

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
 Data File : BF097876.D
 Acq On : 19 Aug 2017 14:03
 Operator : SJ/JU
 Sample : I4852-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-242

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-BF081517.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	4.957	484	488	497	rVB	426320	593627	14.74%	1.420%
2	5.369	552	558	561	rBV	3202155	3331031	82.69%	7.968%
3	6.398	727	733	736	rVB	3245473	3736275	92.75%	8.937%
4	6.534	750	756	759	rBV	3106456	3533687	87.72%	8.453%
5	6.757	790	794	798	rBV	1147944	1076080	26.71%	2.574%
6	6.916	816	821	825	rBV	2665413	2561116	63.58%	6.126%
7	7.328	885	891	894	rBV	2213644	2413003	59.90%	5.772%
8	7.410	900	905	908	rBV	45488	49256	1.22%	0.118%
9	8.045	1007	1013	1015	rBV	1562029	1510964	37.51%	3.614%
10	9.122	1190	1196	1199	rBV	4089553	4028309	100.00%	9.636%
11	9.510	1258	1262	1266	rVB	818028	734889	18.24%	1.758%
12	9.792	1304	1310	1314	rBV	1653383	1662153	41.26%	3.976%
13	9.828	1314	1316	1319	rVB	102999	83541	2.07%	0.200%
14	9.998	1341	1345	1349	rBV2	143249	136453	3.39%	0.326%
15	10.233	1382	1385	1388	rVB	59836	52834	1.31%	0.126%
16	10.339	1400	1403	1406	rBV	111100	97672	2.42%	0.234%
17	10.581	1439	1444	1447	rBV	2310953	2392110	59.38%	5.722%
18	10.704	1462	1465	1473	rVB	103527	112217	2.79%	0.268%
19	10.886	1490	1496	1499	rBV4	29742	50225	1.25%	0.120%
20	11.151	1539	1541	1543	rBV	60346	49171	1.22%	0.118%
21	11.169	1543	1544	1549	rVB2	61450	55153	1.37%	0.132%
