

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
 Data File : BF097113.D
 Acq On : 27 Jul 2017 9:02
 Operator : SJ/JU
 Sample : I4443-11
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-M7-NSW

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	4.640	465	468	478	rBV	217484	323214	12.55%	1.569%
2	4.716	478	481	488	rVB	32792	39822	1.55%	0.193%
3	5.098	541	546	570	rBV	2269448	2428228	94.32%	11.788%
4	6.157	722	726	737	rBV	2204285	2574440	100.00%	12.498%
5	6.239	737	740	741	rBV	52116	41074	1.60%	0.199%
6	6.269	741	745	748	rVB	2449354	2207193	85.73%	10.715%
7	6.492	780	783	791	rBV	760188	713087	27.70%	3.462%
8	6.651	806	810	820	rBV	1962756	1828224	71.01%	8.875%
9	6.828	836	840	844	rBV	37699	39811	1.55%	0.193%
10	7.063	872	880	883	rBV	1740173	1699995	66.03%	8.253%
11	7.275	912	916	919	rBV	28188	29270	1.14%	0.142%
12	7.780	998	1002	1005	rBV	823666	781435	30.35%	3.794%
13	8.492	1120	1123	1127	rVB	37585	31843	1.24%	0.155%
14	8.586	1136	1139	1143	rBV	51382	46772	1.82%	0.227%
15	8.857	1181	1185	1188	rBV	2056491	1775938	68.98%	8.622%
16	9.122	1226	1230	1235	rBV	24390	33602	1.31%	0.163%
17	9.192	1239	1242	1245	rBV2	35500	37568	1.46%	0.182%
18	9.257	1249	1253	1255	rVV	288336	259093	10.06%	1.258%
19	9.304	1259	1261	1267	rVB7	19363	27209	1.06%	0.132%
20	9.522	1294	1298	1303	rBV	764677	753019	29.25%	3.656%
21	9.980	1373	1376	1381	rVB	58402	45920	1.78%	0.223%
22	10.198	1409	1413	1416	rVB2	28456	38061	1.48%	0.185%
23	10.310	1428	1432	1442	rBV	1234392	1151000	44.71%	5.588%
24	10.451	1453	1456	1457	rBV	43491	37761	1.47%	0.183%
25	10.927	1534	1537	1542	rVB	30974	35404	1.38%	0.172%
26	10.998	1545	1549	1552	rBV	730343	598915	23.26%	2.908%
27	11.074	1559	1562	1568	rBV3	25157	43577	1.69%	0.212%
28	11.557	1641	1644	1647	rBV	83038	76301	2.96%	0.370%
29	11.639	1656	1658	1663	rVB4	24409	25789	1.00%	0.125%
30	11.739	1671	1675	1680	rVB4	126855	135931	5.28%	0.660%
31	11.857	1691	1695	1700	rBV	89066	80455	3.13%	0.391%
32	12.204	1750	1754	1758	rBV	20549	32249	1.25%	0.157%
33	12.427	1789	1792	1798	rBV	135954	132191	5.13%	0.642%
34	12.580	1814	1818	1822	rBV	1068791	1037200	40.29%	5.035%

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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	12.963	1880	1883	1888	rBV5	24601	36958	1.44%	0.179%
36	13.133	1909	1912	1915	rBV	84688	84970	3.30%	0.413%
37	13.251	1929	1932	1934	rBV3	28755	37968	1.47%	0.184%
38	13.498	1971	1974	1982	rVB2	73934	101973	3.96%	0.495%
39	13.621	1992	1995	1999	rBV	476100	500334	19.43%	2.429%
40	14.127	2078	2081	2087	rBV7	27006	42148	1.64%	0.205%
41	14.292	2101	2109	2111	rBV9	40367	108244	4.20%	0.525%
42	14.415	2128	2130	2134	rVB2	35353	41707	1.62%	0.202%
43	14.974	2221	2225	2232	rBV	361048	419874	16.31%	2.038%
44	15.427	2299	2302	2306	rBV6	24978	45956	1.79%	0.223%
45	15.927	2383	2387	2389	rBV5	27852	36872	1.43%	0.179%

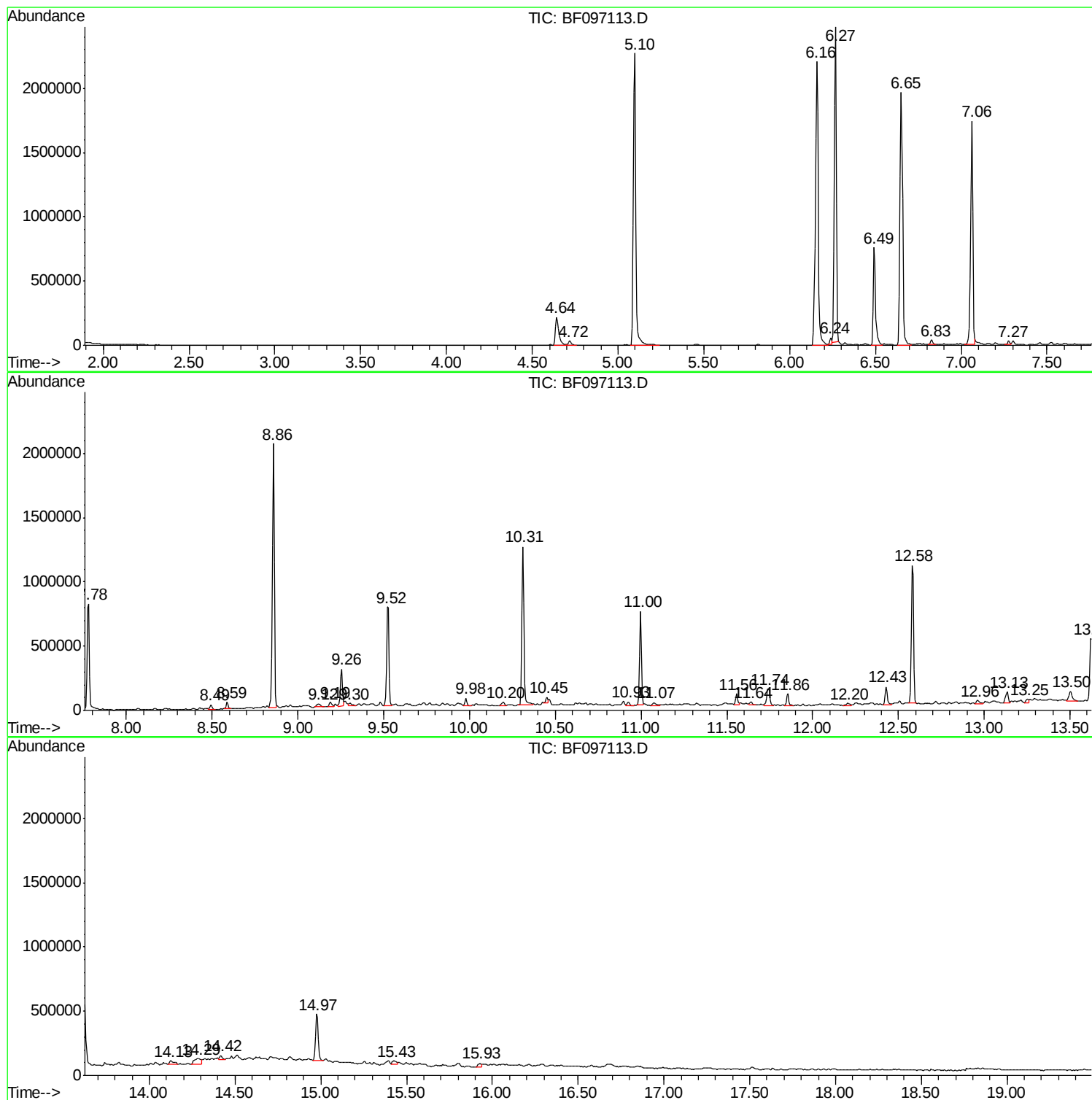
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
E2-M7-NSW

