

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
 Data File : BF097134.D
 Acq On : 27 Jul 2017 20:41
 Operator : SJ/JU
 Sample : I4422-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-201-COMP

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-BF072517.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	4.622	462	465	476	rBV	132997	215541	8.85%	1.013%
2	5.081	539	543	560	rBV	2020164	2321465	95.34%	10.914%
3	6.151	720	725	739	rBV	2274756	2434937	100.00%	11.447%
4	6.257	739	743	747	rBV	2237705	2253801	92.56%	10.596%
5	6.487	779	782	791	rVB	679809	579249	23.79%	2.723%
6	6.640	804	808	812	rBV	1645334	1590308	65.31%	7.476%
7	7.057	874	879	882	rBV	1434163	1445291	59.36%	6.795%
8	7.769	996	1000	1008	rBV	983096	799768	32.85%	3.760%
9	8.216	1071	1076	1083	rBV5	16298	28962	1.19%	0.136%
10	8.851	1179	1184	1187	rBV	2321280	2287890	93.96%	10.756%
11	9.245	1245	1251	1254	rBV	299481	247787	10.18%	1.165%
12	9.516	1293	1297	1303	rVB	829670	752436	30.90%	3.537%
13	9.751	1334	1337	1341	rBV	74500	63736	2.62%	0.300%
14	9.969	1371	1374	1377	rBV	34308	28360	1.16%	0.133%
15	10.186	1406	1411	1414	rBV	19357	25729	1.06%	0.121%
