

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020718\
 Data File : BF102835.D
 Acq On : 8 Feb 2018 00:50
 Operator : SJ/JU
 Sample : J1473-09
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B3

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-BF020318.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	2.175	9	15	27	rVB	469341	639734	12.95%	1.452%
2	3.452	229	232	255	rBV	269339	594020	12.03%	1.348%
3	5.122	513	516	525	rVB	141300	183944	3.72%	0.417%
4	5.510	576	582	585	rBV	4487447	4938995	100.00%	11.209%
5	6.516	747	753	756	rBV	4203189	4763188	96.44%	10.810%
6	6.657	772	777	780	rBV	4728727	4741073	95.99%	10.759%
7	6.887	812	816	819	rBV	1331637	1156904	23.42%	2.626%
8	7.040	838	842	846	rBV	3786069	3619212	73.28%	8.214%
9	7.445	906	911	914	rBV	2884123	3070107	62.16%	6.967%
10	8.169	1030	1034	1037	rBV	1643279	1473395	29.83%	3.344%
11	9.245	1211	1217	1220	rBV	4289781	4372385	88.53%	9.923%
12	9.316	1226	1229	1231	rVB	103463	77652	1.57%	0.176%
13	9.633	1279	1283	1285	rBV	247639	242948	4.92%	0.551%
14	9.845	1311	1319	1322	rBV	257396	213850	4.33%	0.485%
15	9.922	1328	1332	1336	rBV2	1578561	1406595	28.48%	3.192%
16	10.169	1371	1374	1378	rBV2	45810	50026	1.01%	0.114%
17	10.345	1401	1404	1407	rVB	276978	205443	4.16%	0.466%
18	10.563	1436	1441	1444	rBV	69828	91913	1.86%	0.209%
19	10.710	1462	1466	1477	rVB	2273252	2294191	46.45%	5.206%