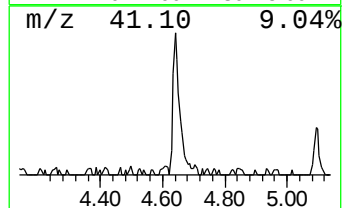
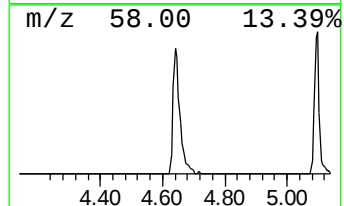
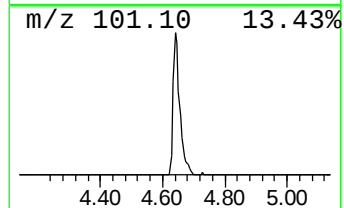
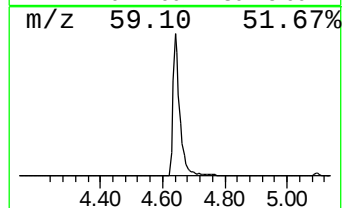
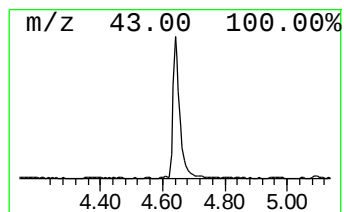
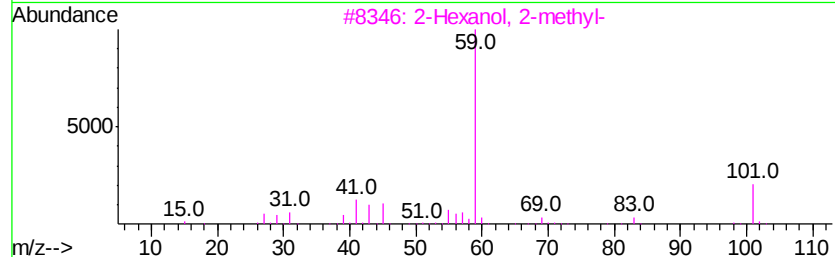
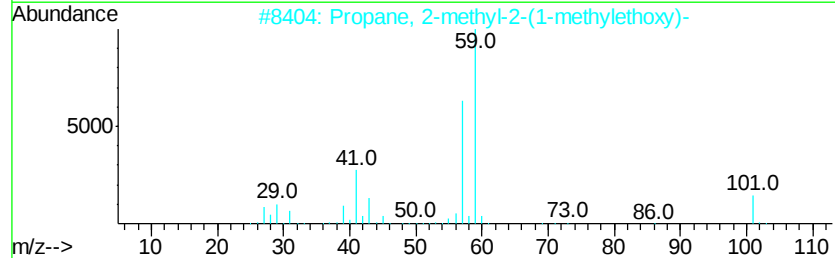
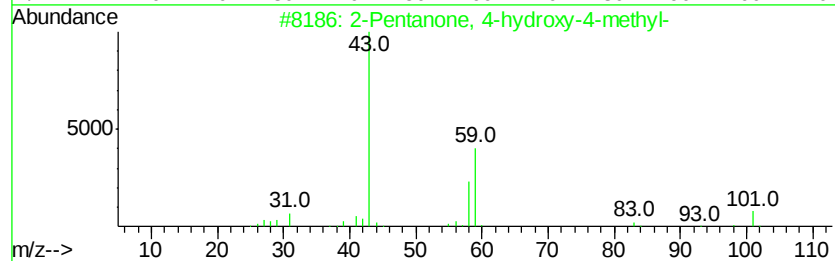
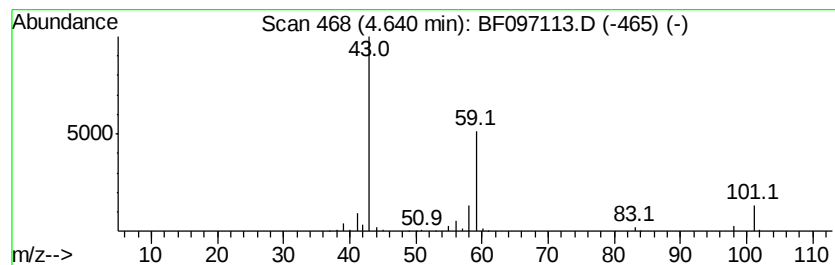
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	9.07 ng	323214	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
5		Hexanamide	115	C6H13NO	000628-02-4	9



