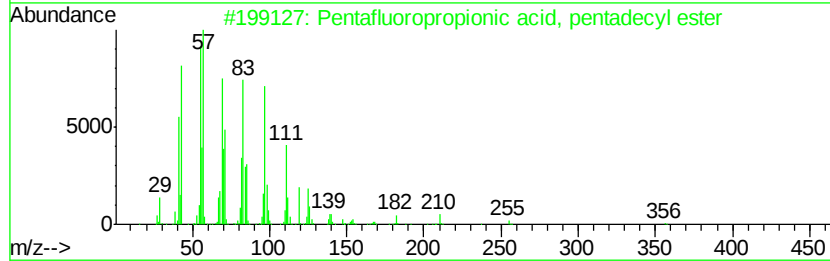
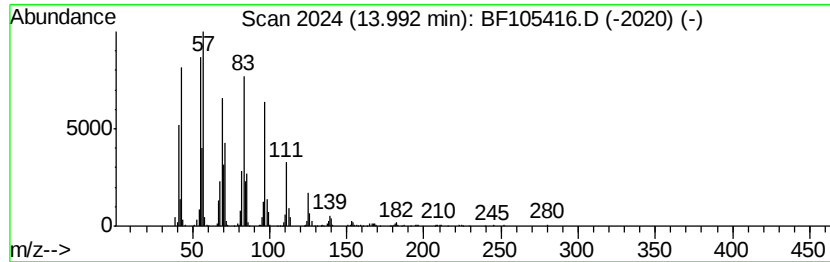
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	16.10 ng	783355	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
3		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
4		1-Docosene	308	C22H44	001599-67-3	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\HPCHEM1\BNA_F\Data\BF051518\
Data File : BF105416.D
Acq On : 15 May 2018 14:44
Operator : JU/SJ
Sample : J2873-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

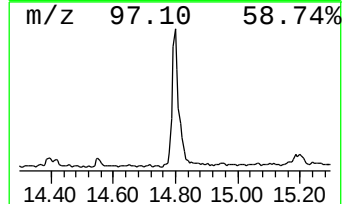
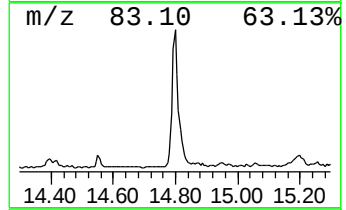
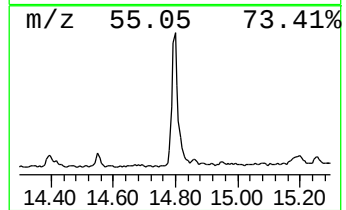
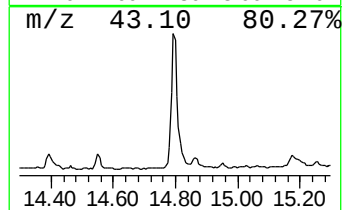
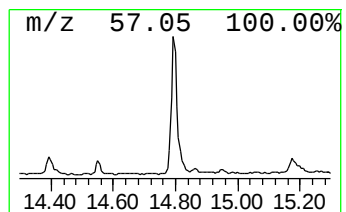
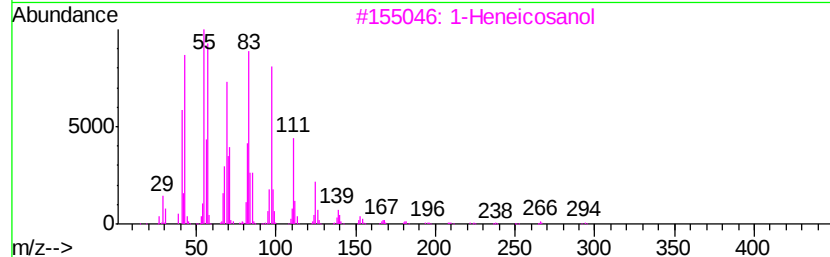
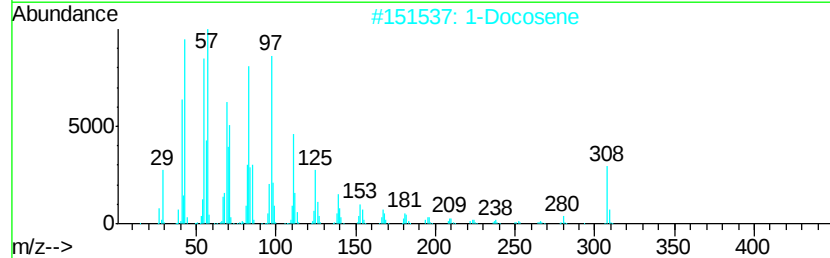
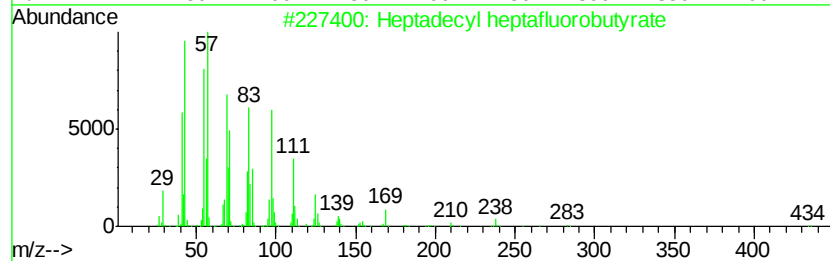