20	10.816	1481	1484	1493	rVB	203392	236579	4.79%	0.537%
21	11.269	1557	1561	1563	rBV	105744	86637	1.75%	0.197%
22	11.298	1563	1566	1572	rVB3	43504	59716	1.21%	0.136%
23	11.410	1581	1585	1588	rBV	1395214	1231898	24.94%	2.796%
24	11.433	1588	1589	1593	rVB	263502	153663	3.11%	0.349%
25	11.639	1617	1624	1630	rBV	44941	64363	1.30%	0.146%
26	11.927	1667	1673	1681	rBV3	251937	298259	6.04%	0.677%
27	12.027	1687	1690	1696	rVB2	42567	56869	1.15%	0.129%
28	12.621	1788	1791	1795	rBV	415586	340862	6.90%	0.774%
29	12.804	1819	1822	1825	rBV2	65070	62719	1.27%	0.142%
30	12.851	1825	1830	1834	rBV	305694	325226	6.58%	0.738%
31	12.998	1850	1855	1860	rVB	3293786	3606663	73.02%	8.185%
32	13.880	2001	2005	2013	rVB	518916	571335	11.57%	1.297%
33	14.051	2029	2034	2037	rBV	1124164	1136303	23.01%	2.579%
34	14.074	2037	2038	2043	rVB	161242	106264	2.15%	0.241%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.145	2048	2050	2055	rVB3	51346	56894	1.15%	0.129%
36	14.510	2110	2112	2118	rVB4	62523	70786	1.43%	0.161%
37	14.668	2136	2139	2144	rVB	404871	358145	7.25%	0.813%
38	15.092	2208	2211	2215	rBV	101981	151099	3.06%	0.343%
39	15.157	2220	2222	2227	rVB2	55555	63997	1.30%	0.145%
40	15.468	2272	2275	2281	rVB	58588	69978	1.42%	0.159%
41	15.533	2281	2286	2295	rBV	583472	820274	16.61%	1.862%

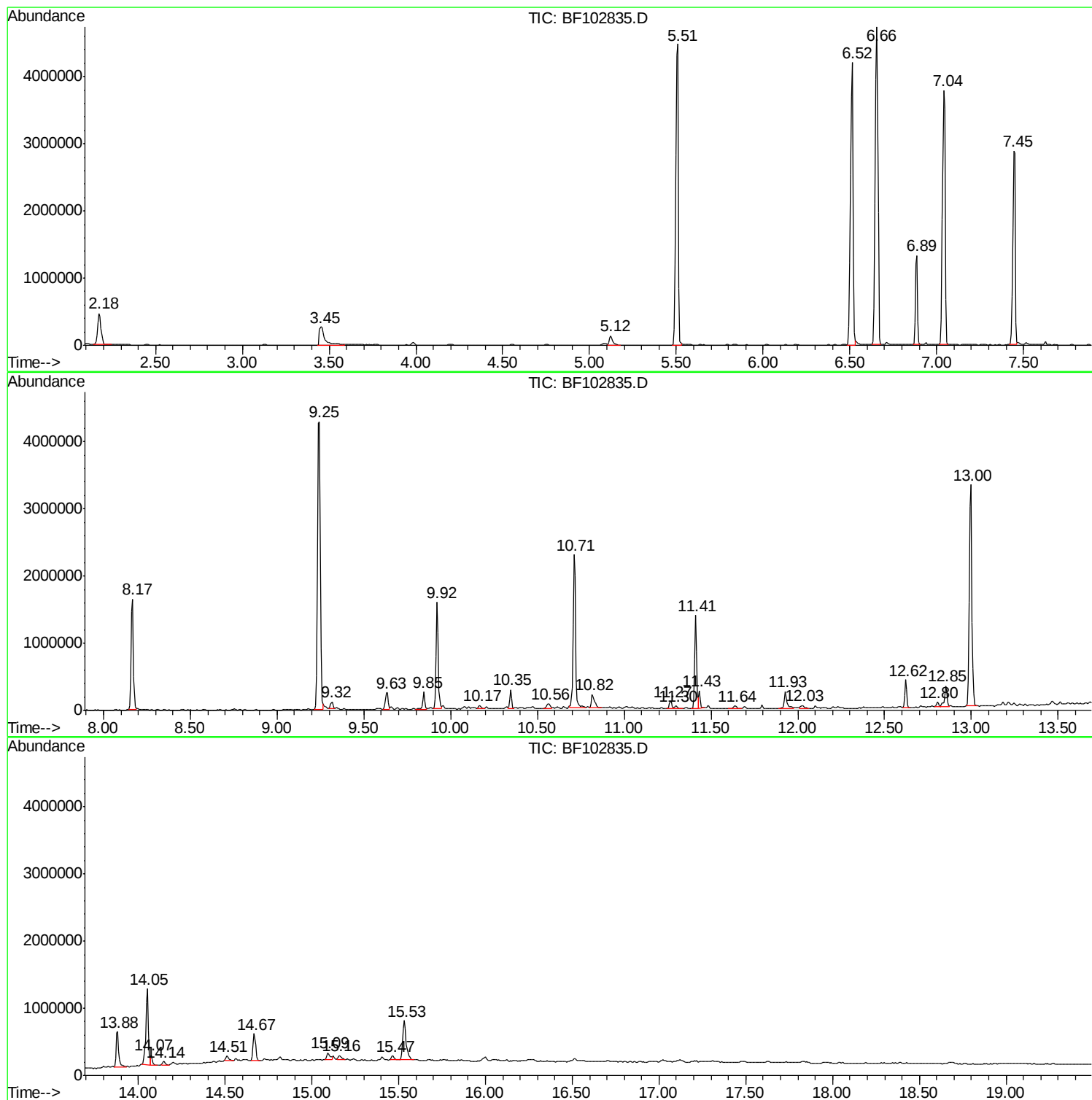