16	10.298	1426	1430	1437	rVB	1241907	1208073	49.61%	5.679%
17	10.439	1451	1454	1460	rBV	48606	58323	2.40%	0.274%
18	10.886	1526	1530	1532	rBV	35881	29939	1.23%	0.141%
19	10.986	1543	1547	1550	rBV	780100	644047	26.45%	3.028%
20	11.545	1639	1642	1648	rBV	136118	131412	5.40%	0.618%
21	12.192	1749	1752	1756	rVB	69249	62339	2.56%	0.293%
22	12.327	1772	1775	1779	rBV2	61843	69461	2.85%	0.327%
23	12.416	1786	1790	1798	rBV	78694	88850	3.65%	0.418%
24	12.574	1812	1817	1820	rBV	1711087	1691536	69.47%	7.952%
25	12.798	1853	1855	1861	rVB4	21608	25048	1.03%	0.118%
26	13.074	1899	1902	1904	rVB4	32575	34110	1.40%	0.160%
27	13.139	1910	1913	1919	rBV3	27975	35927	1.48%	0.169%
28	13.480	1968	1971	1979	rVB	187048	214118	8.79%	1.007%
29	13.610	1989	1993	1996	rBV	710366	664766	27.30%	3.125%
30	13.816	2024	2028	2031	rBV5	23797	27356	1.12%	0.129%
31	14.116	2075	2079	2085	rBV	166626	206762	8.49%	0.972%
32	14.386	2123	2125	2127	rBV3	26609	25001	1.03%	0.118%
33	14.604	2158	2162	2168	rBV	60630	111885	4.59%	0.526%
34	14.692	2174	2177	2178	rBV3	37161	36997	1.52%	0.174%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.851	2201	2204	2211	rVB3	42986	69274	2.85%	0.326%