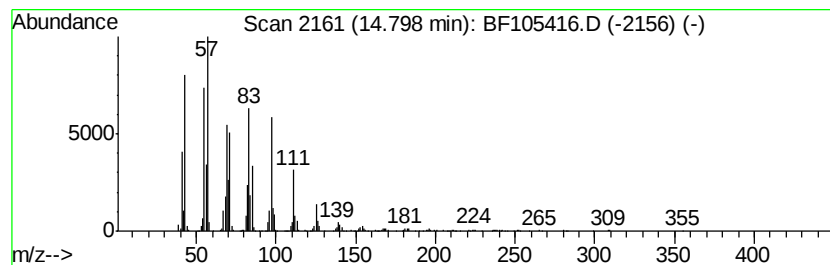
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	27.81 ng	1353460	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		1-Docosene	308	C22H44	001599-67-3	93
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



Data Path : Z:\HPCHEM1\BNA_F\Data\BF051518\
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Sample : J2873-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

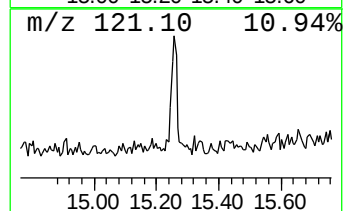
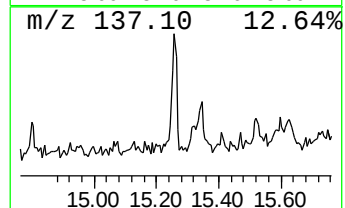
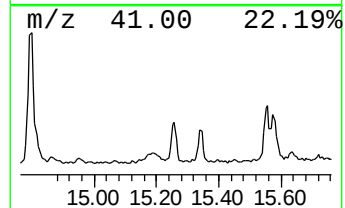
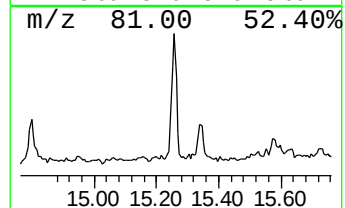
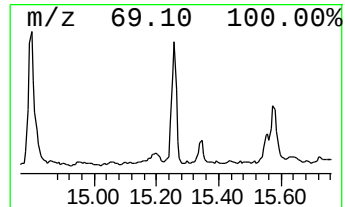
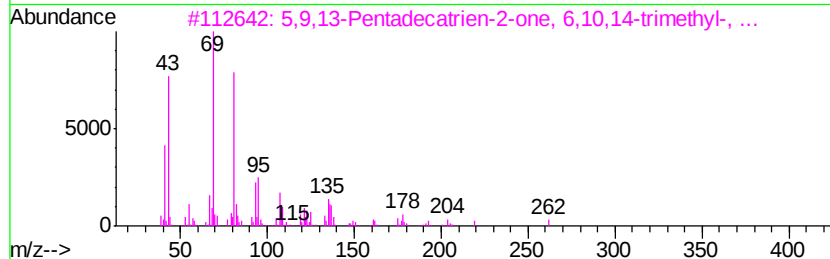
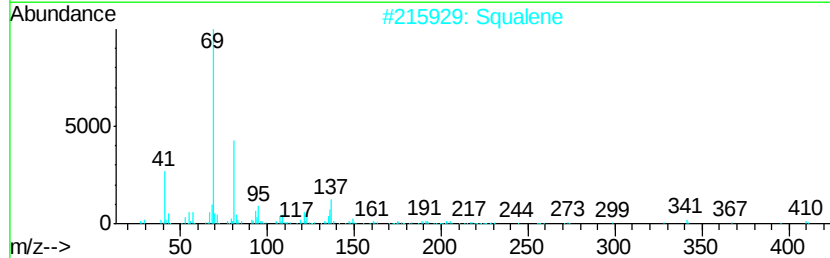
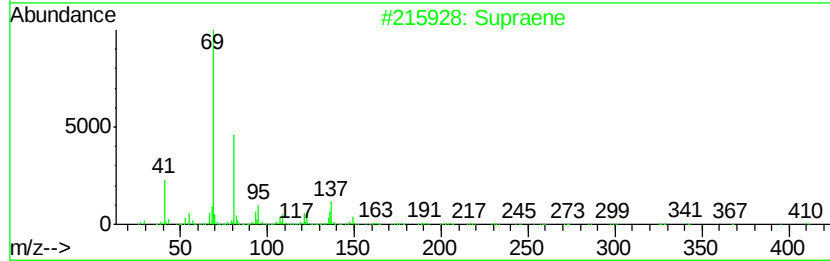
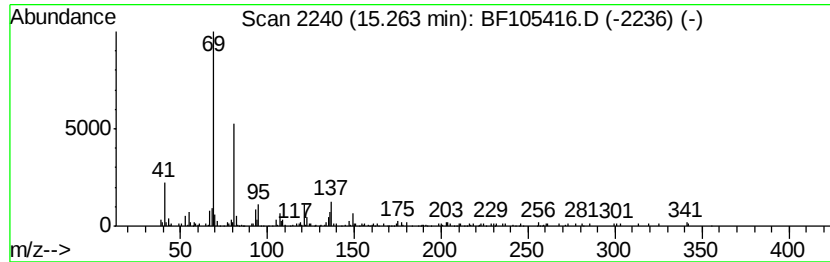