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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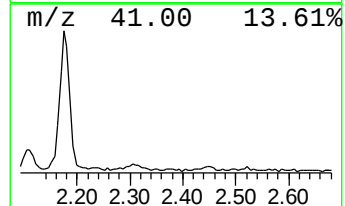
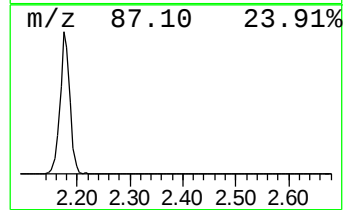
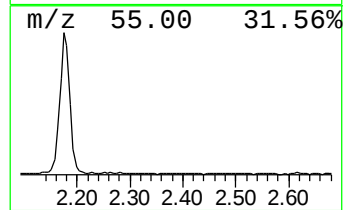
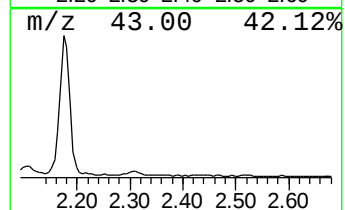
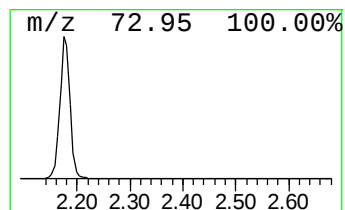
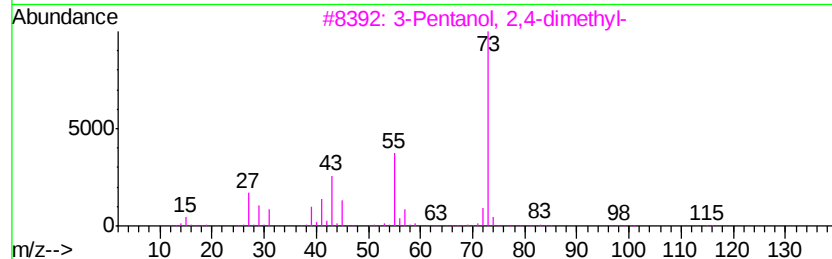
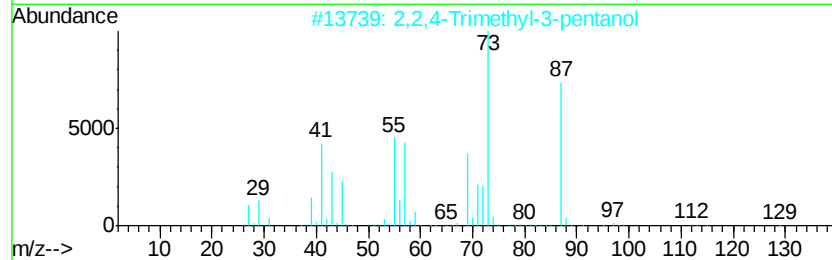
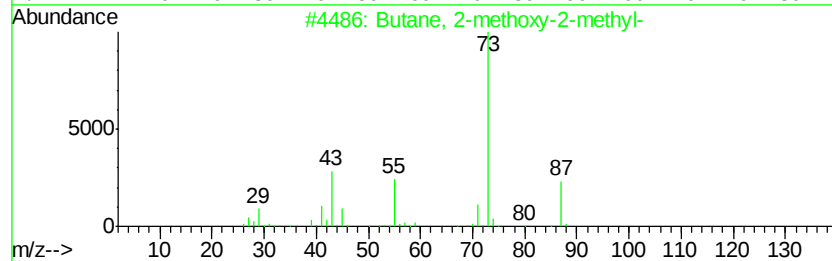
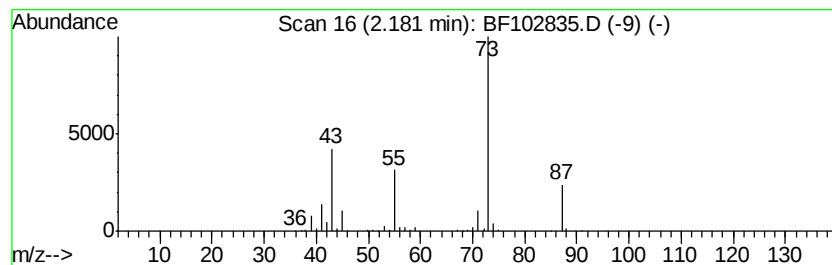
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	11.06 ng	639734	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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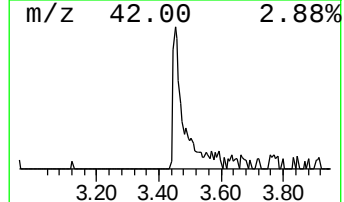
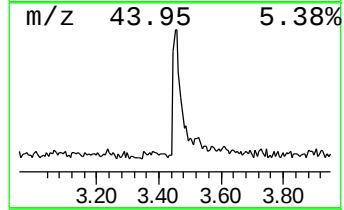
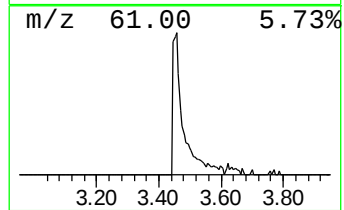
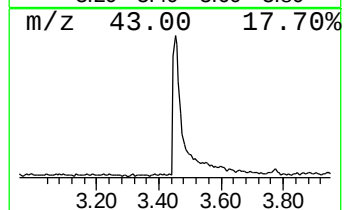
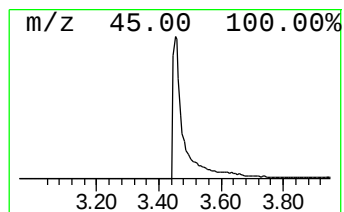
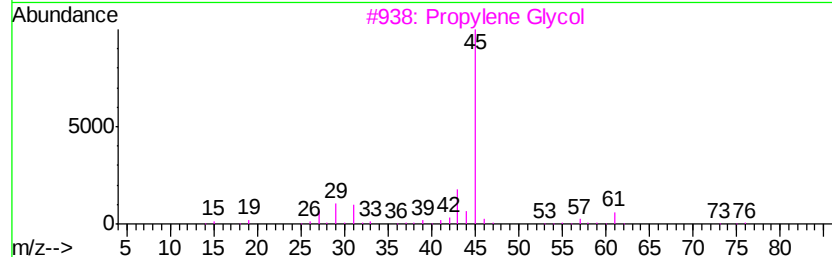
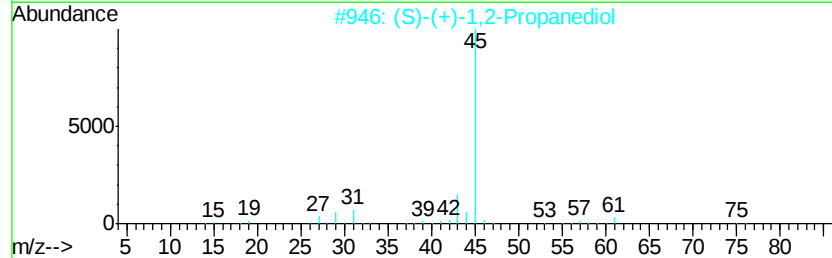
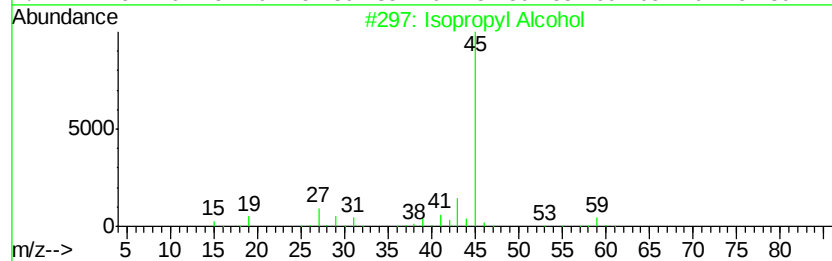
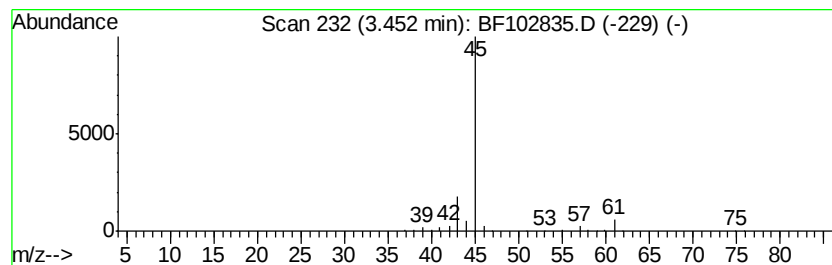
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.45	10.27 ng	594020	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	80
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3		Propylene Glycol	76	C3H8O2	000057-55-6	46
4		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9



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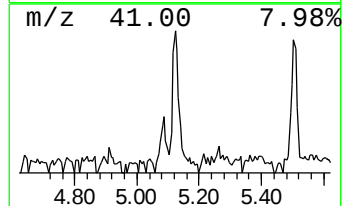