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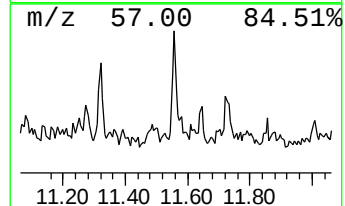
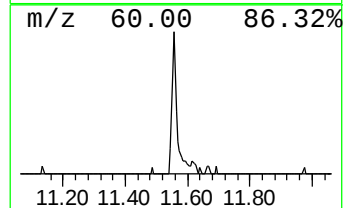
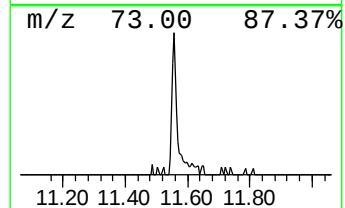
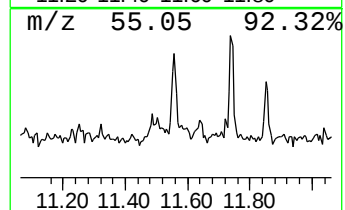
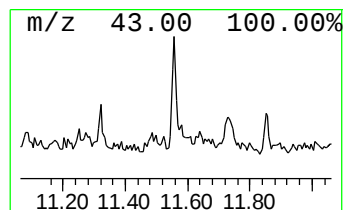
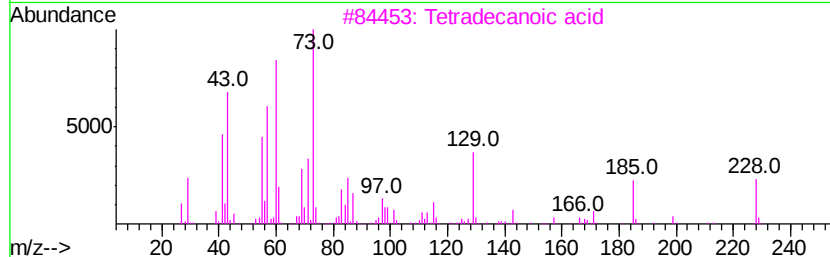
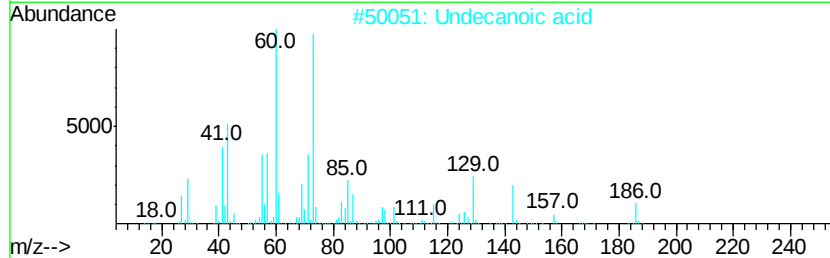
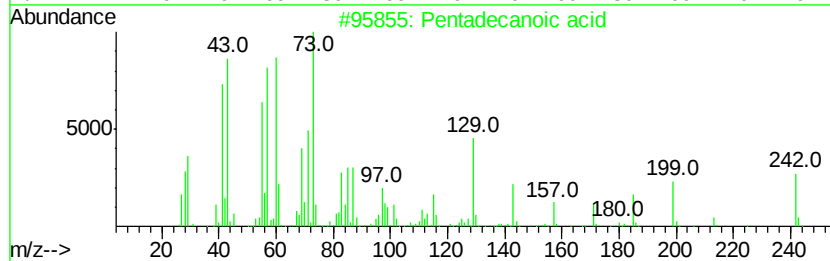
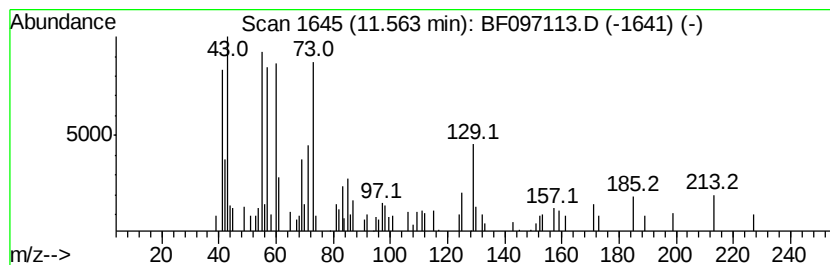
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.56	2.55 ng	76301	Phenanthrene-d10		11.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2	Undecanoic acid	186	C11H22O2	000112-37-8	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64