36	14.910	2211	2214	2217	rBV	45403	61613	2.53%	0.290%
37	14.957	2218	2222	2227	rBV	451927	521442	21.42%	2.451%
38	15.451	2305	2306	2310	rBV4	34657	44318	1.82%	0.208%
39	15.751	2355	2357	2359	rBV3	25577	34506	1.42%	0.162%
40	16.180	2429	2430	2436	rVB6	32804	33511	1.38%	0.158%
41	17.280	2614	2617	2622	rBV6	29701	65138	2.68%	0.306%

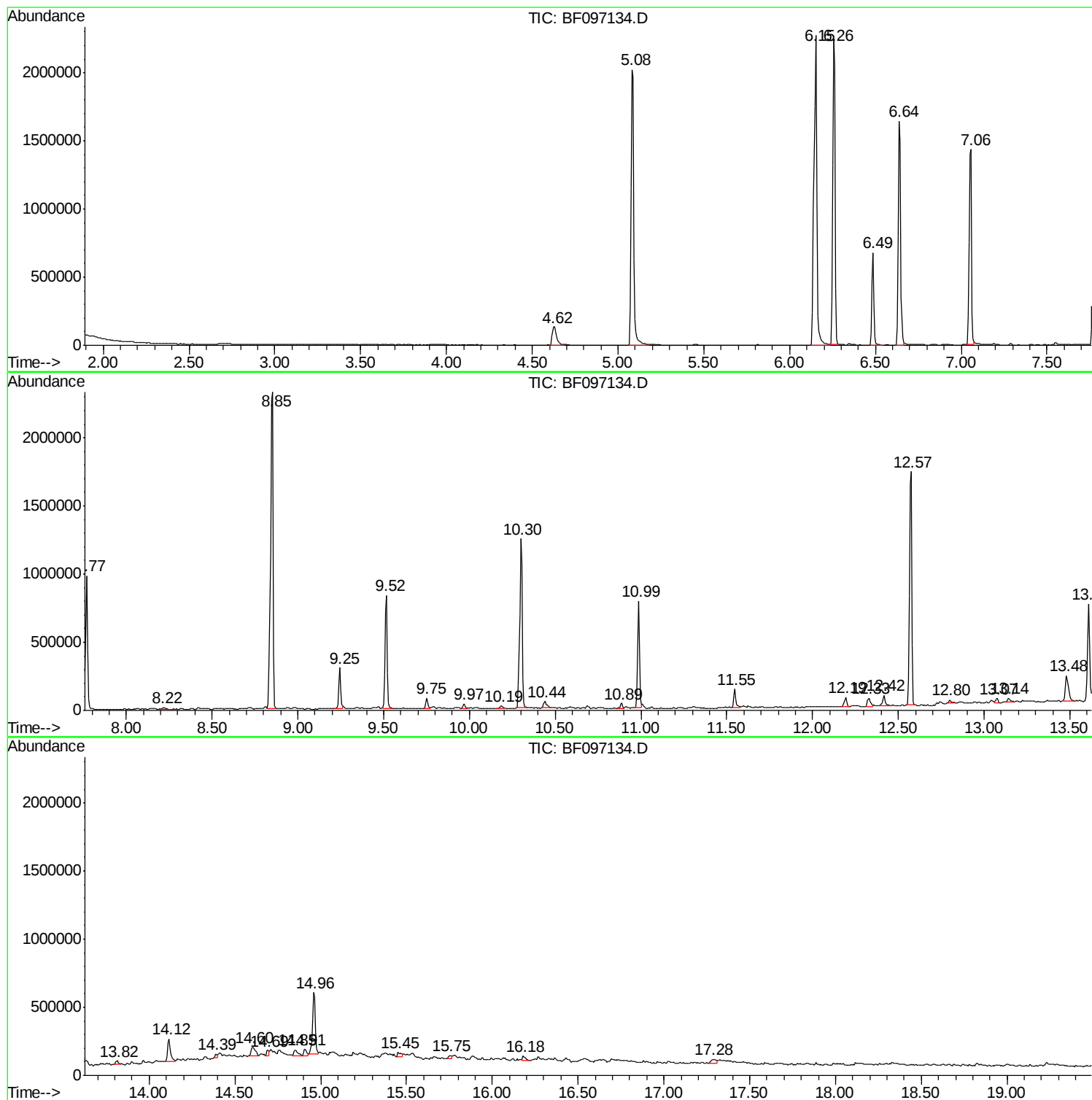
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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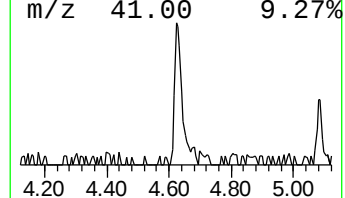
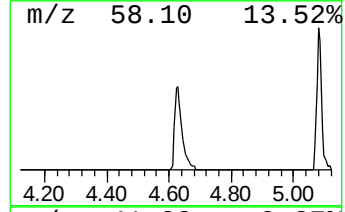
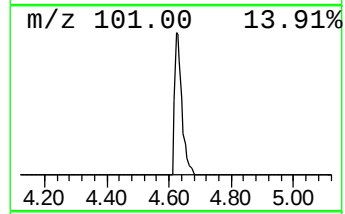
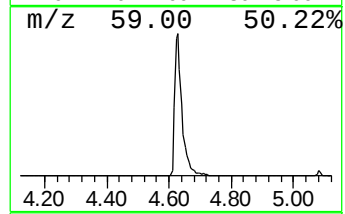
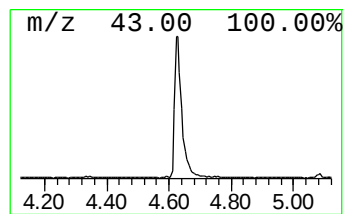
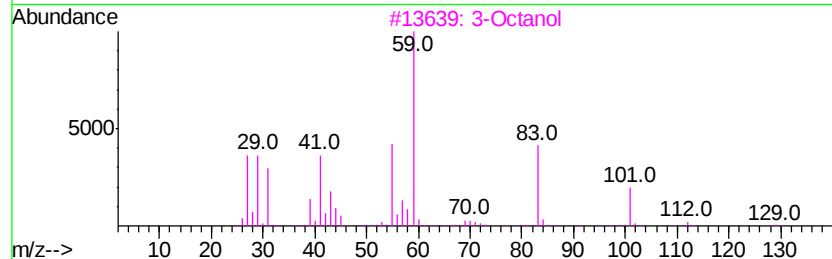
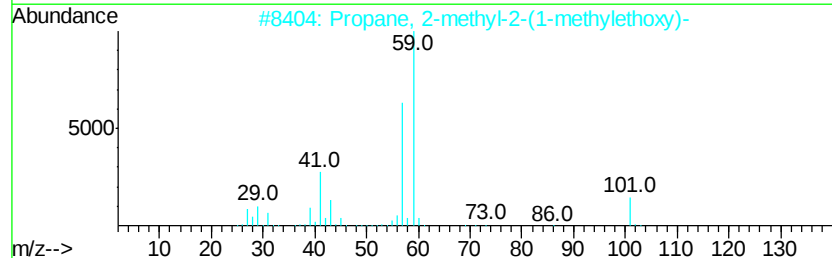
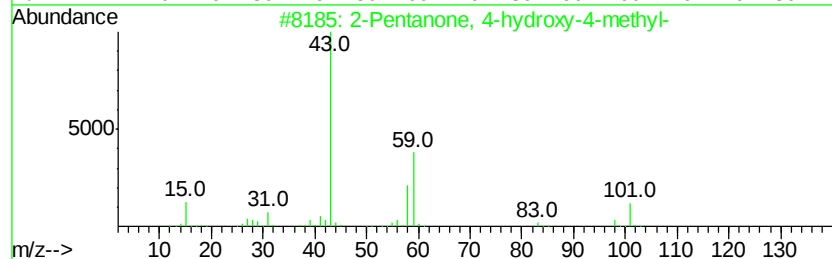
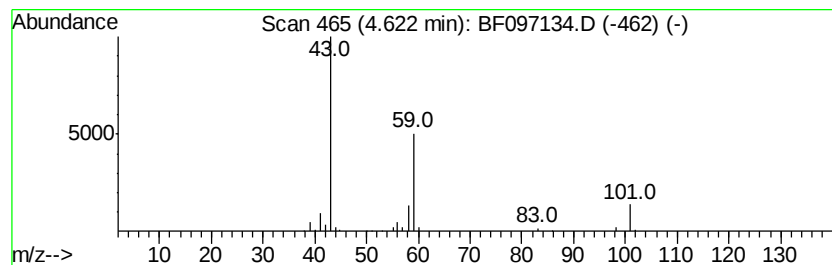
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.62	7.44 ng	215541	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Octanol	130	C8H18O	000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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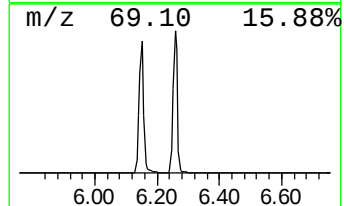