22	11.275	1558	1562	1564	rBV	1745079	1557702	38.67%	3.726%
23	11.298	1564	1566	1569	rVV	855405	628591	15.60%	1.504%
24	11.345	1572	1574	1578	rVB	235039	192742	4.78%	0.461%
25	11.504	1595	1601	1603	rBV	63936	68932	1.71%	0.165%
26	11.575	1610	1613	1616	rBV2	46034	40324	1.00%	0.096%
27	11.775	1643	1647	1649	rBV	91912	77732	1.93%	0.186%
28	11.804	1649	1652	1656	rVV	117201	110490	2.74%	0.264%
29	11.845	1656	1659	1662	rVV2	56107	53552	1.33%	0.128%
30	11.886	1662	1666	1668	rVV	158134	161884	4.02%	0.387%
31	11.910	1668	1670	1674	rVB	54870	46088	1.14%	0.110%
32	12.069	1694	1697	1699	rBV	71667	63460	1.58%	0.152%
33	12.322	1737	1740	1743	rBV	61343	57167	1.42%	0.137%
34	12.404	1751	1754	1759	rVB3	43405	49914	1.24%	0.119%

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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	12.480	1763	1767	1771	rVV	904470	773443	19.20%	1.850%
36	12.527	1772	1775	1781	rVB4	47810	57146	1.42%	0.137%
37	12.633	1786	1793	1797	rBV2	41145	63036	1.56%	0.151%
38	12.710	1800	1806	1809	rBV	759785	778468	19.32%	1.862%
39	12.763	1812	1815	1819	rVB2	42825	52605	1.31%	0.126%
40	12.827	1823	1826	1828	rBV	48645	53565	1.33%	0.128%
41	12.863	1828	1832	1835	rVV	3126006	2996868	74.40%	7.169%
42	12.933	1838	1844	1847	rBV2	52740	83557	2.07%	0.200%
43	13.039	1859	1862	1865	rVB	137684	123594	3.07%	0.296%
44	13.104	1870	1873	1875	rBV	127003	102106	2.53%	0.244%
45	13.139	1875	1879	1882	rBV2	84852	90912	2.26%	0.217%
46	13.651	1962	1966	1969	rBV2	60570	80067	1.99%	0.192%