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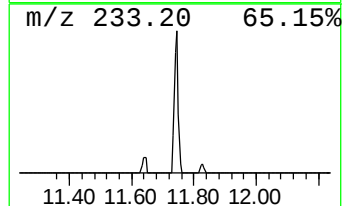
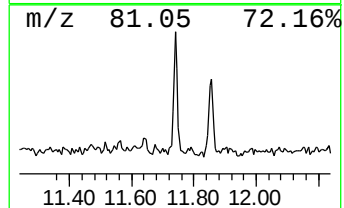
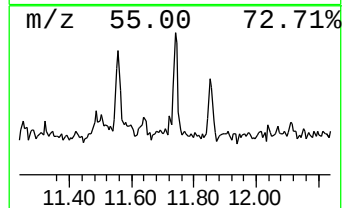
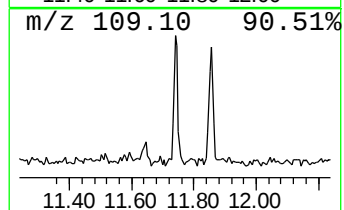
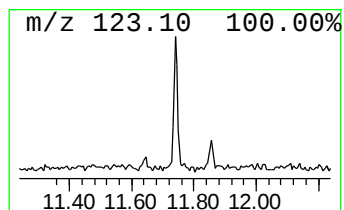
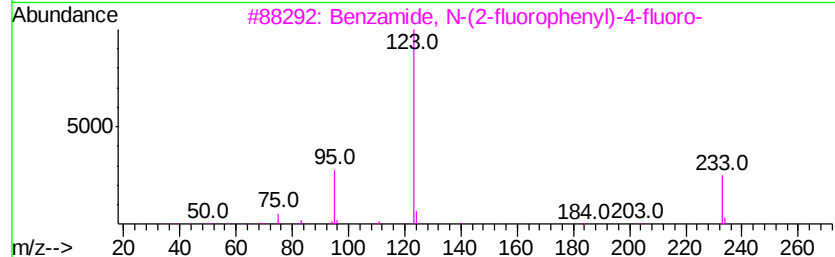
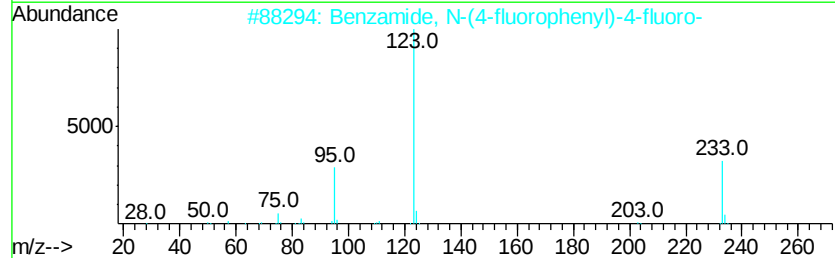
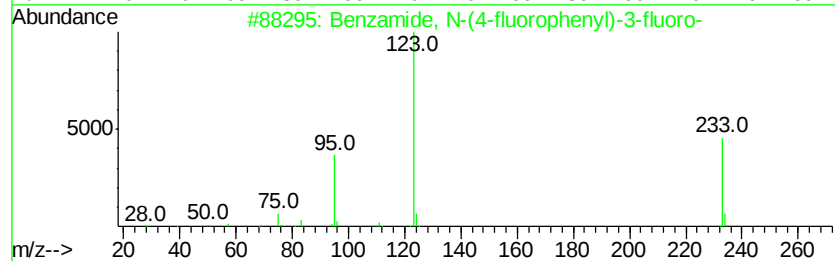
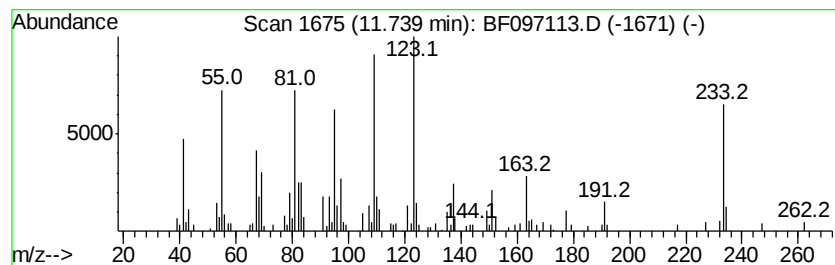
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown11.74 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	4.54 ng	135931	Phenanthrene-d10	11.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-(4-fluorophenyl)-3-...	233	C13H9F2NO	1000307-16-3	35
2			Benzamide, N-(4-fluorophenyl)-4-...	233	C13H9F2NO	1000307-10-1	35
3			Benzamide, N-(2-fluorophenyl)-4-...	233	C13H9F2NO	1000308-30-2	35
4			Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	27
5			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	25



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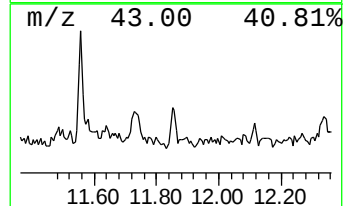
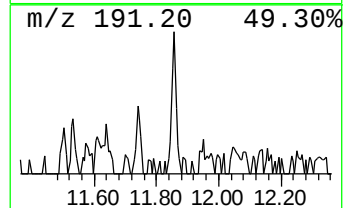
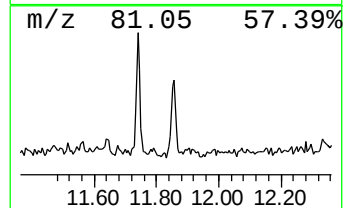
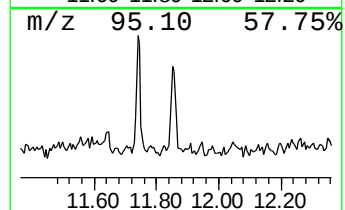
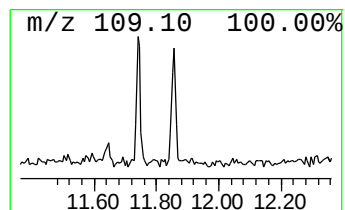
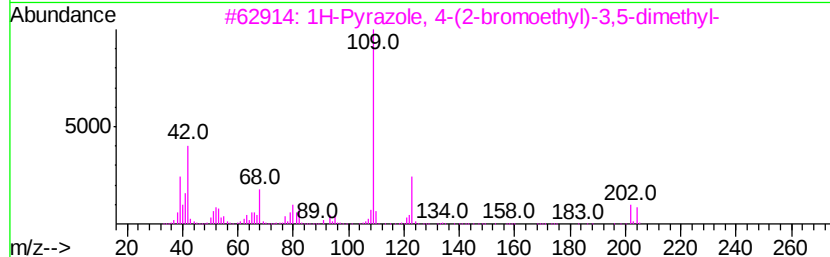
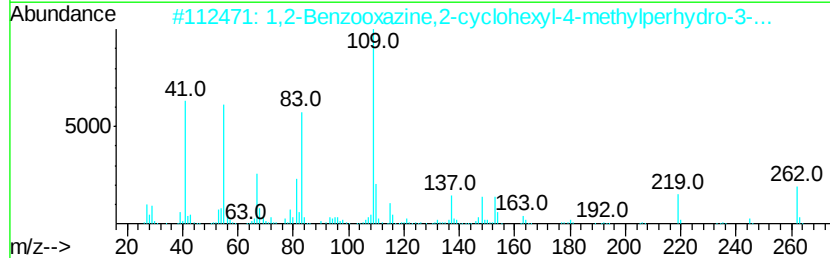
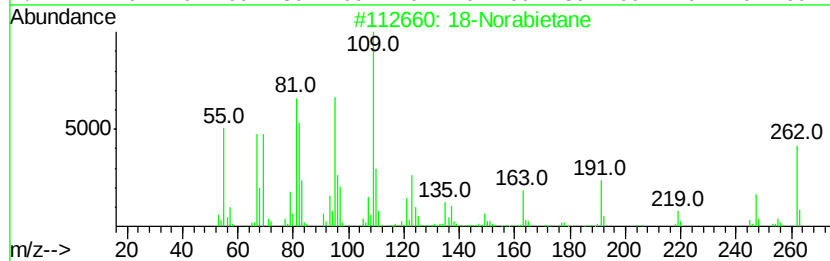
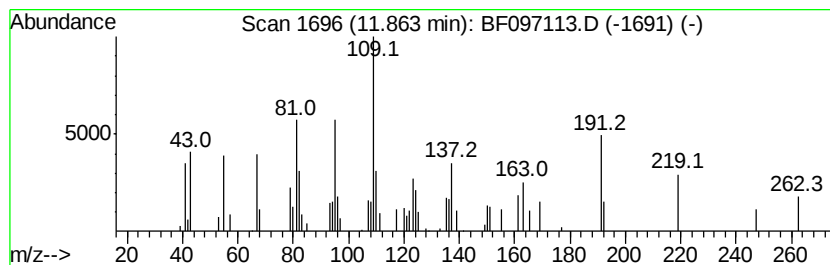
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 18-Norabietane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.69 ng	80455	Phenanthrene-d10	11.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	18-Norabietane		262	C19H34	1000293-16-6	81
2	1,2-Benzooxazine,2-cyclohexyl-4-...		262	C16H26N2O	037898-39-8	38
3	1H-Pyrazole, 4-(2-bromoethyl)-3,...		202	C7H11BrN2	083467-28-1	27
4	Ketone, isopropylidenecyclopropyl...		124	C8H12O	029765-67-1	25
5	Cyclopentane, 2-ethylidene-1,1-d...		124	C9H16	056324-66-4	22