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	4.93 ng	212731	Perylene-d12	15.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	72
4		Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59
5		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	58



Data Path : Z:\HPCHEM1\BNA_F\Data\BF051518\
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Acq On : 15 May 2018 14:44
Operator : JU/SJ
Sample : J2873-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

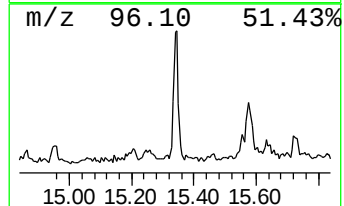
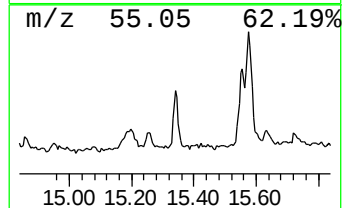
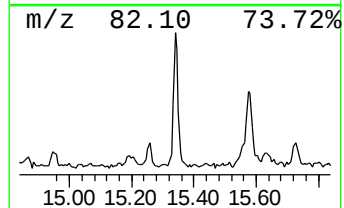
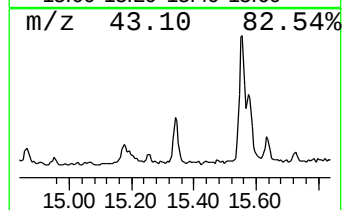
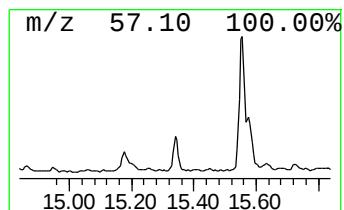
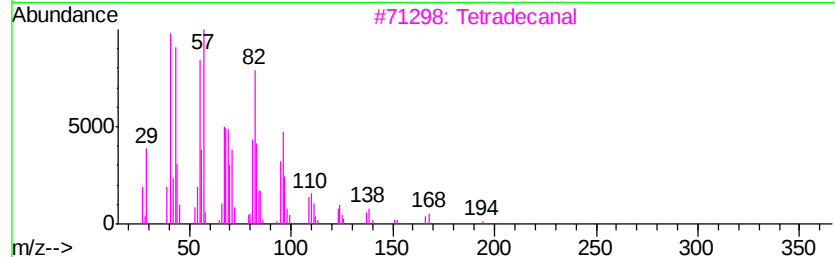
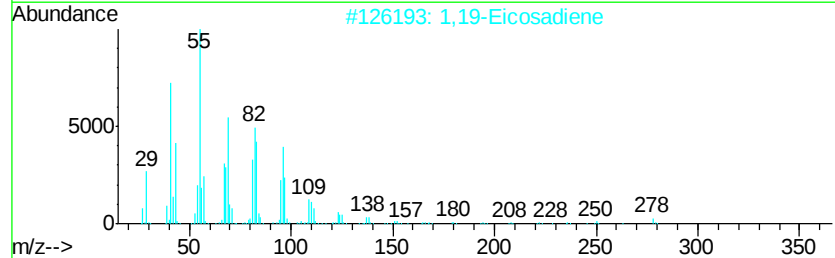
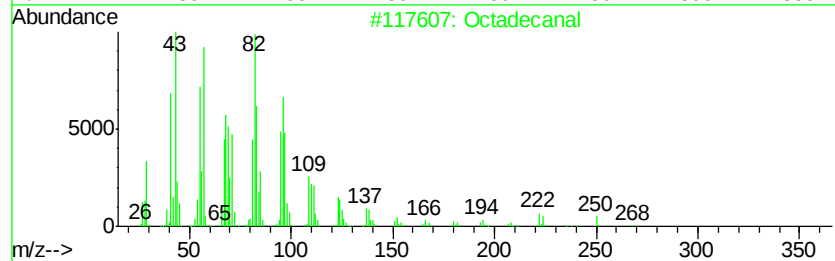
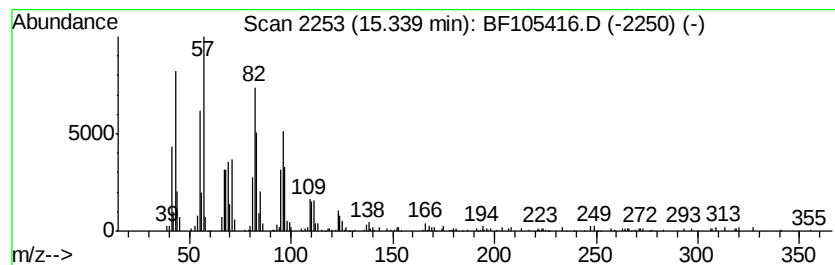