47	13.757	1981	1984	1990	rVB3	177204	205202	5.09%	0.491%
48	13.904	2004	2009	2012	rBV2	1149953	1346637	33.43%	3.221%
49	13.927	2012	2013	2019	rVB	295437	241185	5.99%	0.577%
50	14.010	2024	2027	2029	rVB	52918	41375	1.03%	0.099%
51	14.286	2072	2074	2078	rVB	50393	48249	1.20%	0.115%
52	14.686	2140	2142	2148	rBV4	31646	46057	1.14%	0.110%
53	14.757	2150	2154	2158	rVB	814027	826609	20.52%	1.977%
54	14.916	2177	2181	2184	rBV	243104	342239	8.50%	0.819%
55	15.016	2195	2198	2205	rVB2	83179	118544	2.94%	0.284%
56	15.204	2227	2230	2236	rVB	165032	206545	5.13%	0.494%
57	15.263	2236	2240	2245	rBV	209290	248840	6.18%	0.595%
58	15.327	2247	2251	2255	rBV	672296	851980	21.15%	2.038%
59	15.792	2326	2330	2334	rBV2	62883	89507	2.22%	0.214%
60	15.833	2334	2337	2348	rVB10	38680	99571	2.47%	0.238%
61	16.010	2364	2367	2377	rVB10	76535	145895	3.62%	0.349%
62	16.704	2480	2485	2492	rVB2	92191	174790	4.34%	0.418%
63	17.115	2551	2555	2565	rBV	69033	147703	3.67%	0.353%

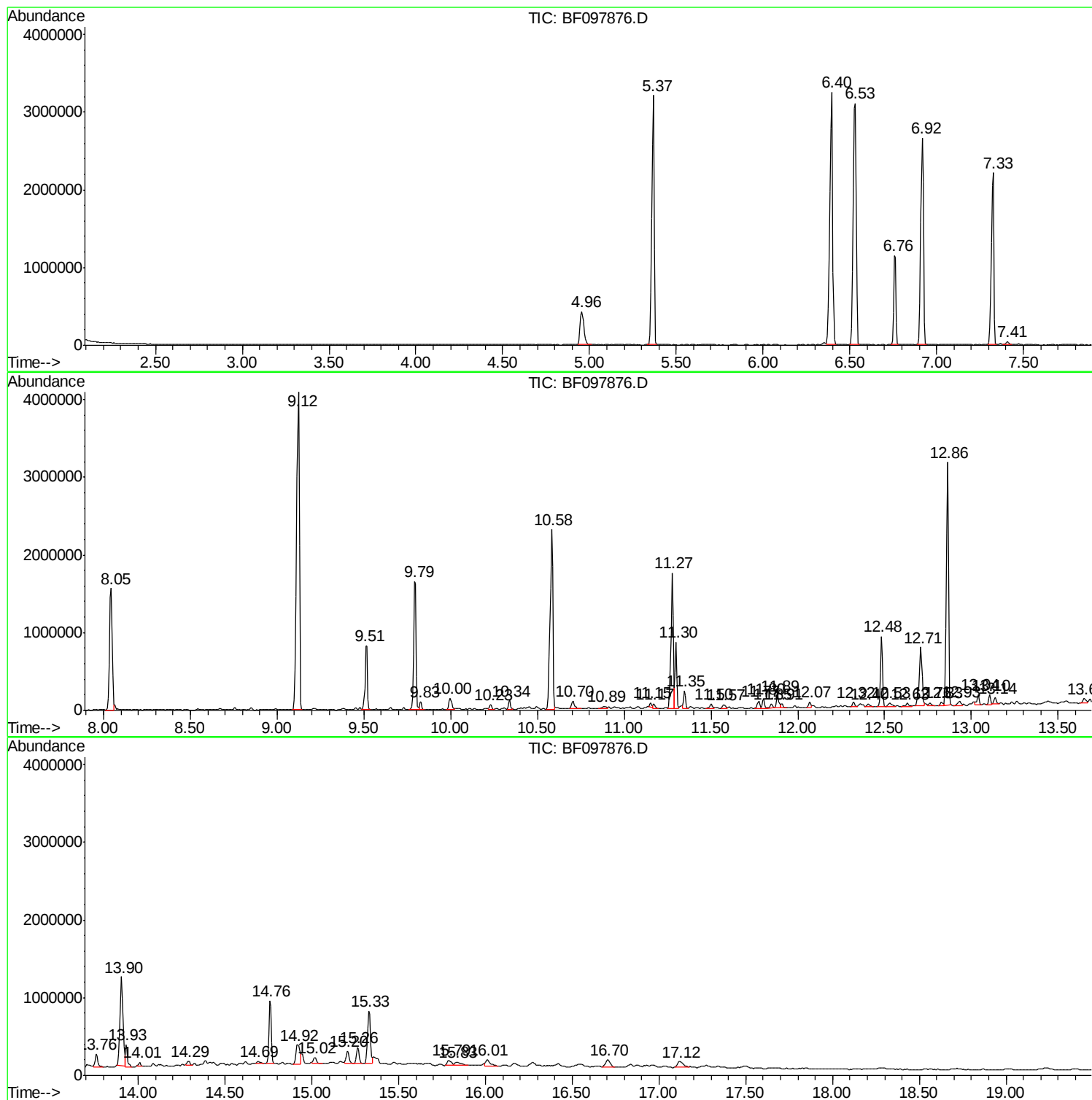
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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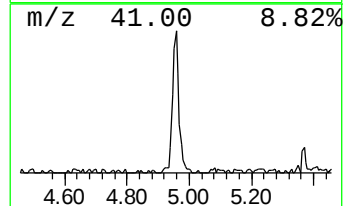
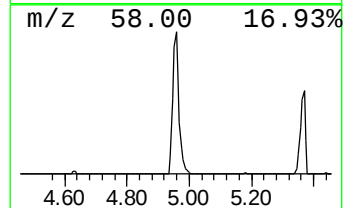
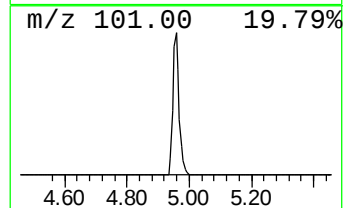
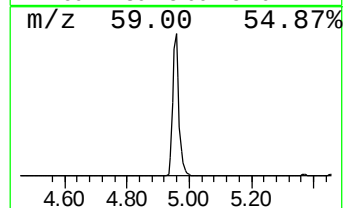
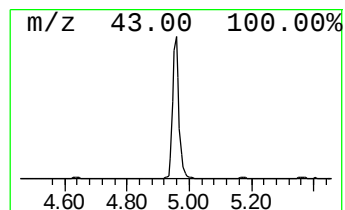
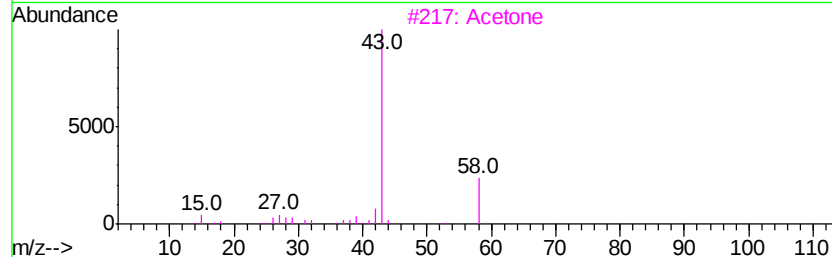
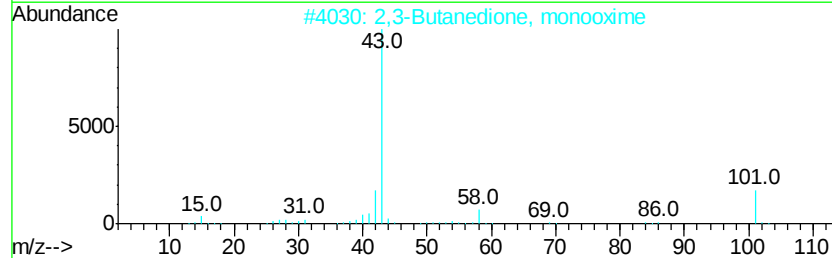
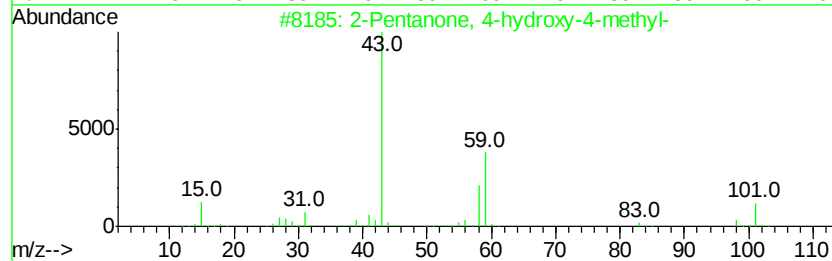
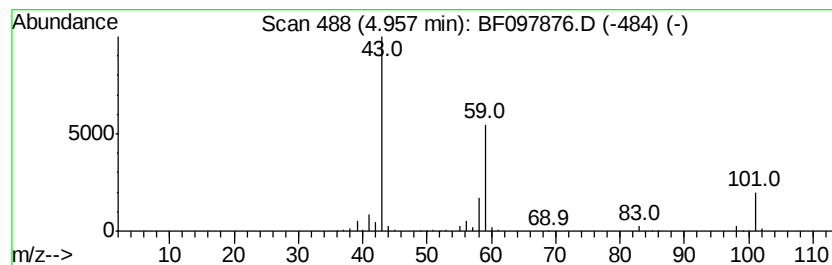