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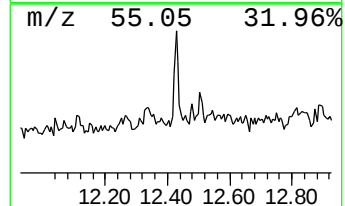
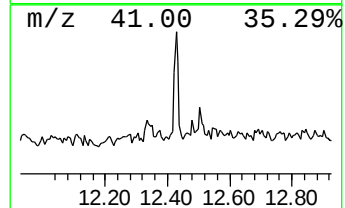
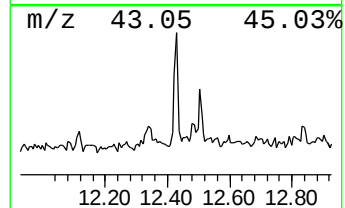
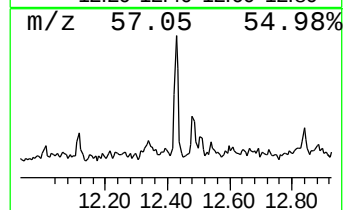
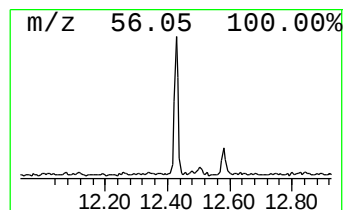
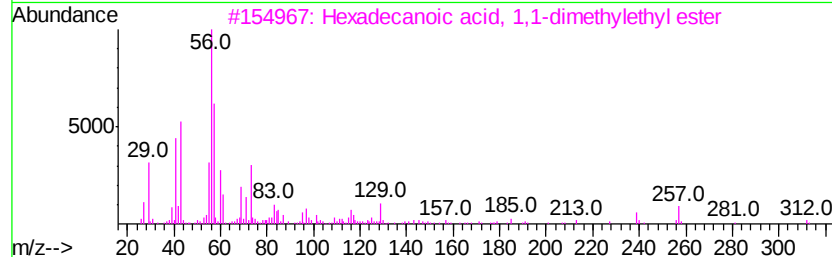
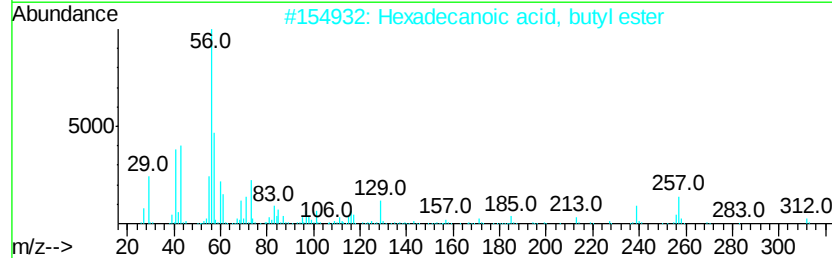
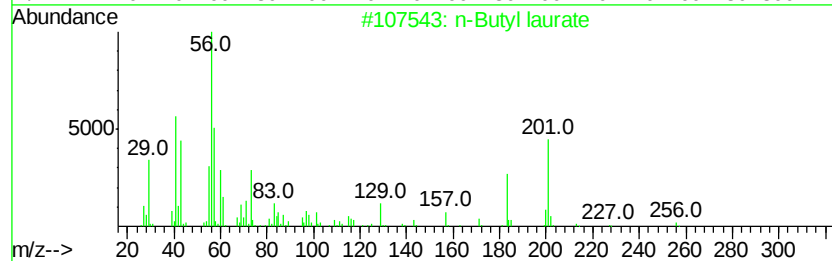
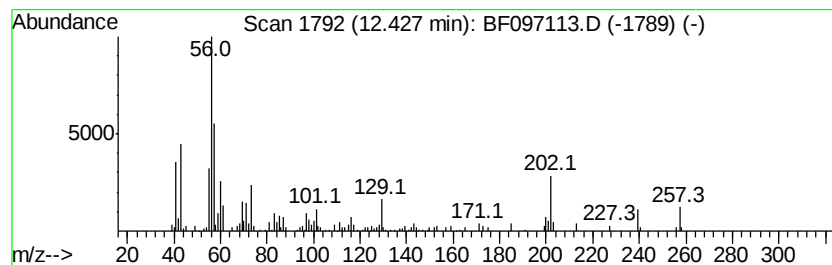
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E2-M7-NSW

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 6 n-Butyl laurate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.43	5.28 ng	132191	Chrysene-d12	13.63		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Butyl laurate	256	C16H32O2	000106-18-3	90
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
4		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	43
5		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097113.D
Acq On : 27 Jul 2017 9:02
Operator : SJ/JU
Sample : I4443-11
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-NSW