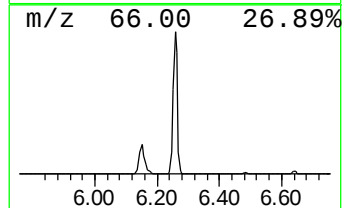
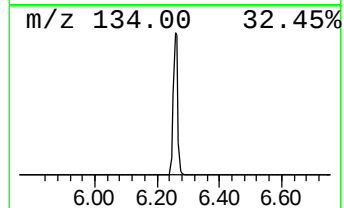
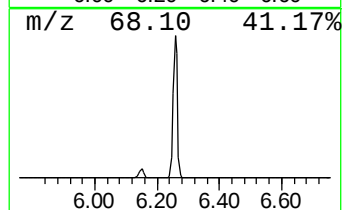
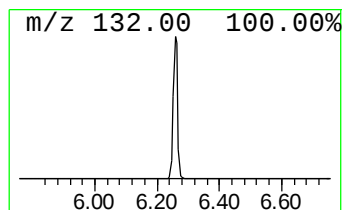
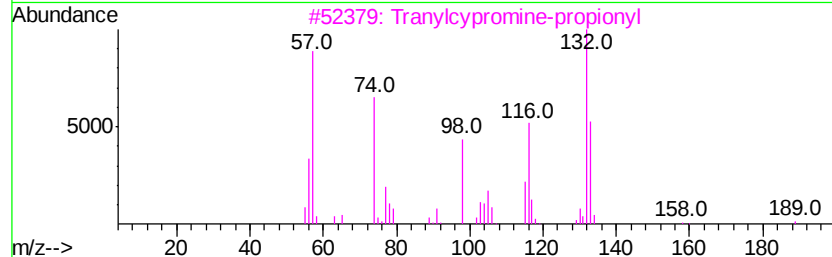
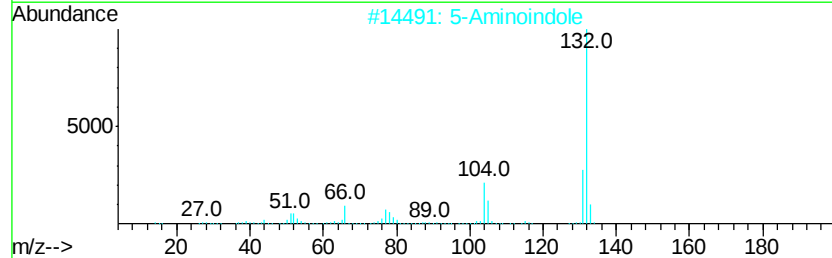
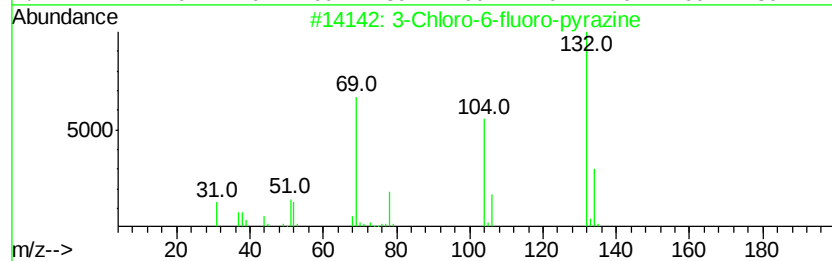
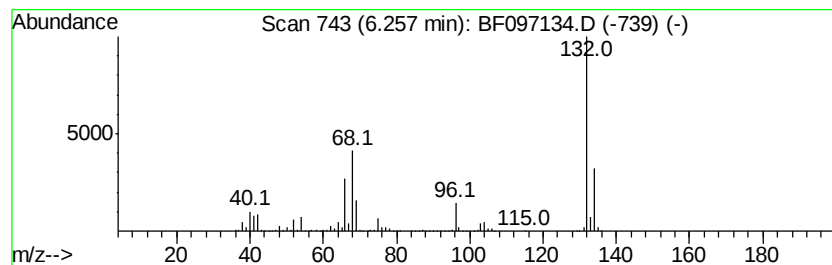
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	77.82 ng	2253800	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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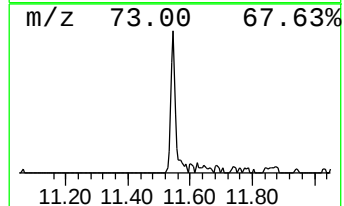
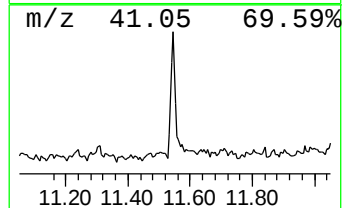
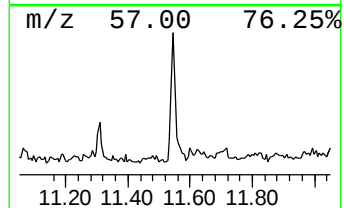
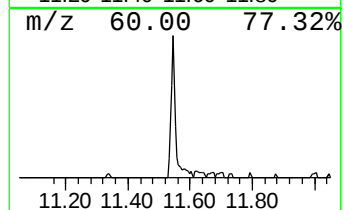
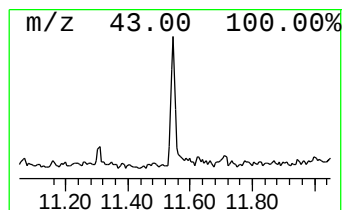
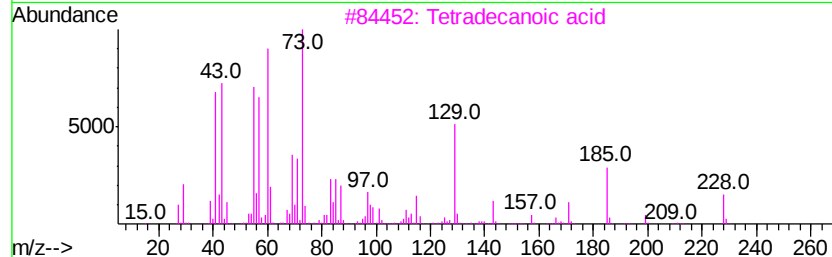
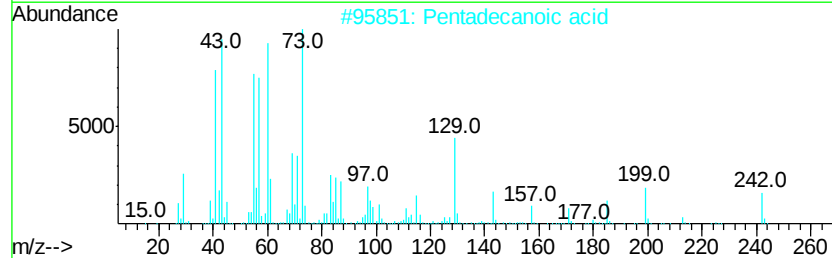
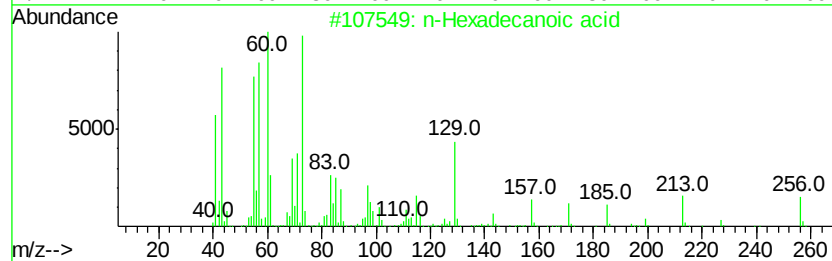
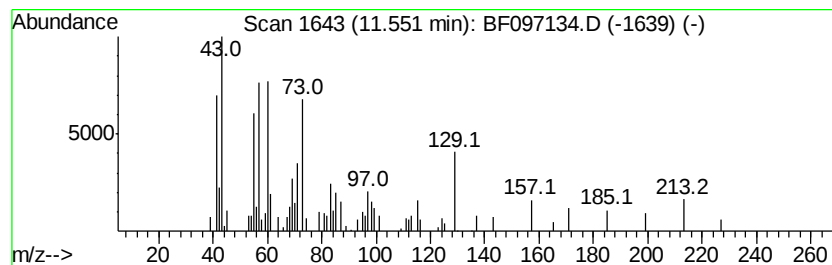
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	4.08 ng	131412	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Maltose	342	C12H22O11	000069-79-4	47