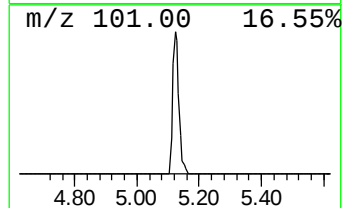
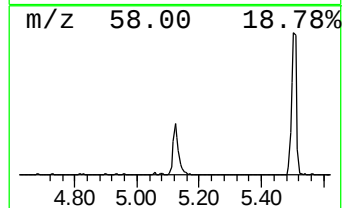
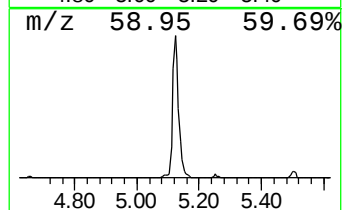
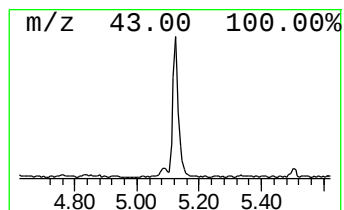
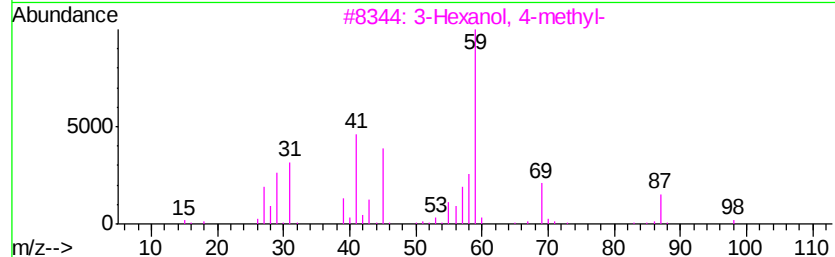
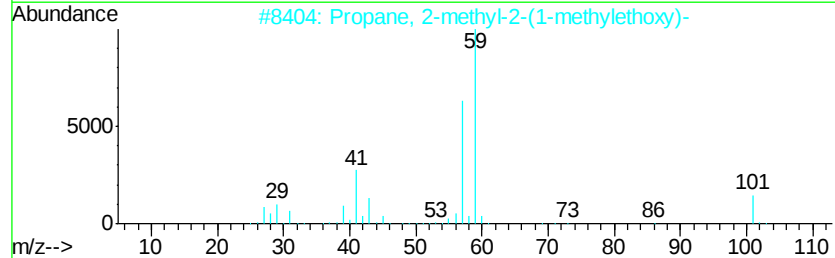
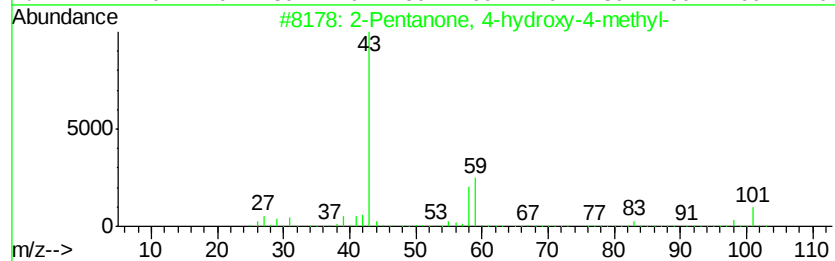
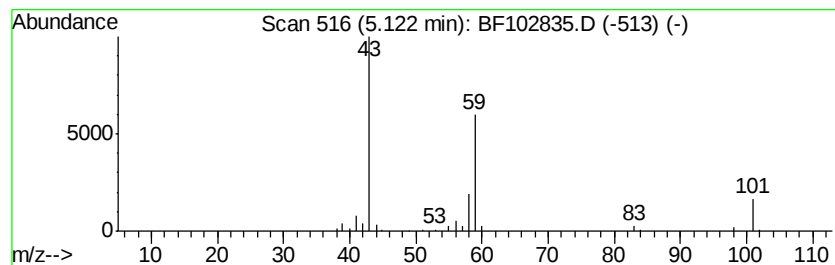
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.18 ng	183944	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
5			3-Hexanol	102	C6H14O	000623-37-0	28



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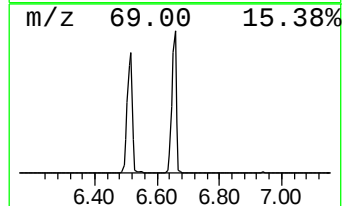
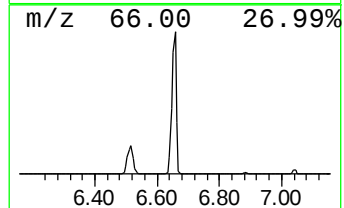
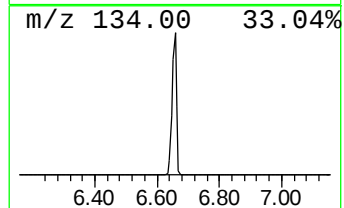
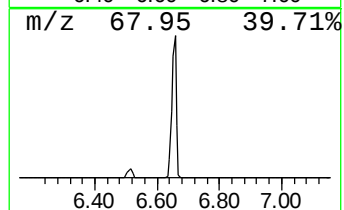
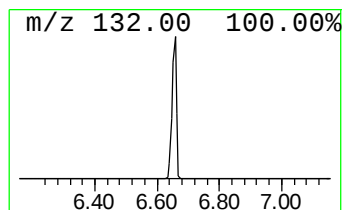
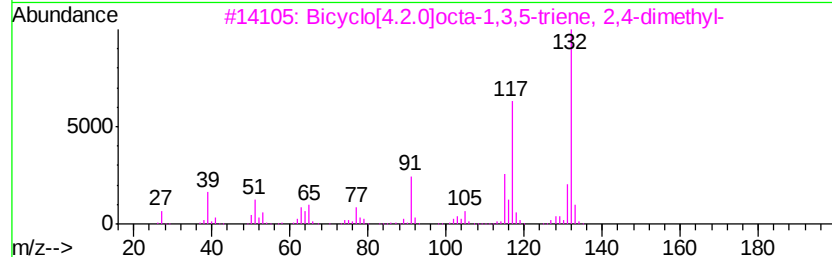
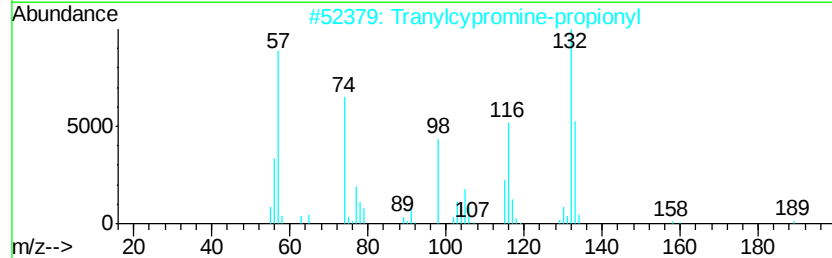
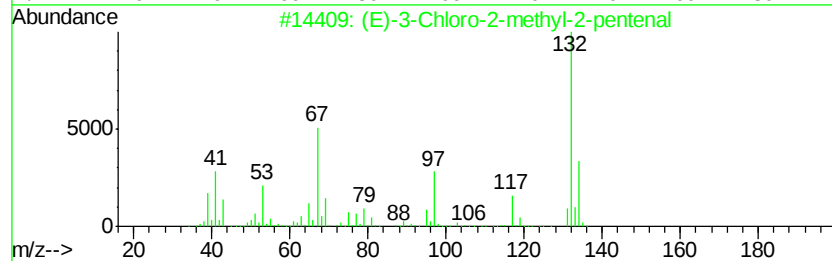
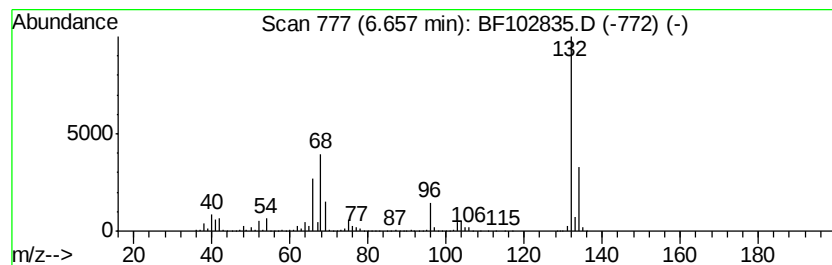
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Peak Number 4 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	81.96 ng	4741070	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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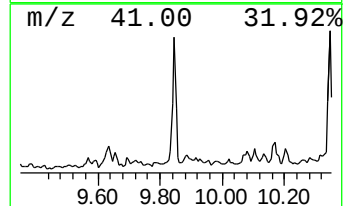
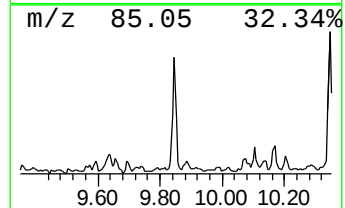
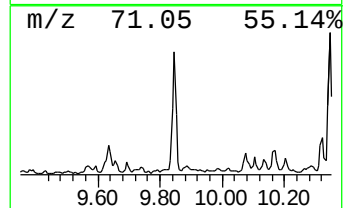
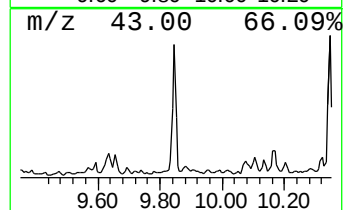
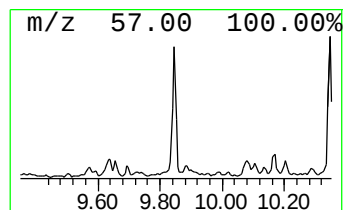