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanal Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	6.57 ng	283566	Perylene-d12	15.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	91
2		1,19-Eicosadiene	278	C20H38	014811-95-1	90
3		Tetradecanal	212	C14H28O	000124-25-4	90
4		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
5		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87



Data Path : Z:\HPCHEM1\BNA_F\Data\BF051518\
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Acq On : 15 May 2018 14:44
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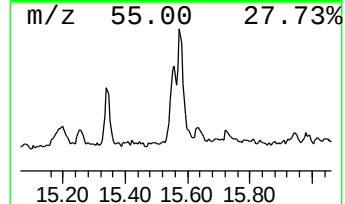
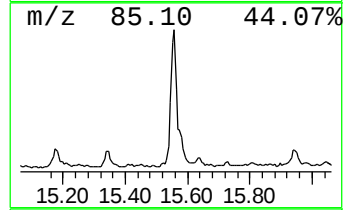
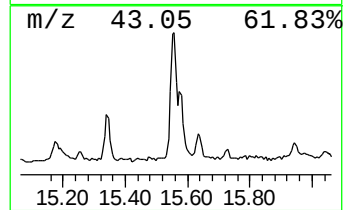
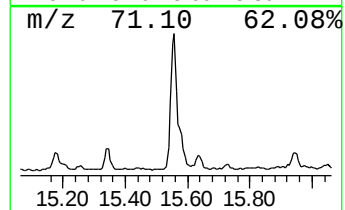
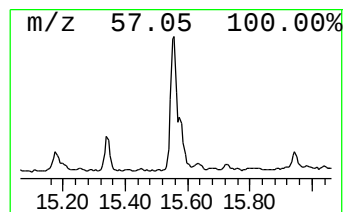
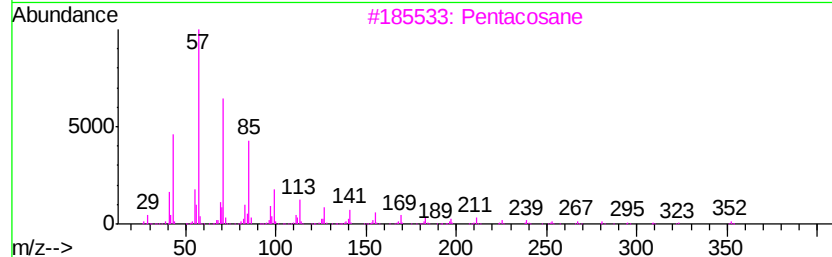
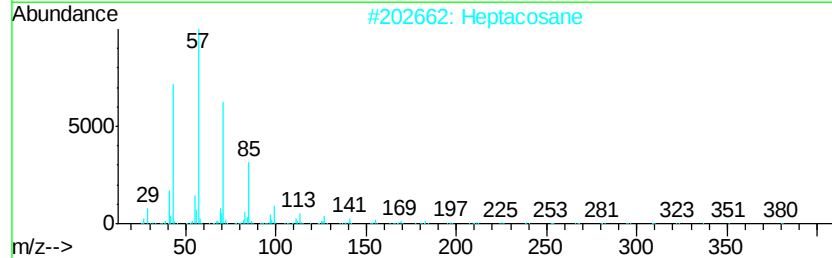
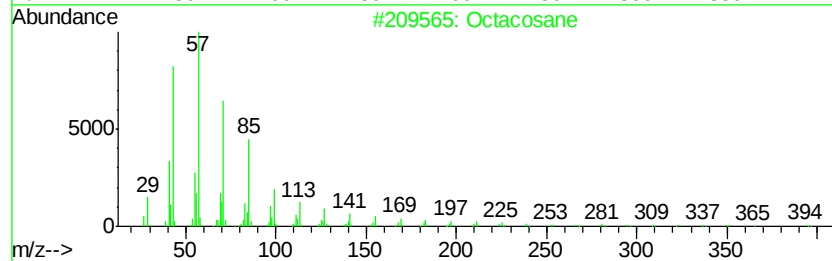