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	11.03 ng	593627	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
3		Acetone	58	C3H6O	000067-64-1	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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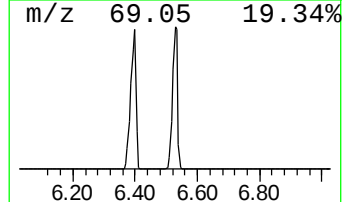
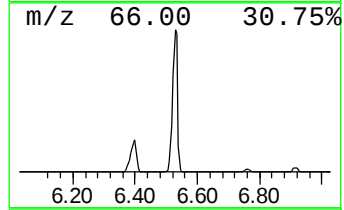
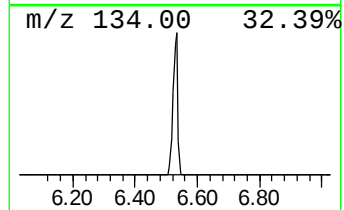
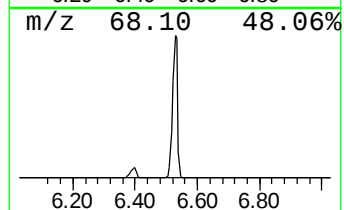
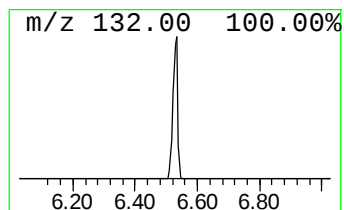
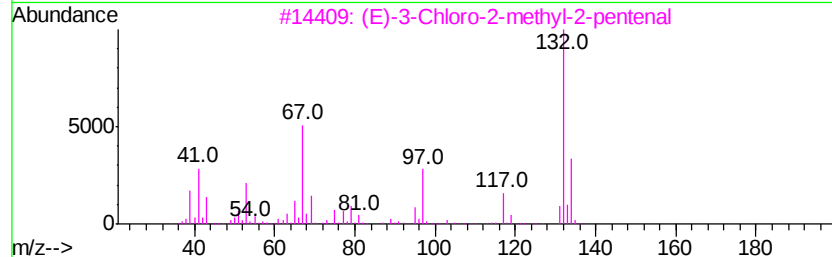
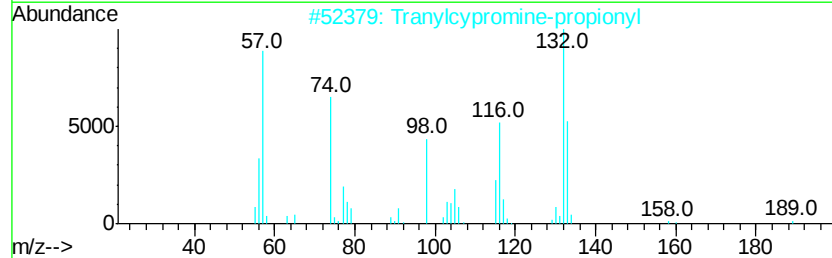
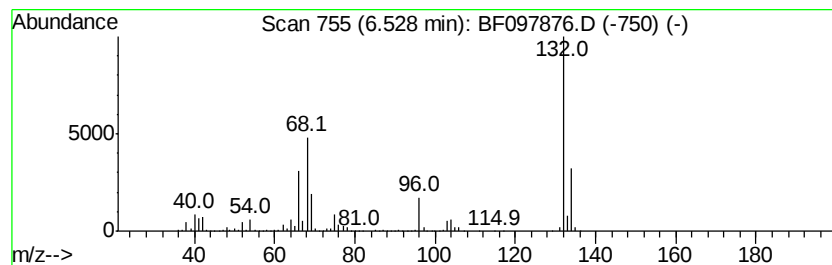
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	65.68 ng	3533690	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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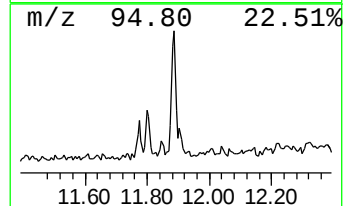
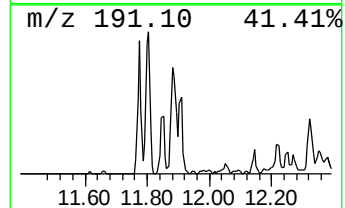
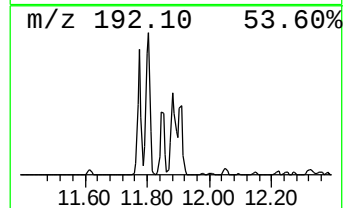
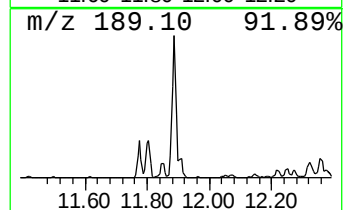
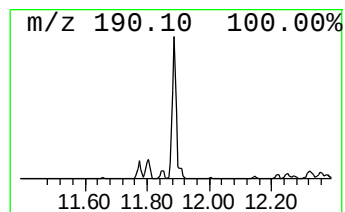
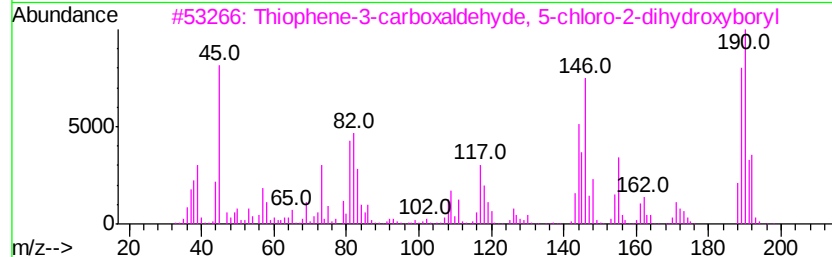
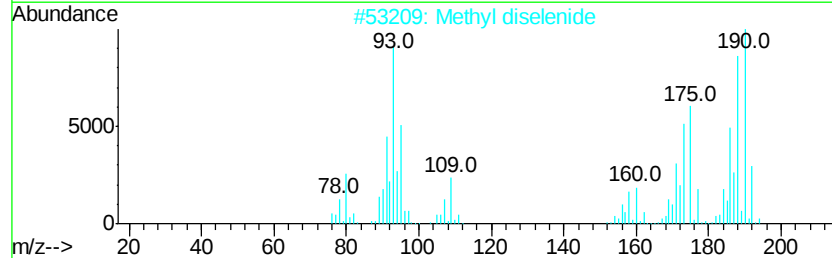
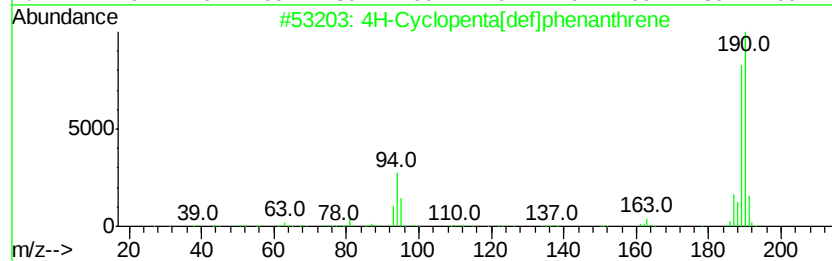
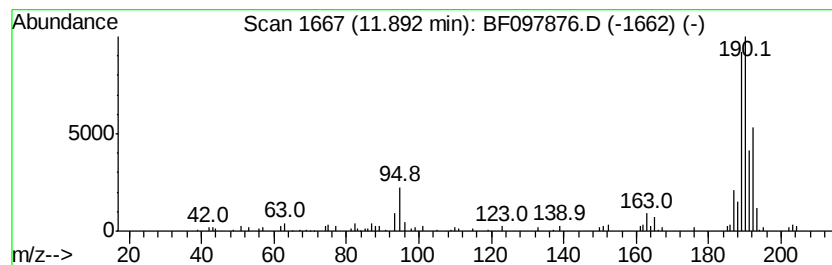
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	2.08 ng	161884	Phenanthrene-d10	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2		Methyl diselenide	190	C2H6Se2	007101-31-7	55
3		Thiophene-3-carboxaldehyde, 5-chloro-2-dihydroxyboryl	190	C5H4BClO3S	036155-87-0	52
4		6H-Cyclobuta[f]phenanthrene	190	C15H10	083469-43-6	50