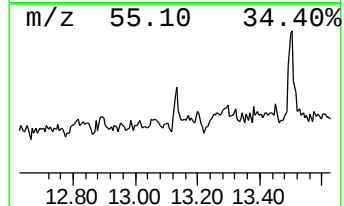
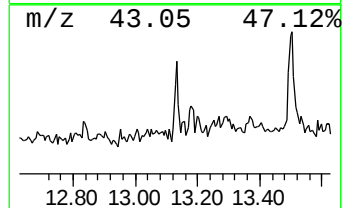
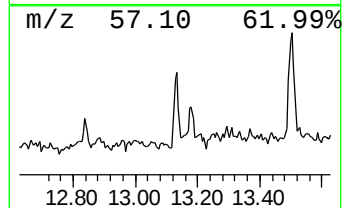
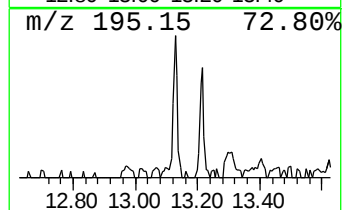
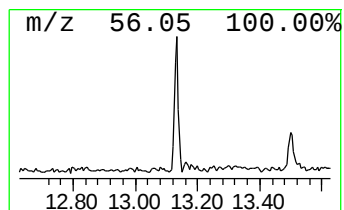
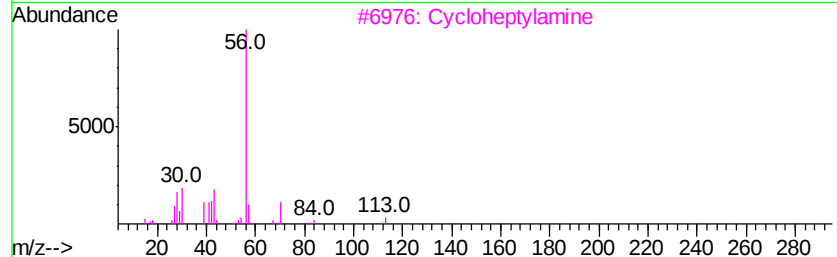
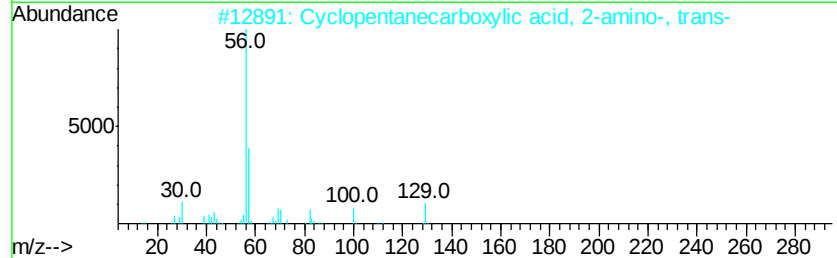
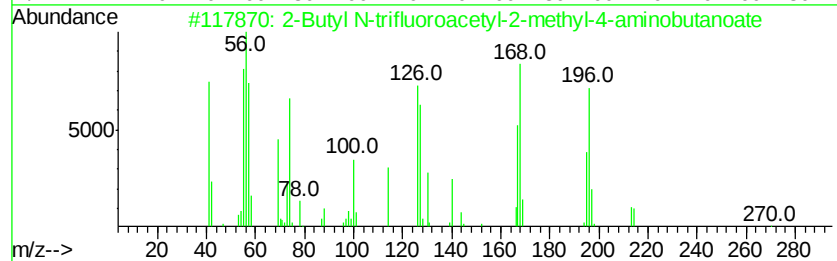
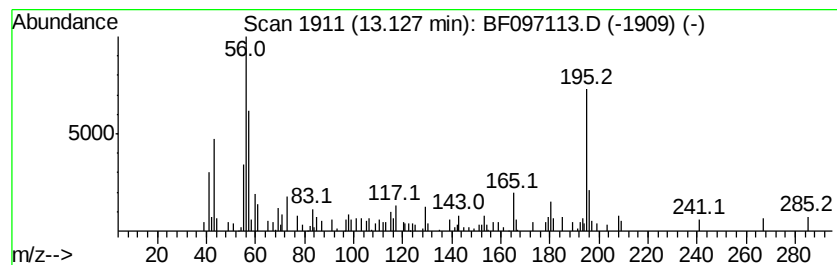
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.13 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	3.40 ng	84970	Chrysene-d12	13.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butyl N-trifluoroacetyl-2-meth...	269	C11H18F3NO3	083556-41-6	35
2		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	35
3		Cycloheptylamine	113	C7H15N	005452-35-7	25
4		Butyl myristate	284	C18H36O2	000110-36-1	25
5		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	25



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Sample : I4443-11
Misc :
ALS Vial : 31 Sample Multiplier: 1

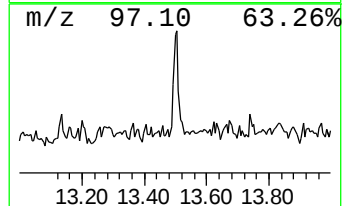
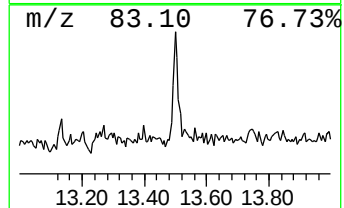
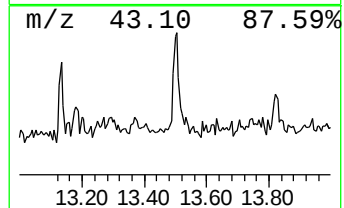
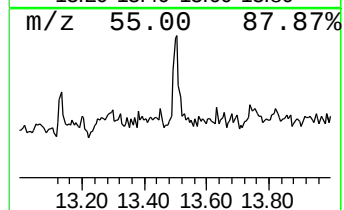
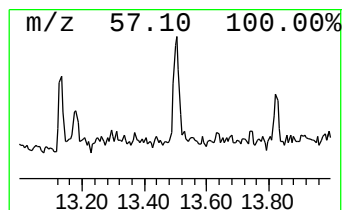
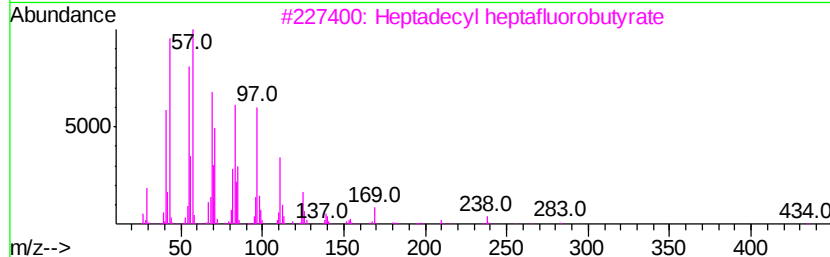
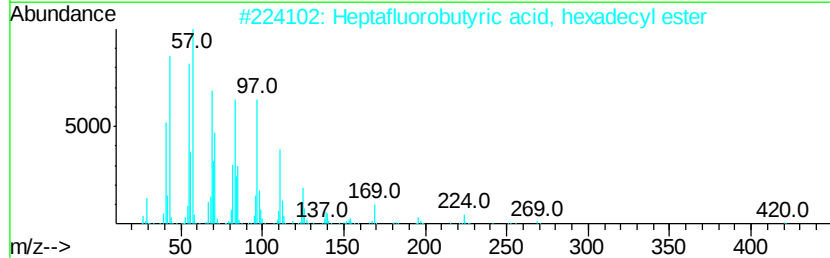
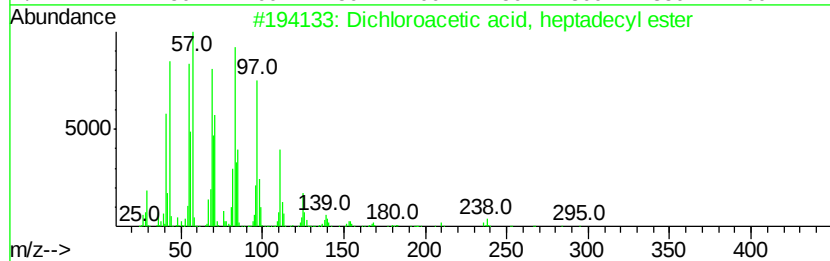
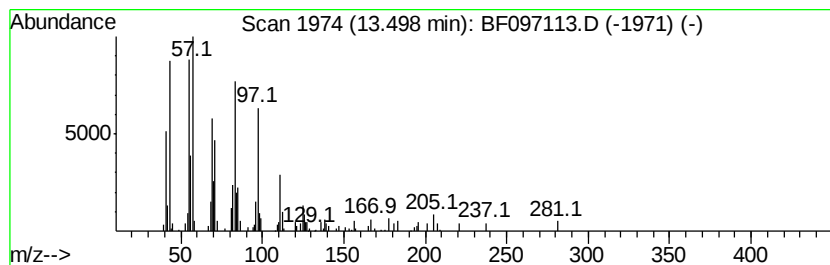
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.50	4.08 ng	101973	Chrysene-d12	13.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	81
3	Heptadecyl heptafluorobutyrat	452	C21H35F7O2	959085-66-6	81
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	68