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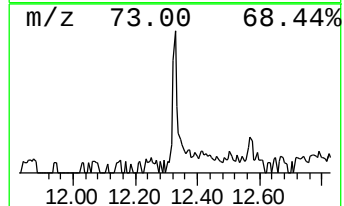
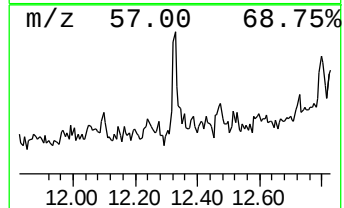
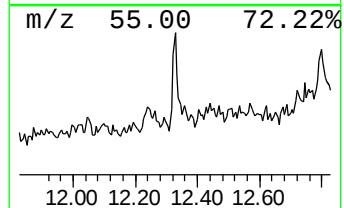
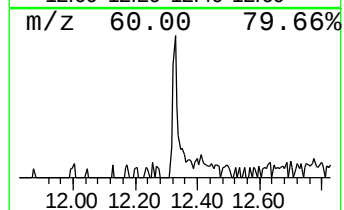
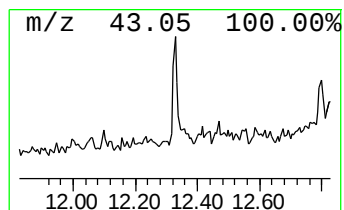
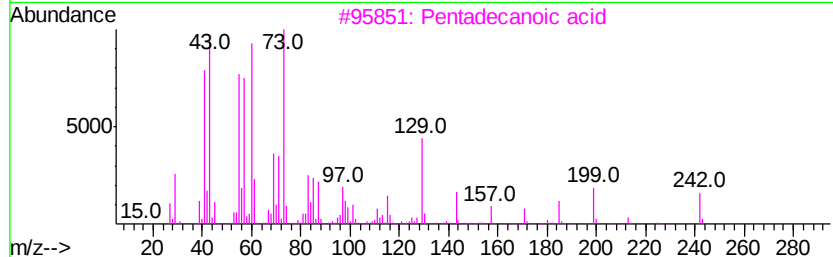
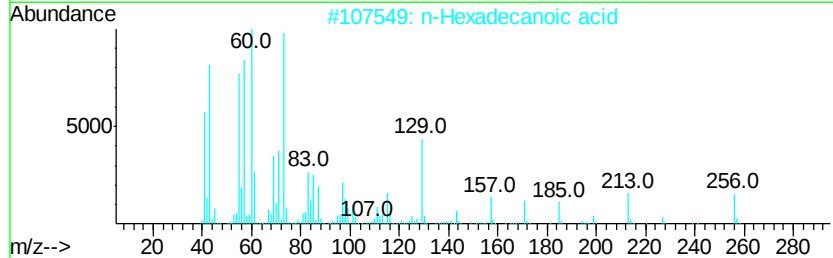
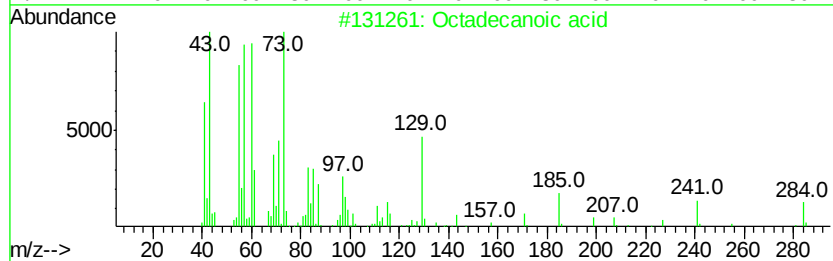
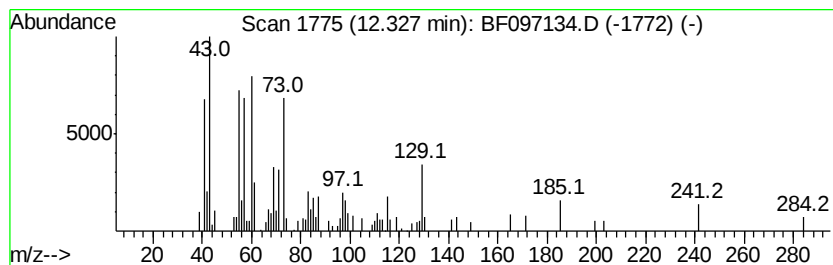
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	2.09 ng	69461	Chrysene-d12	13.61

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		Tridecanoic acid	214	C13H26O2	000638-53-9	58



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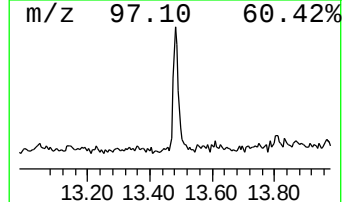
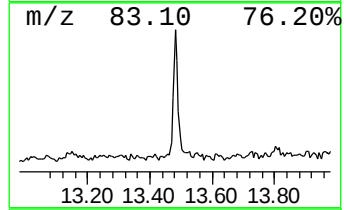
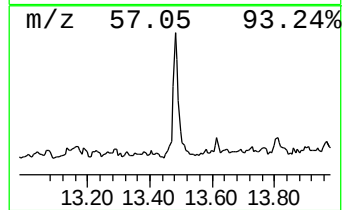
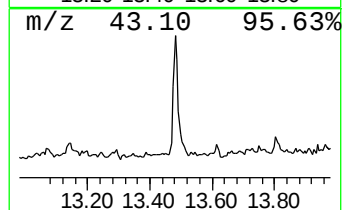
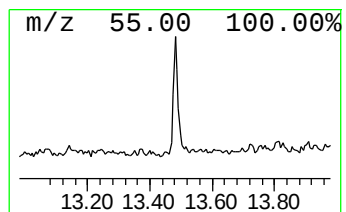
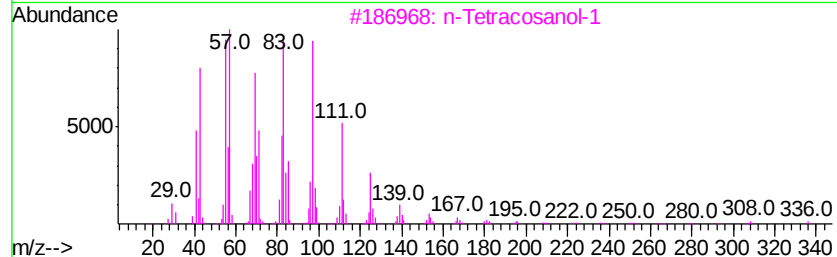
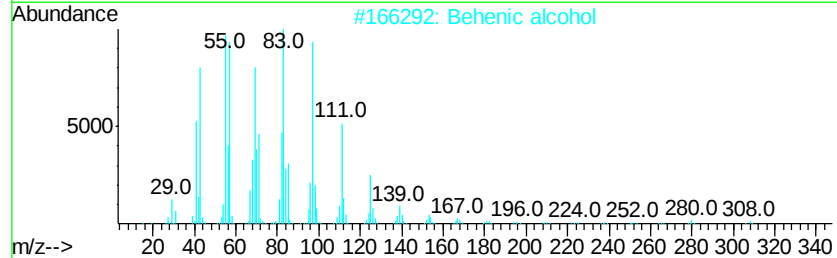
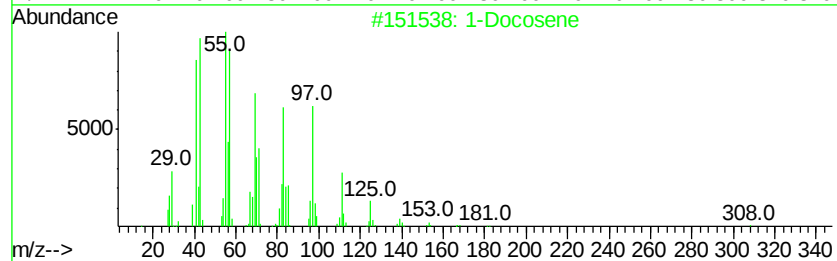
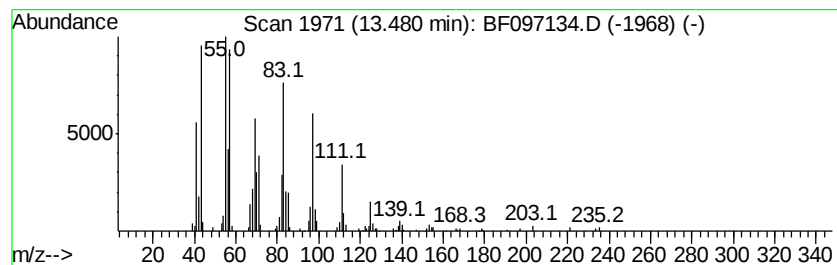