5		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42



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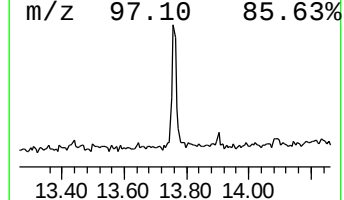
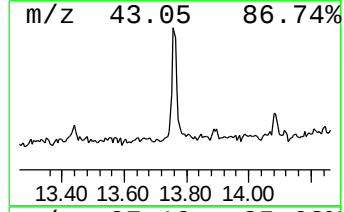
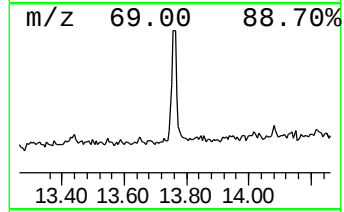
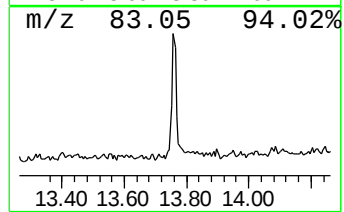
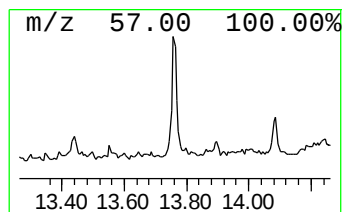
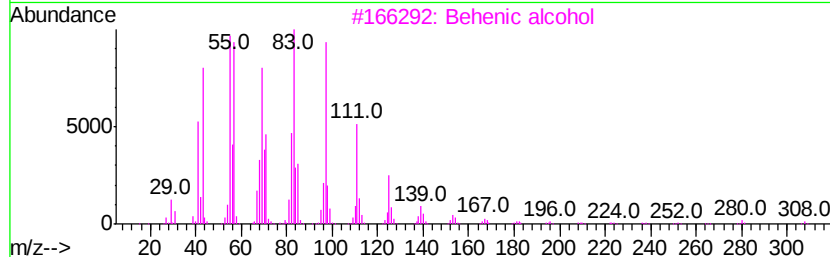
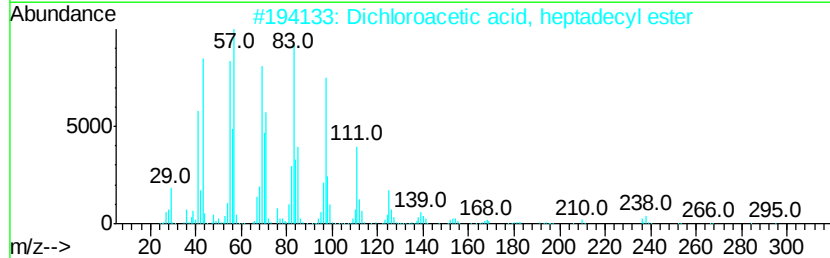
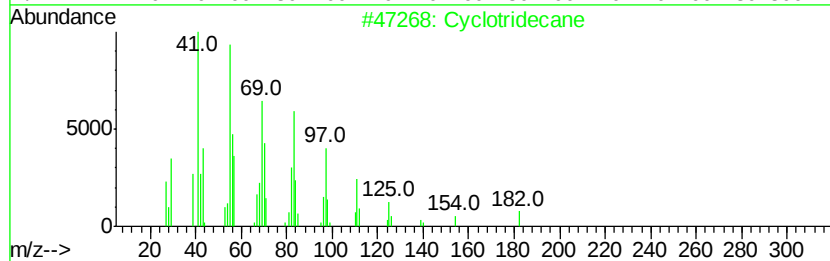
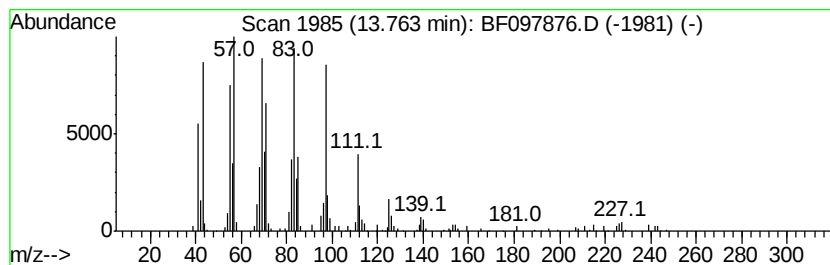
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclotridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.76	3.05 ng	205202	Chrysene-d12	13.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotridecane	182	C13H26	000295-02-3	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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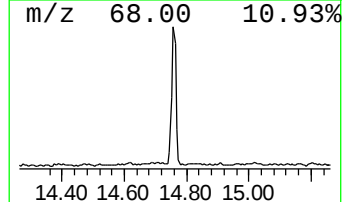
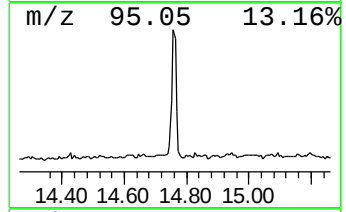
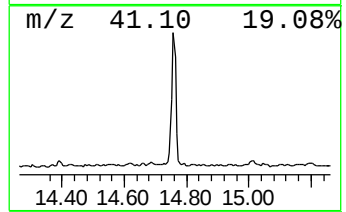
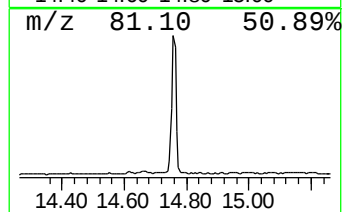
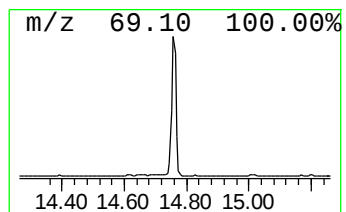
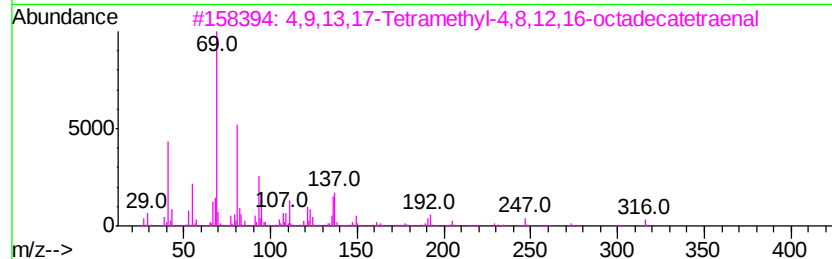
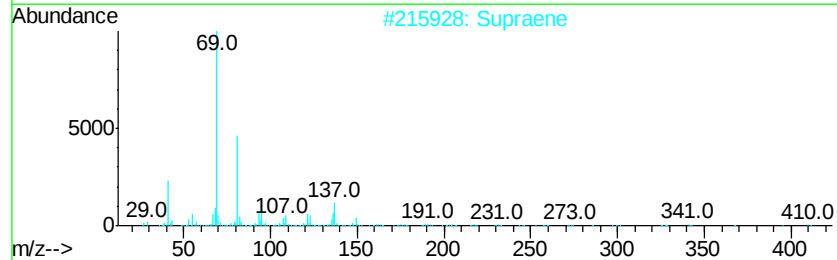
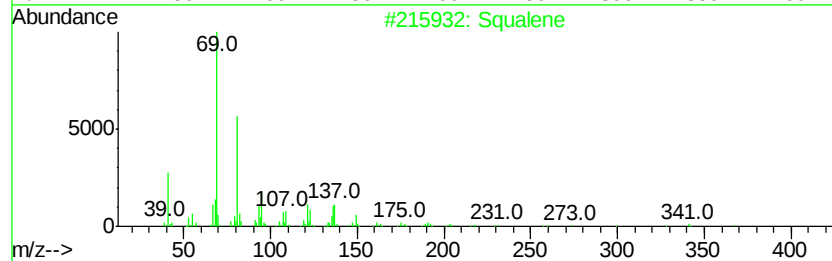
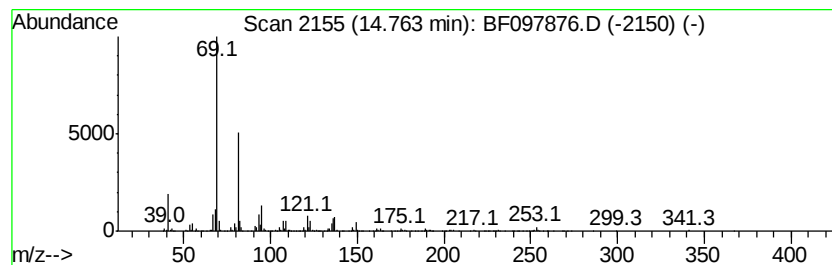
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	19.40 ng	826609	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4		1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	53
5		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
Data File : BF097876.D
Acq On : 19 Aug 2017 14:03
Operator : SJ/JU