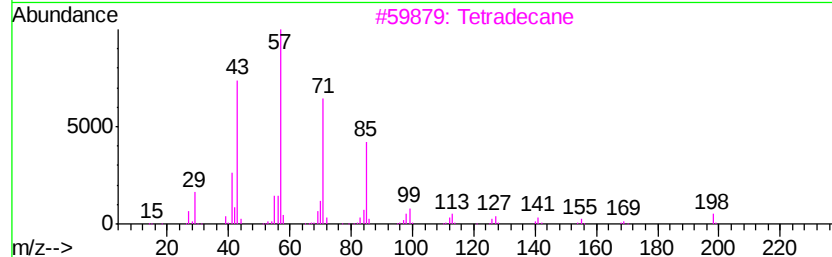
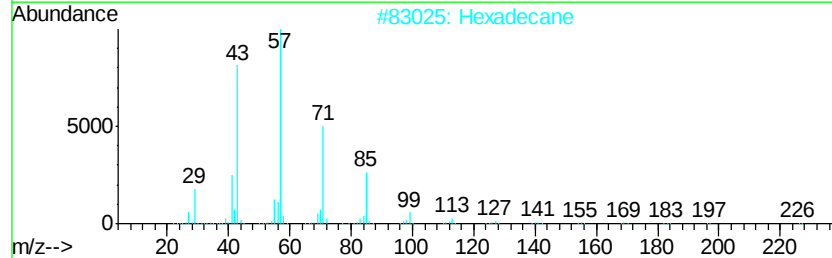
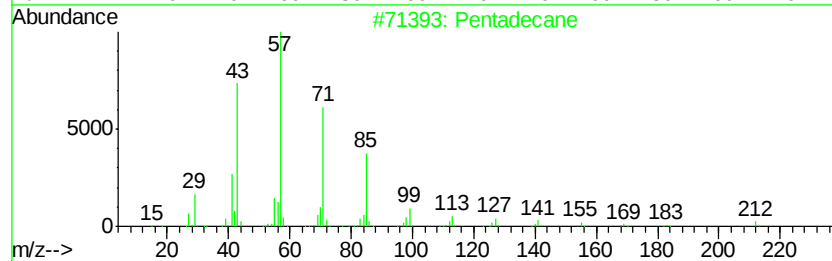
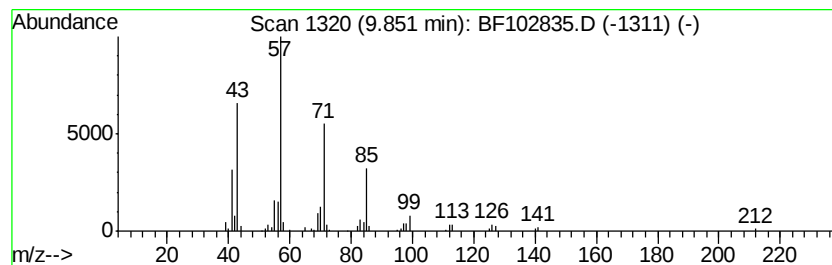
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	3.04 ng	213850	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	94
2	Hexadecane		226	C16H34	000544-76-3	91
3	Tetradecane		198	C14H30	000629-59-4	86
4	Heneicosane		296	C21H44	000629-94-7	86
5	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020718\
Data File : BF102835.D
Acq On : 8 Feb 2018 00:50
Operator : SJ/JU
Sample : J1473-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

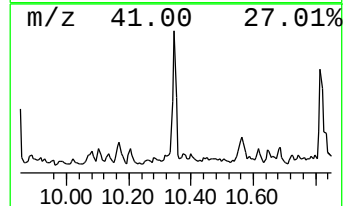
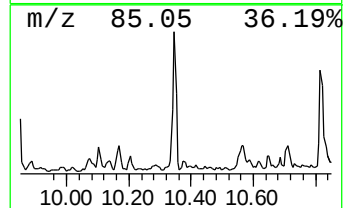
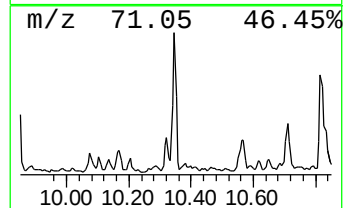
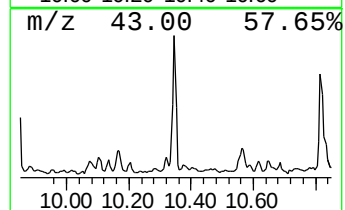
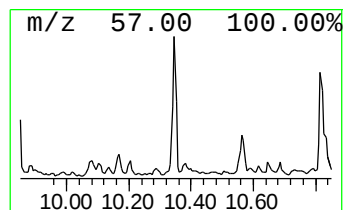
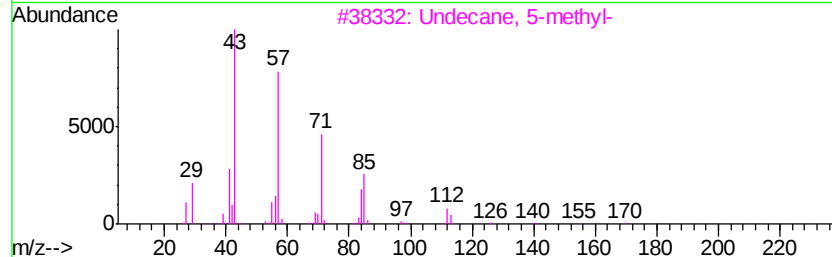
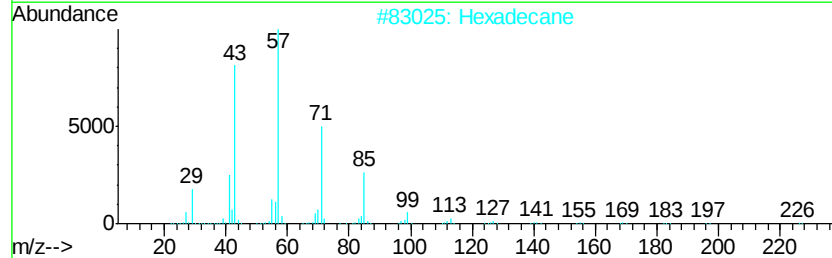
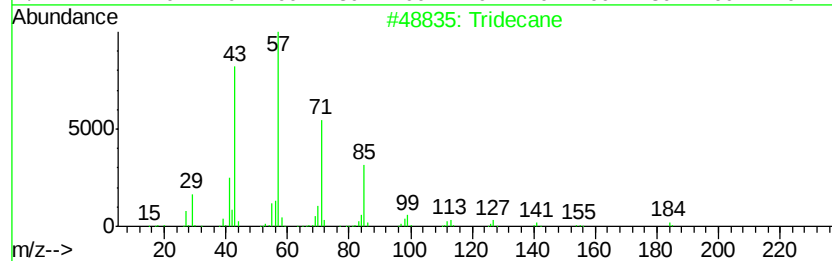
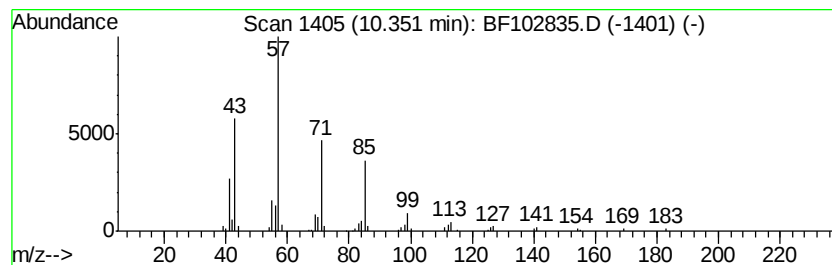
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.92 ng	205443	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Tridecane	184 C13H28	000629-50-5	90
2	Hexadecane	226 C16H34	000544-76-3	86
3	Undecane, 5-methyl-	170 C12H26	001632-70-8	80
4	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	80
5	Pentadecane	212 C15H32	000629-62-9	80