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Sample : I4443-11
Misc :
ALS Vial : 31 Sample Multiplier: 1

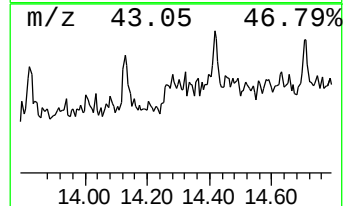
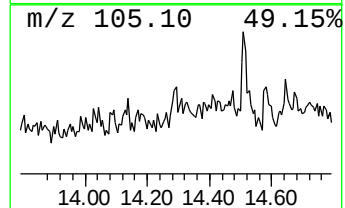
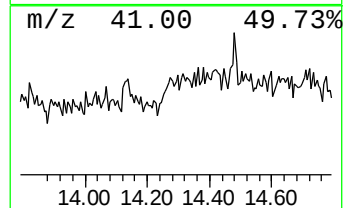
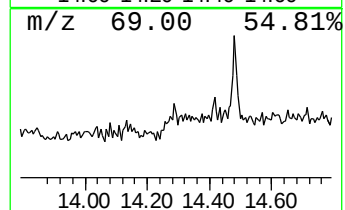
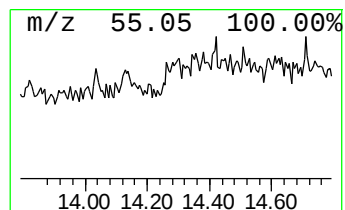
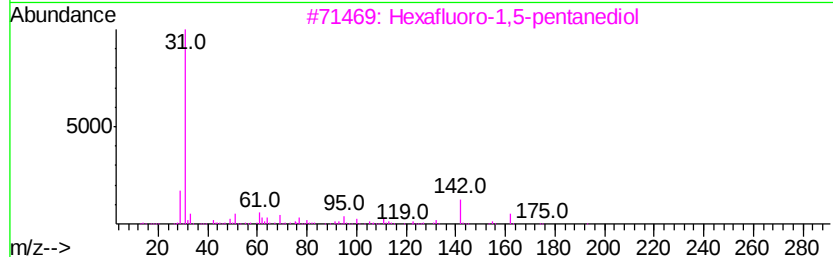
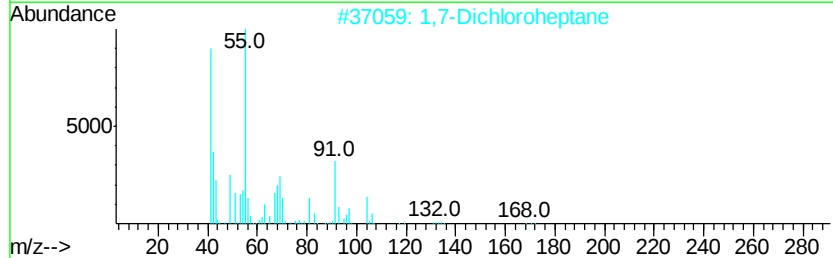
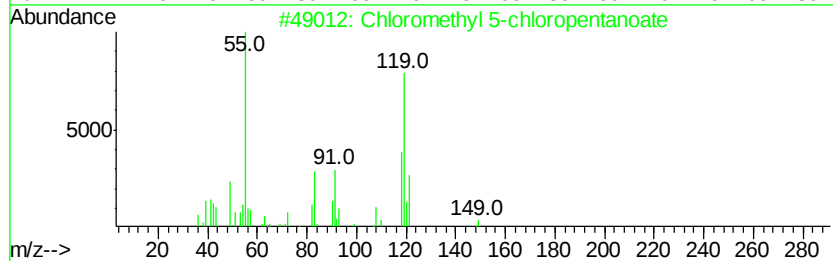
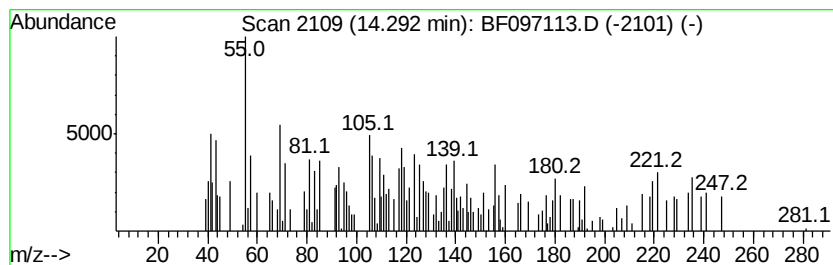
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 9 unknown14.29 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.29	4.33 ng	108244	Chrysene-d12	13.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chloromethyl 5-chloropentanoate	184	C6H10Cl2O2	080482-35-5	12
2	1,7-Dichloroheptane	168	C7H14Cl2	000821-76-1	9
3	Hexafluoro-1,5-pentanediol	212	C5H6F6O2	000376-90-9	9
4	Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	9
5	Propane, 1,3-dichloro-2-methyl-	126	C4H8Cl2	000616-19-3	9