Sample : I4852-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

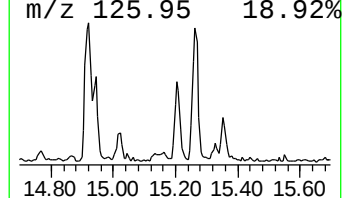
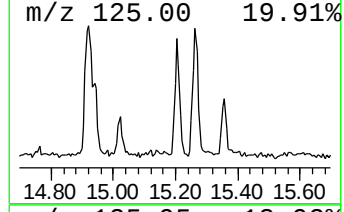
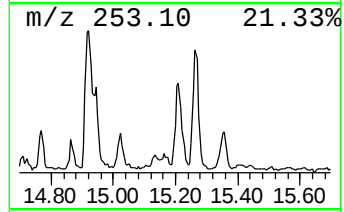
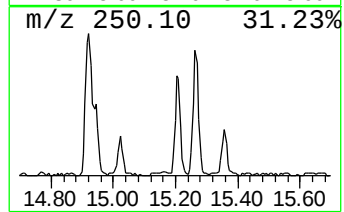
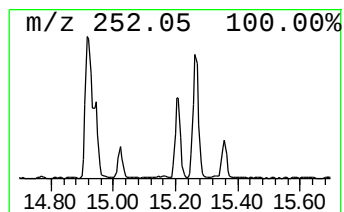
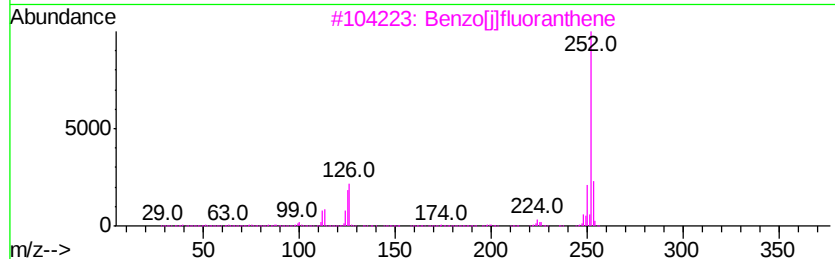
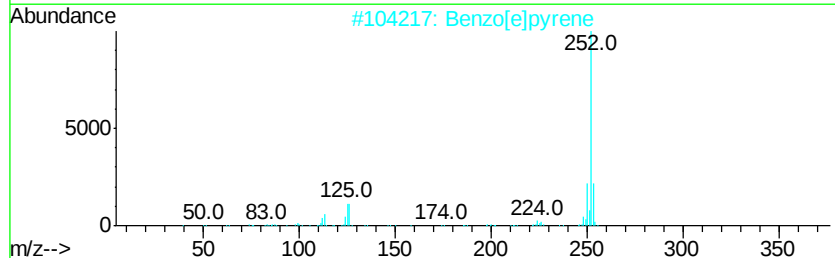
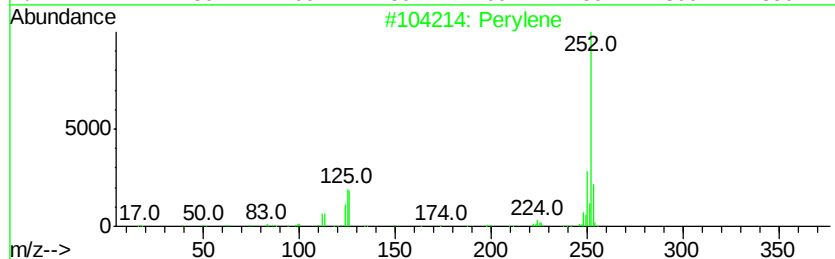
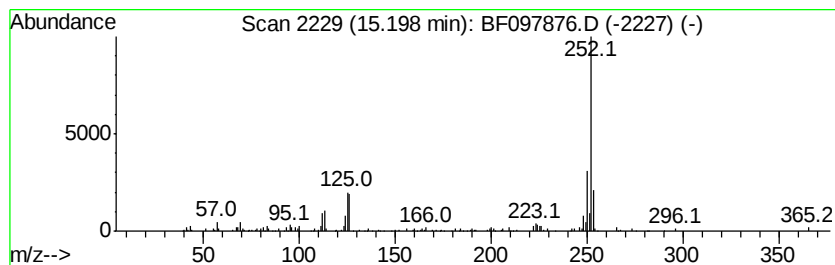
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	4.85 ng	206545	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	99
2		Benzo[e]pyrene	252	C20H12	000192-97-2	98
3		Benzo[i]fluoranthene	252	C20H12	000205-82-3	97
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
5		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081917\
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Operator : SJ/JU
Sample : I4852-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

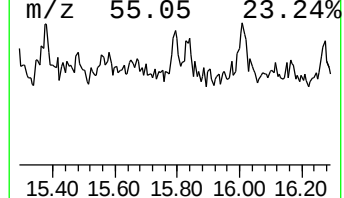
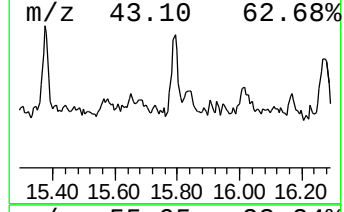
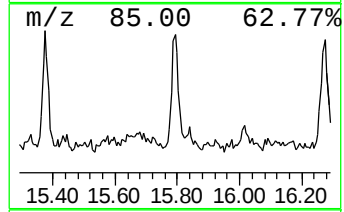
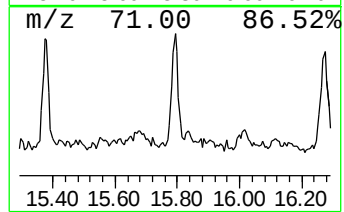
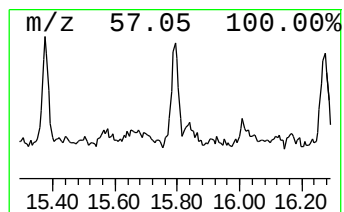
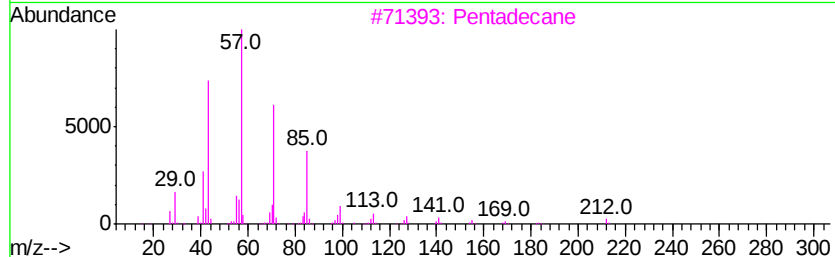
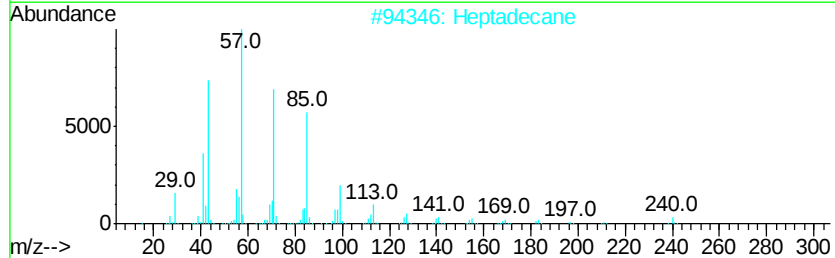
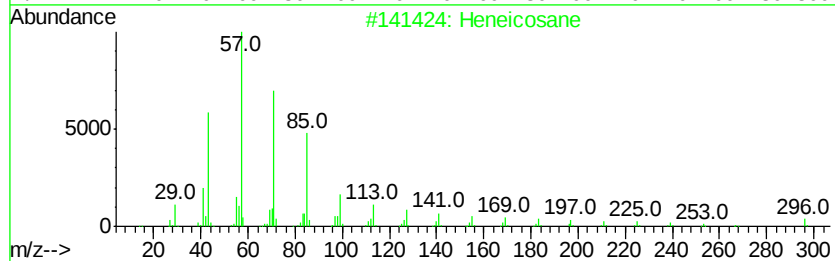
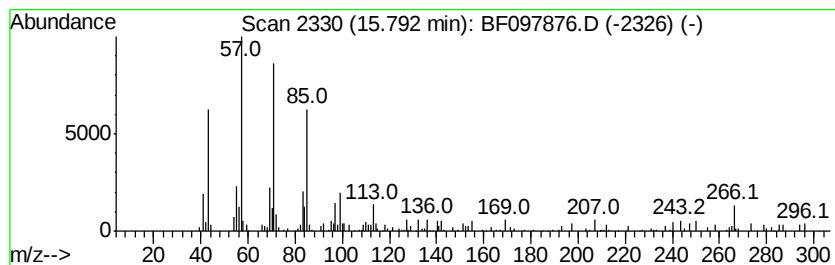
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ClientSampleId :
VNJ-242

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.10 ng	89507	Perylene-d12	15.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296	C21H44	000629-94-7 90