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	6.44 ng	214118	Chrysene-d12	13.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	95
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5		1-Octadecanol	270	C18H38O	000112-92-5	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072717\
Data File : BF097134.D
Acq On : 27 Jul 2017 20:41
Operator : SJ/JU
Sample : I4422-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-201-COMP

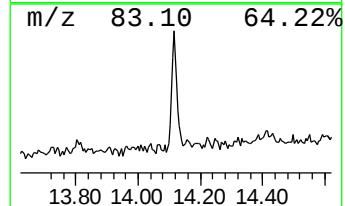
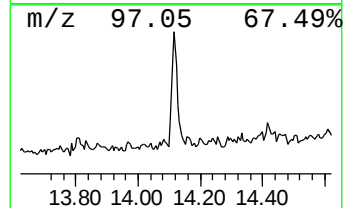
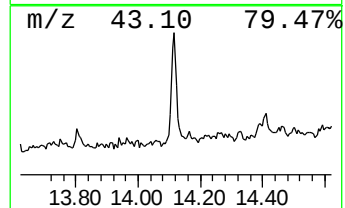
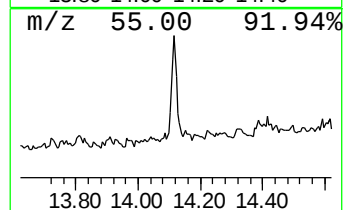
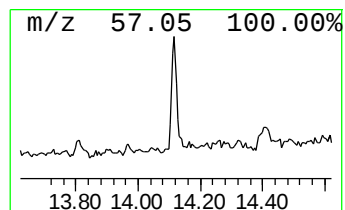
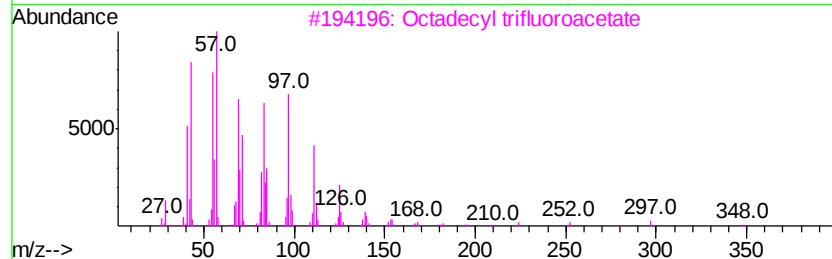
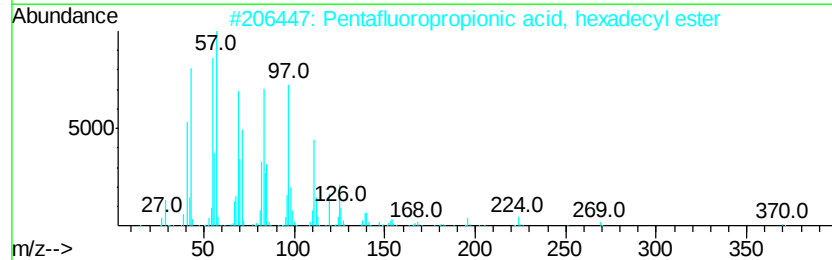
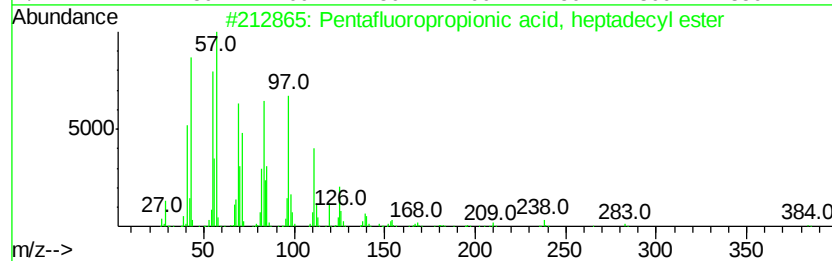
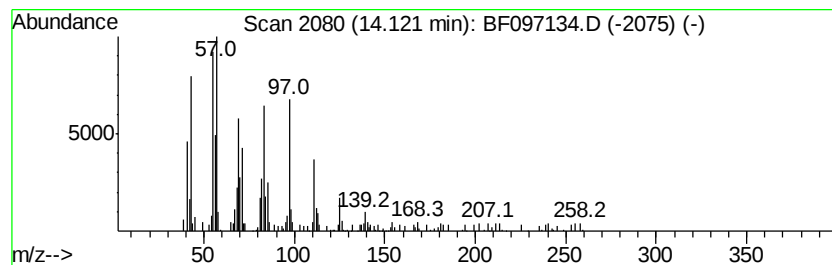
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.12	6.22 ng	206762	Chrysene-d12	13.61

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91



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Sample : I4422-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-201-COMP

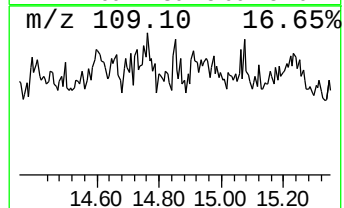
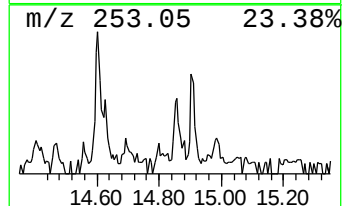