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Sample : I4443-11
Misc :
ALS Vial : 31 Sample Multiplier: 1

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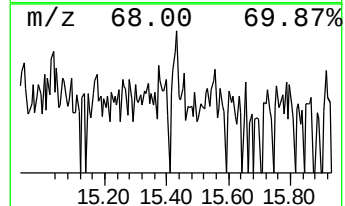
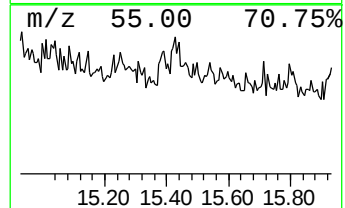
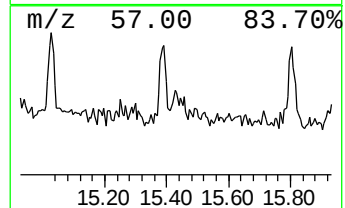
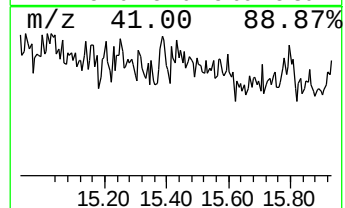
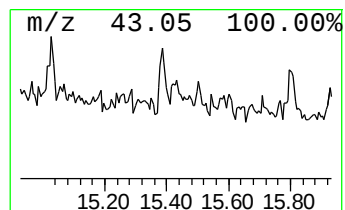
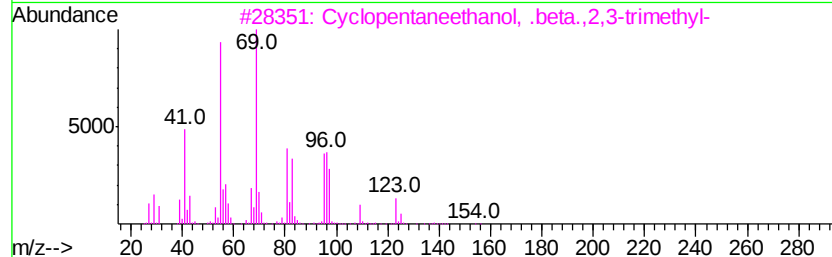
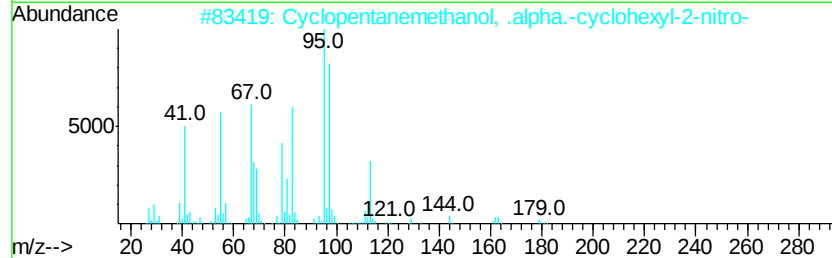
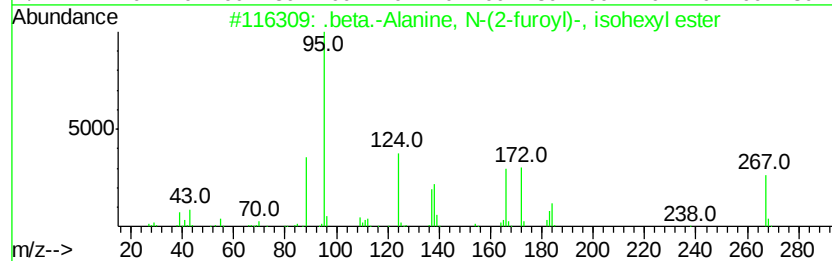
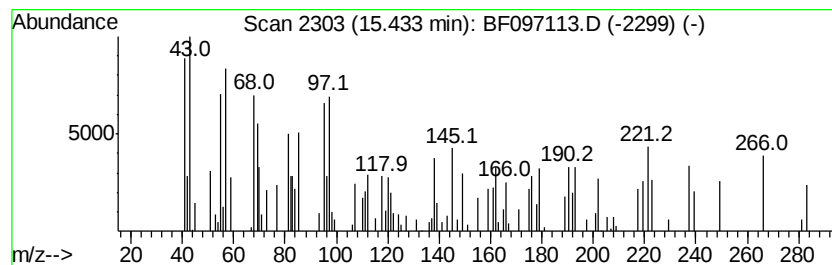
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown15.43 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.43	2.19 ng	45956	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Alanine, N-(2-furoyl)-, i...	267	C14H21N04	1000321-97-6	22
2		Cyclopentanemethanol, .alpha.-cy...	227	C12H21N03	103077-58-3	12
3		Cyclopentaneethanol, .beta.,2,3-...	156	C10H20O	021721-18-6	12
4		E-8-Methyl-7-dodecen-1-ol acetate	240	C15H28O2	1000131-32-2	12
5		6-Octenoic acid, 3,7-dimethyl-	170	C10H18O2	000502-47-6	11



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Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.64	9.1 ng		323214	1	6.49	713087	20.0
Pentadecanoic acid	11.56	2.5 ng		76301	4	11.00	598915	20.0
unknown11.74	11.74	4.5 ng		135931	4	11.00	598915	20.0
18-Norabietane	11.86	2.7 ng		80455	4	11.00	598915	20.0
n-Butyl laurate	12.43	5.3 ng		132191	5	13.63	500334	20.0
unknown13.13	13.13	3.4 ng		84970	5	13.63	500334	20.0
Dichloroacetic ac...	13.50	4.1 ng		101973	5	13.63	500334	20.0
unknown14.29	14.29	4.3 ng		108244	5	13.63	500334	20.0
unknown15.43	15.43	2.2 ng		45956	6	14.97	419874	20.0