2	Heptadecane	240	C17H36	000629-78-7 89
3	Pentadecane	212	C15H32	000629-62-9 68
4	Octacosane	394	C28H58	000630-02-4 64
5	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7 64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
Data File : BF097876.D
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Operator : SJ/JU
Sample : I4852-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

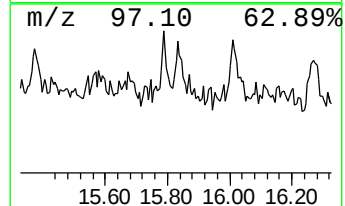
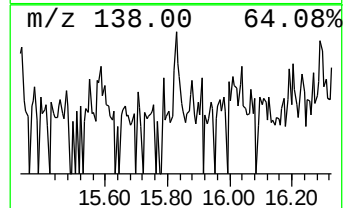
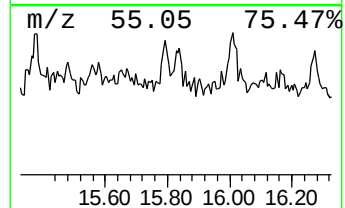
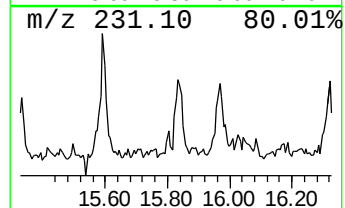
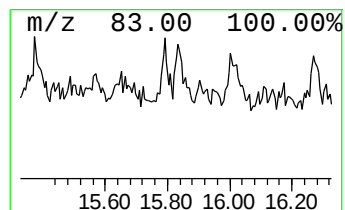
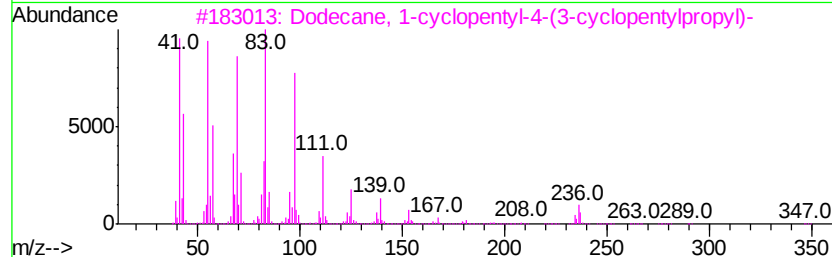
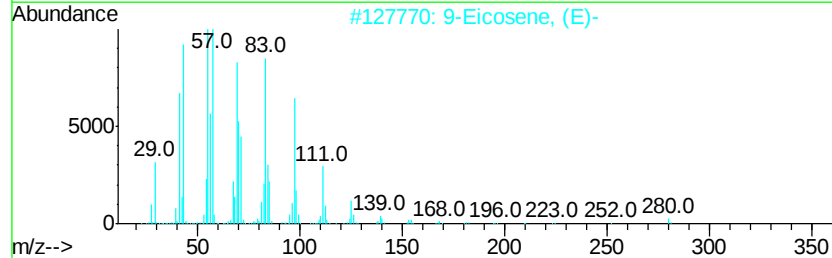
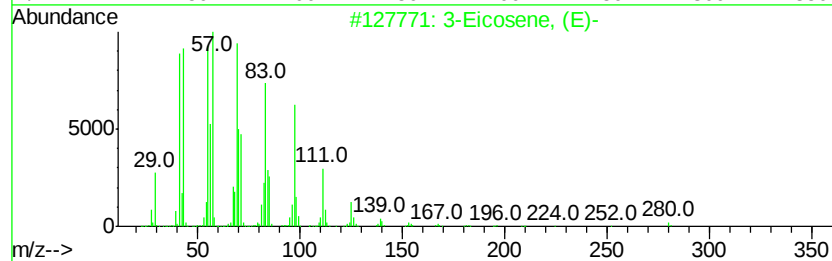
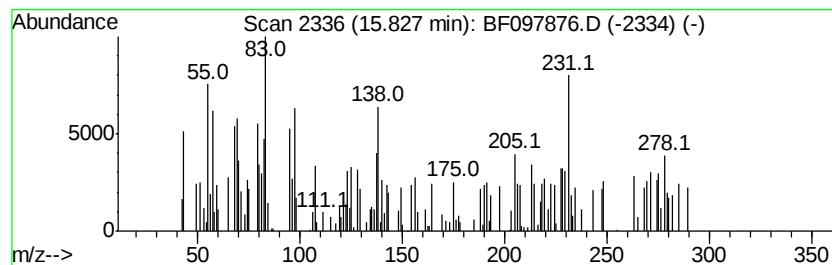
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 3-Eicosene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	2.34 ng	99571	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	64
2		9-Eicosene, (E)-	280	C20H40	074685-29-3	58
3		Dodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-	348	C25H48	007225-68-5	52
4		Methyl 2-hydroxy-pentadecanoate	272	C16H32O3	1000336-35-7	52
5		Cyclopentanecarboxylic acid, 3-p...	230	C15H18O2	1000282-59-3	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
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Sample : I4852-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VNJ-242

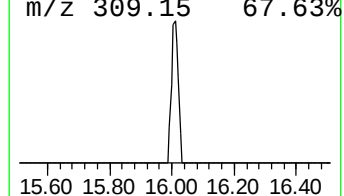