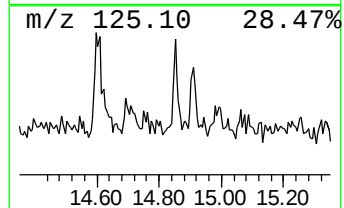
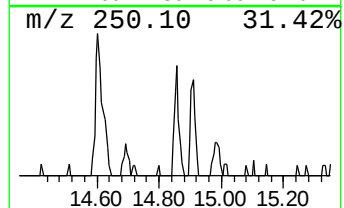
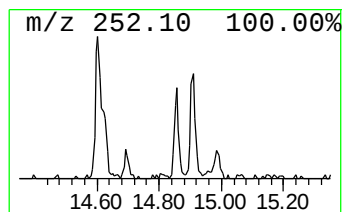
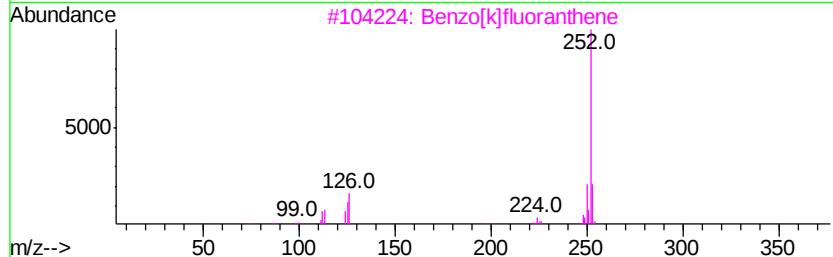
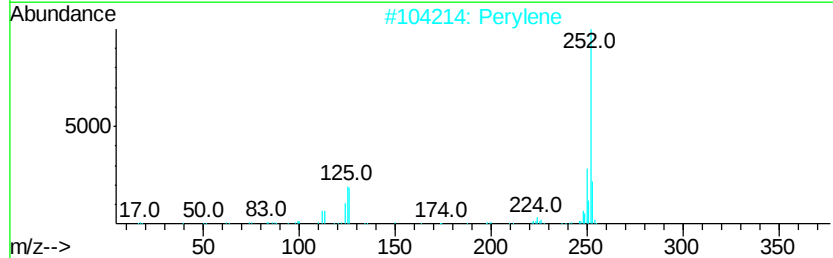
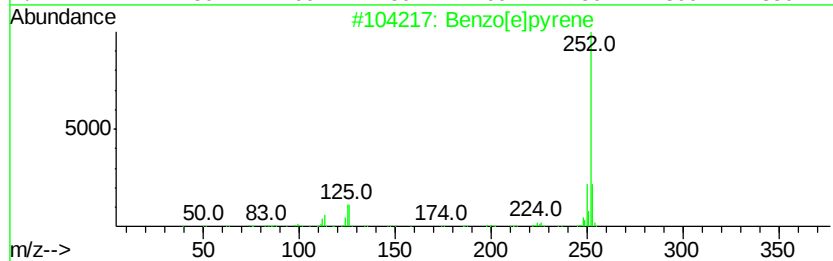
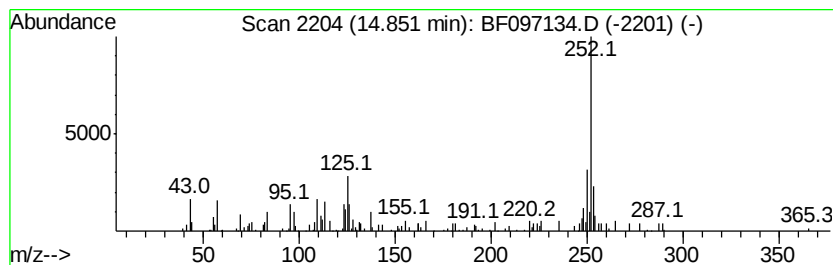
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	2.66 ng	69274	Perylene-d12	14.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	68
2		Perylene	252	C20H12	000198-55-0	64
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	64
4		Benzo[a]pyrene	252	C20H12	000050-32-8	60
5		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	58



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Sample : I4422-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-201-COMP

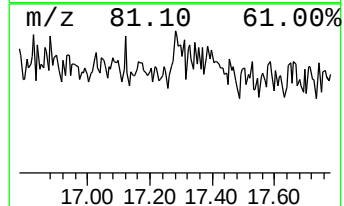
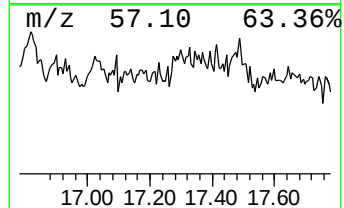
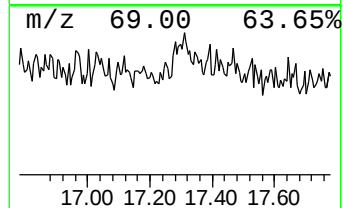
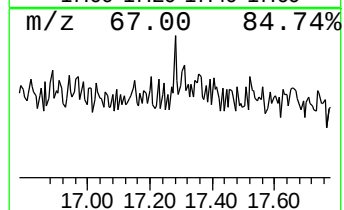
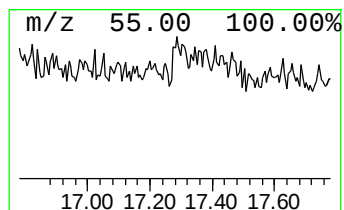
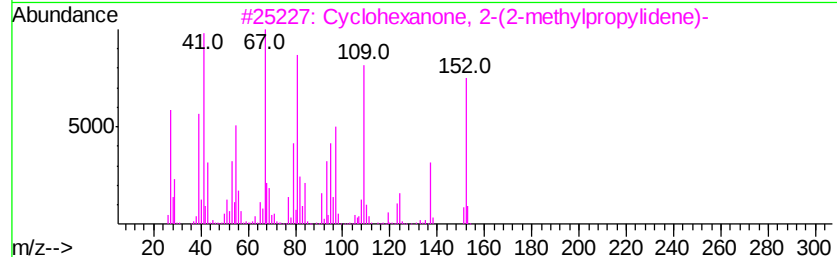
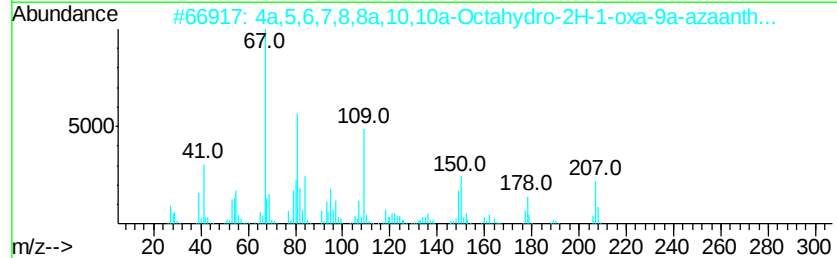
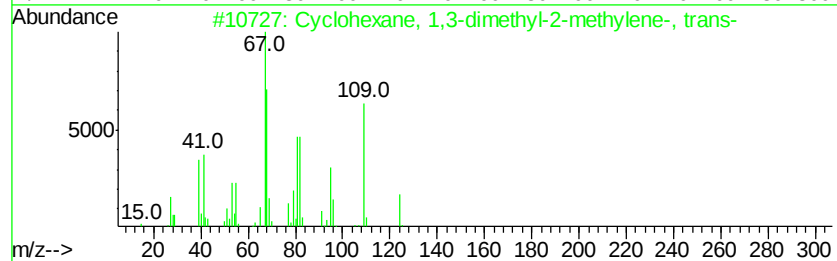