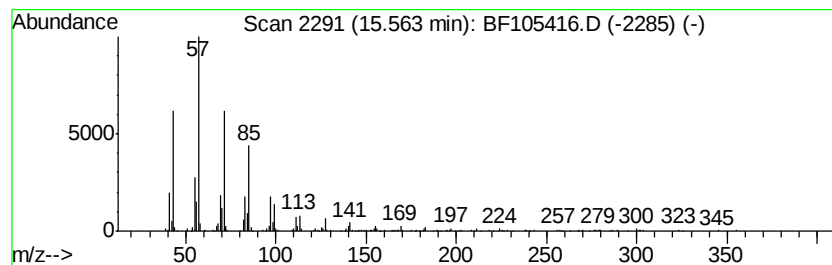
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	13.15 ng	567275	Perylene-d12	15.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Eicosane	282	C20H42	000112-95-8	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\HPCHEM1\BNA_F\Data\BF051518\
Data File : BF105416.D
Acq On : 15 May 2018 14:44
Operator : JU/SJ
Sample : J2873-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051018.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown15.57 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	7.70 ng	332391	Perylene-d12	15.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	49
2		6-Bromo-2,2-dimethylcyclohexanone	204	C8H13BrO	021690-26-6	43
3		Cyclohexadecane	224	C16H32	000295-65-8	41
4		Cycloheptane, methyl-	112	C8H16	004126-78-7	38
5		4-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-9	38