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Sample : J1473-09
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Instrument :
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ClientSampleId :
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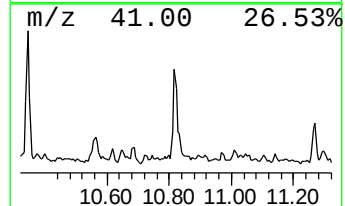
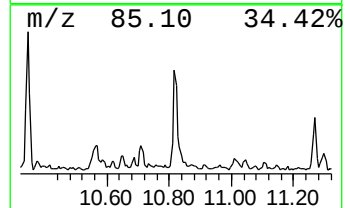
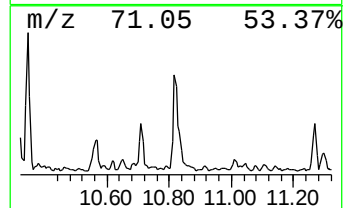
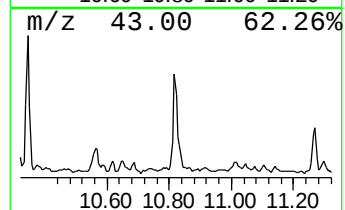
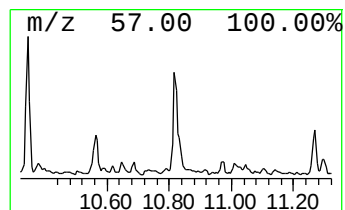
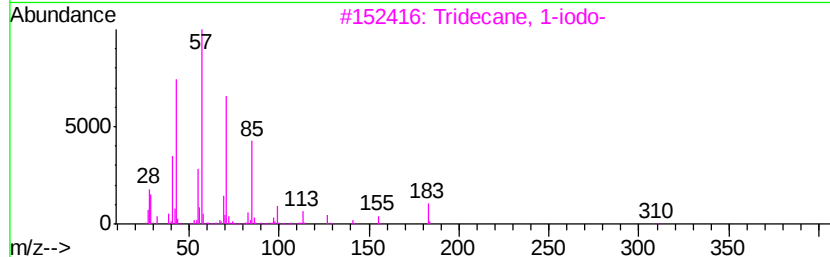
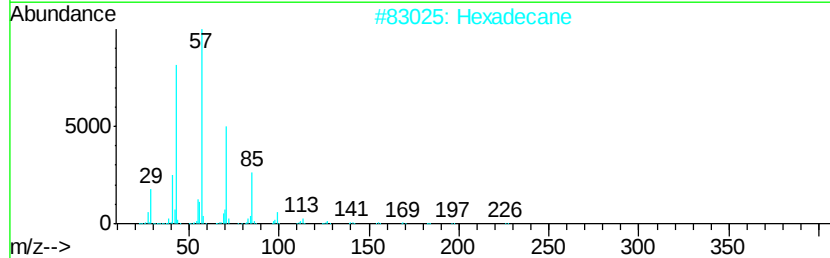
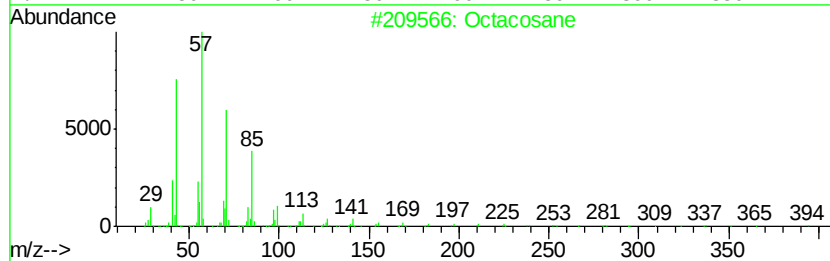
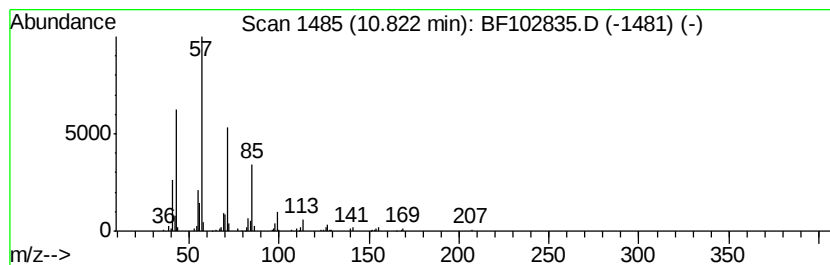
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.84 ng	236579	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	83
4	Eicosane		282	C20H42	000112-95-8	83
5	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	80



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Acq On : 8 Feb 2018 00:50
Operator : SJ/JU
Sample : J1473-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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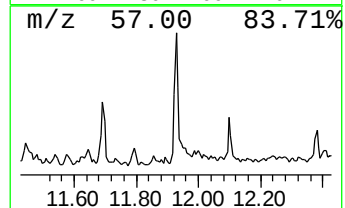
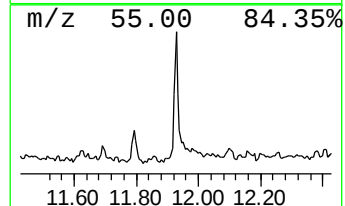
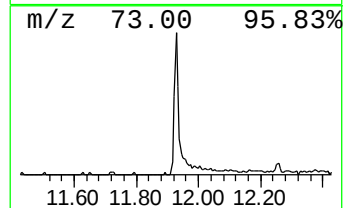
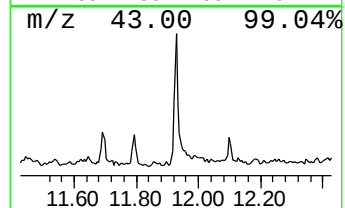
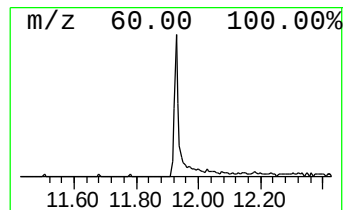
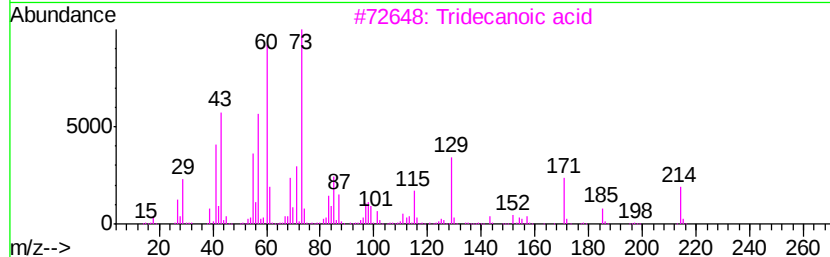
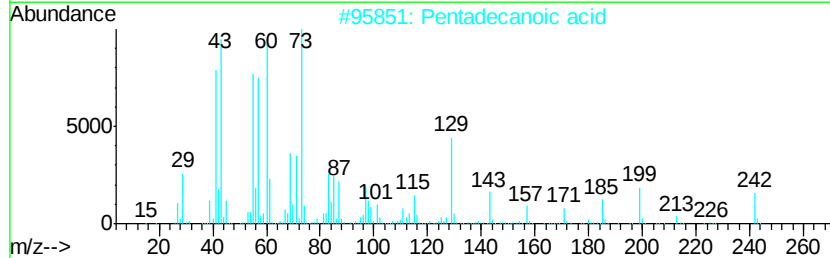