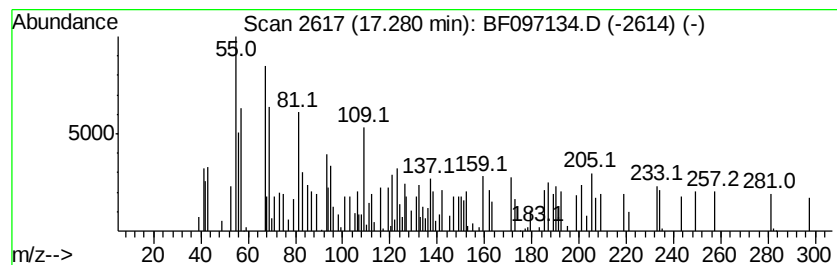
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.28 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.28	2.50 ng	65138	Perylene-d12	14.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,3-dimethyl-2-meth...	124	C9H16	020348-74-7	41
2		4a,5,6,7,8,8a,10,10a-Octahydro-2...	207	C12H17N02	1000194-96-9	38
3		Cyclohexanone, 2-(2-methylpropyl)-	152	C10H16O	043108-69-6	35
4		2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	35
5		3-Undecyne	152	C11H20	060212-30-8	35



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Sample : I4422-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-201-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.62	7.4	ng	215541	1	6.49	579249	20.0
unknown6.26	6.26	77.8	ng	2253800	1	6.49	579249	20.0
n-Hexadecanoic acid	11.55	4.1	ng	131412	4	10.99	644047	20.0
Octadecanoic acid	12.33	2.1	ng	69461	5	13.61	664766	20.0
1-Docosene	13.48	6.4	ng	214118	5	13.61	664766	20.0
Pentafluoropropio...	14.12	6.2	ng	206762	5	13.61	664766	20.0
Benzo[e]pyrene	14.85	2.7	ng	69274	6	14.96	521442	20.0
unknown17.28	17.28	2.5	ng	65138	6	14.96	521442	20.0