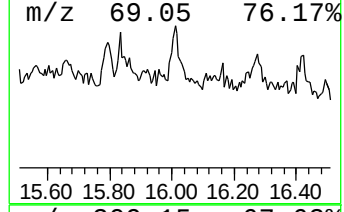
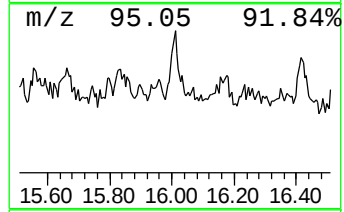
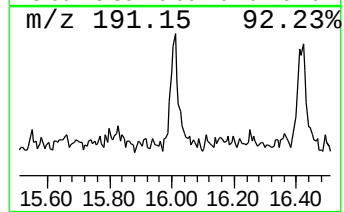
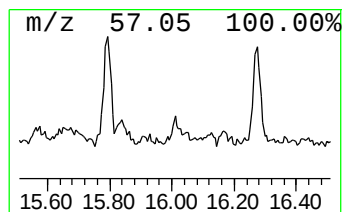
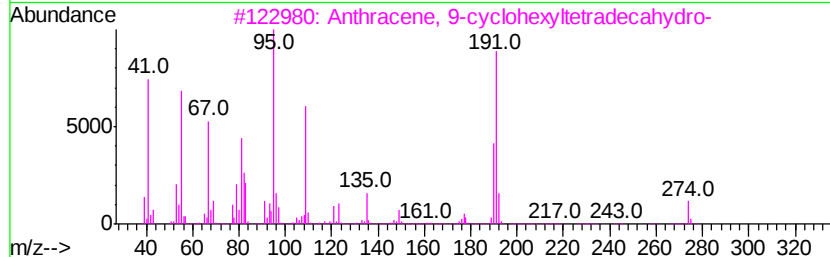
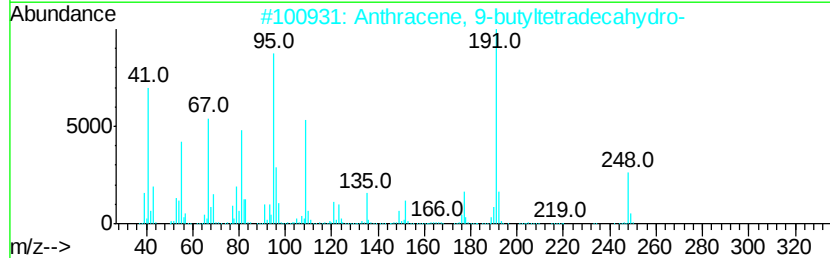
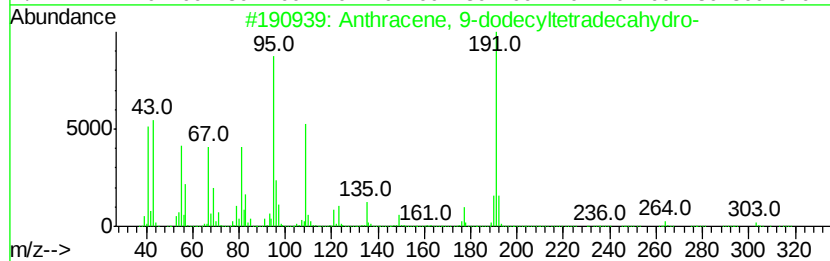
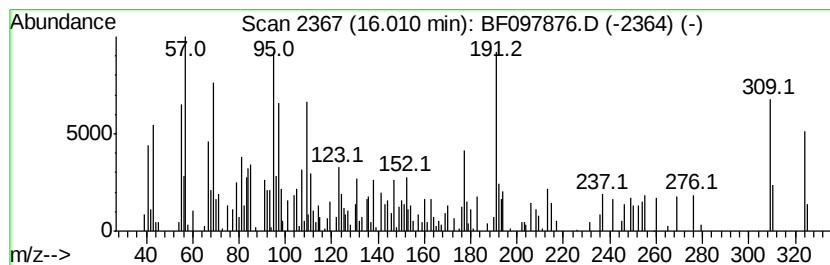
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	3.42 ng	145895	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-dodecyltetradeca...	360	C26H48	055401-75-7	43
2		Anthracene, 9-butyltetradeca...	248	C18H32	055133-89-6	43
3		Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	38
4		1,4-Methanonaphthalene, 6,7-diet...	206	C15H26	016539-02-9	30
5		5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081917\
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 Acq On : 19 Aug 2017 14:03
 Operator : SJ/JU
 Sample : I4852-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-242

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
2-Pentanone, 4-hy...	4.96	11.0	ng	593627	1	6.76	1076080	20.0
unknown6.53	6.53	65.7	ng	3533690	1	6.76	1076080	20.0
4H-Cyclopenta[def...	11.89	2.1	ng	161884	4	11.27	1557700	20.0
Cyclotridecane	13.76	3.0	ng	205202	5	13.90	1346640	20.0
Squalene	14.76	19.4	ng	826609	6	15.33	851980	20.0
Perylene	15.20	4.8	ng	206545	6	15.33	851980	20.0
Heneicosane	15.79	2.1	ng	89507	6	15.33	851980	20.0
3-Eicosene, (E)-	15.83	2.3	ng	99571	6	15.33	851980	20.0
unknown16.01	16.01	3.4	ng	145895	6	15.33	851980	20.0