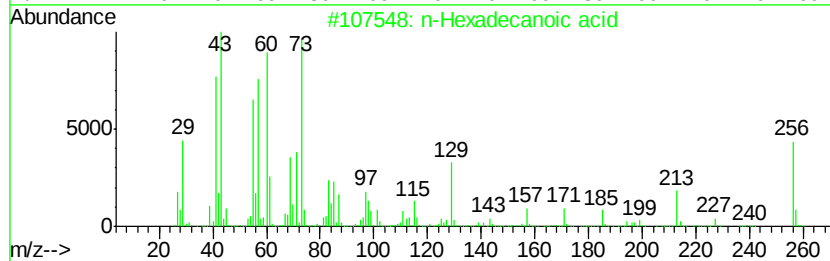
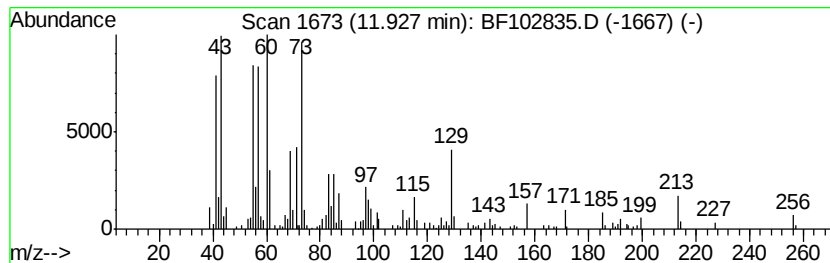
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	4.84 ng	298259	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		n-Decanoic acid	172	C10H20O2	000334-48-5	64
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020718\
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Acq On : 8 Feb 2018 00:50
Operator : SJ/JU
Sample : J1473-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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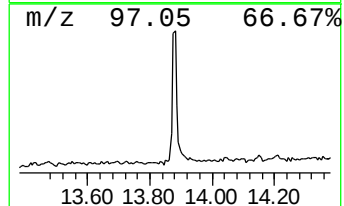
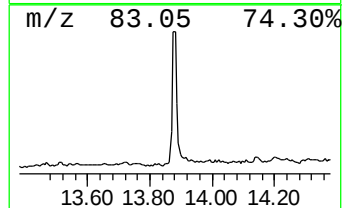
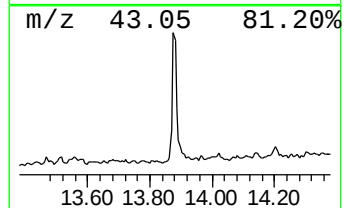
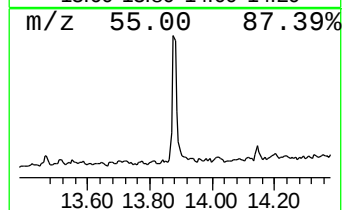
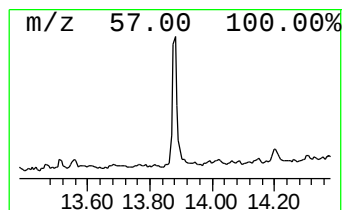
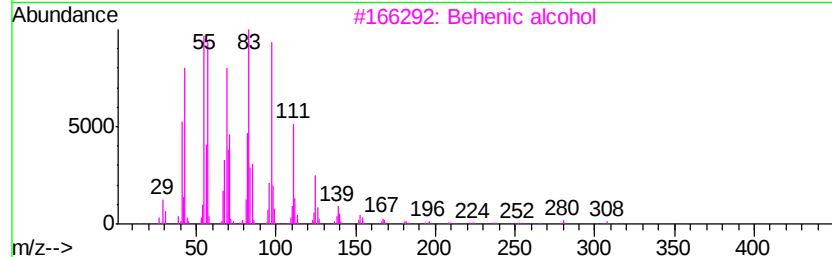
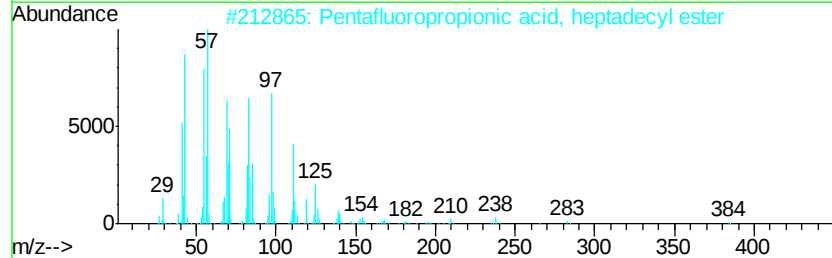
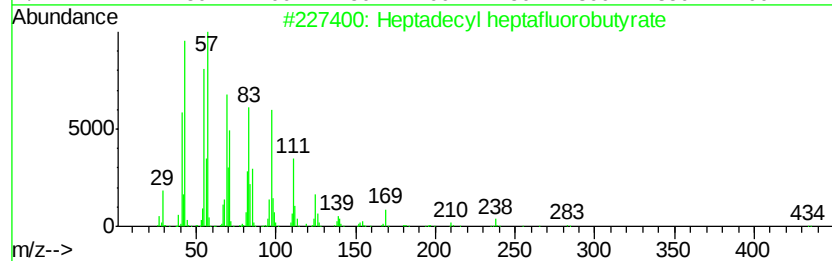
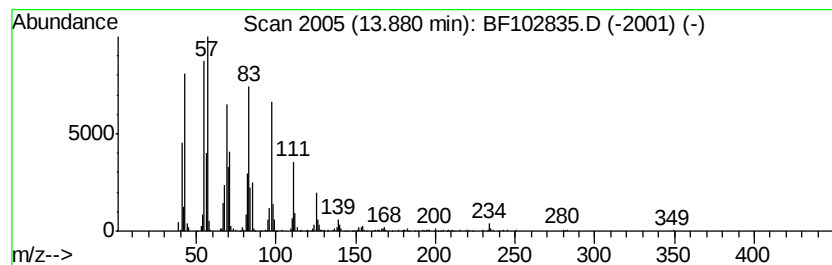
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	10.06 ng	571335	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5		Cyclotetracosane	336	C24H48	000297-03-0	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020718\
Data File : BF102835.D
Acq On : 8 Feb 2018 00:50
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ALS Vial : 19 Sample Multiplier: 1

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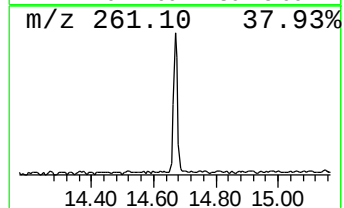
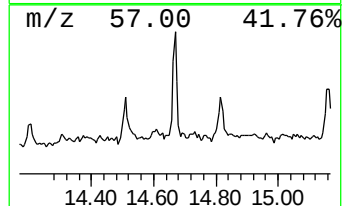
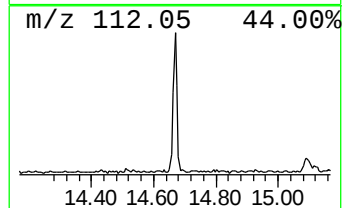
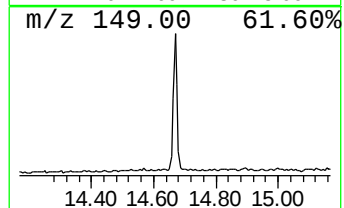
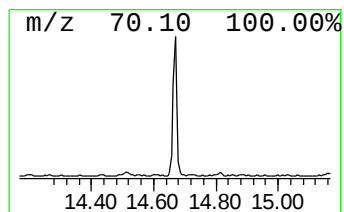
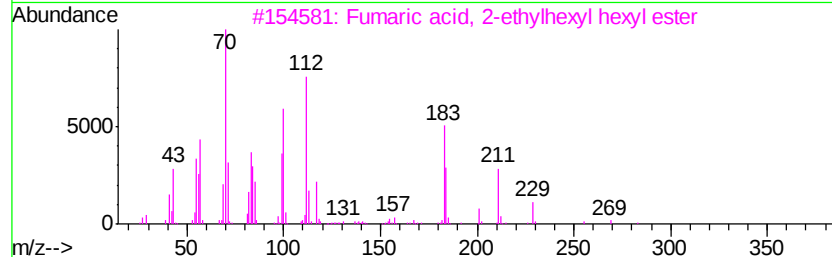
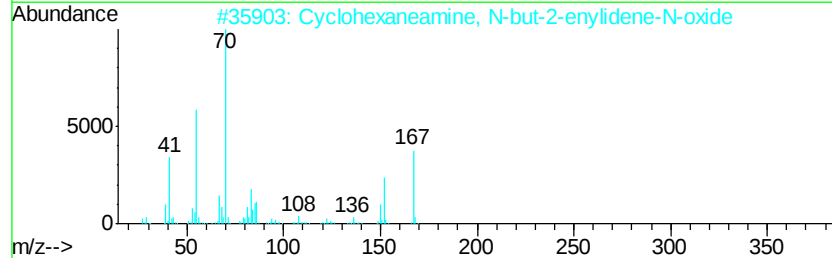
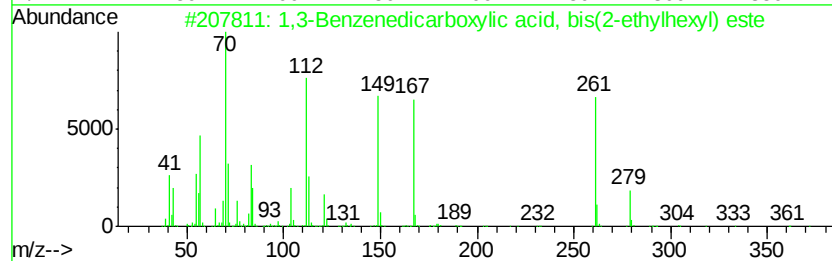
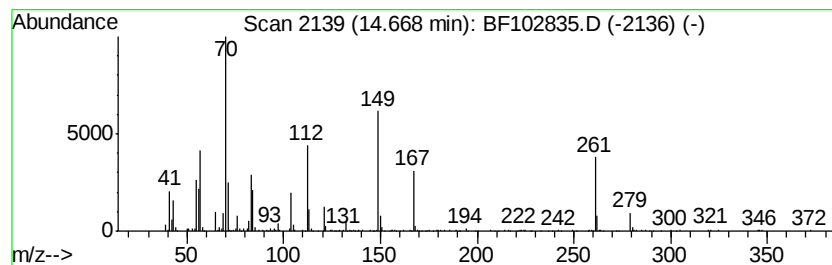
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,3-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	6.30 ng	358145	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	50
2		Cyclohexanamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	27
3		Fumaric acid, 2-ethylhexyl hexyl...	312	C18H32O4	1000339-14-1	22
4		Carbonic acid, propanoyl 2-ethyl...	212	C12H20O3	1000357-90-9	22
5		9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	22



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.18	11.1	ng	639734	1	6.89	1156900	20.0
Isopropyl Alcohol	3.45	10.3	ng	594020	1	6.89	1156900	20.0
2-Pentanone, 4-hy...	5.12	3.2	ng	183944	1	6.89	1156900	20.0
unknown6.66	6.66	82.0	ng	4741070	1	6.89	1156900	20.0
Pentadecane	9.85	3.0	ng	213850	3	9.92	1406600	20.0
Tridecane	10.35	2.9	ng	205443	3	9.92	1406600	20.0
Octacosane	10.82	3.8	ng	236579	4	11.41	1231900	20.0
n-Hexadecanoic acid	11.93	4.8	ng	298259	4	11.41	1231900	20.0
Heptadecyl heptaf...	13.88	10.1	ng	571335	5	14.05	1136300	20.0
1,3-Benzenedicarb...	14.67	6.3	ng	358145	5	14.05	1136300	20.0