

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
 Data File : BF102895.D
 Acq On : 9 Feb 2018 18:10
 Operator : SJ/JU
 Sample : J1506-08
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-22(8-10)

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	2.163	6	13	21	rVB	555677	740015	14.58%	1.716%
2	5.122	513	516	525	rVB	159439	212528	4.19%	0.493%
3	5.510	576	582	585	rBV	4692308	5075519	100.00%	11.772%
4	6.516	747	753	756	rBV	4179652	4993305	98.38%	11.582%
5	6.657	772	777	780	rBV	4764621	4876364	96.08%	11.310%
6	6.886	812	816	819	rBV	1301652	1125866	22.18%	2.611%
7	6.939	821	825	834	rBV	87178	80321	1.58%	0.186%
8	7.045	838	843	846	rBV	3606972	3552936	70.00%	8.241%
9	7.451	906	912	915	rBV	3235238	3331500	65.64%	7.727%
10	8.169	1030	1034	1037	rBV	1724030	1441582	28.40%	3.344%
11	9.245	1212	1217	1220	rBV	4568594	4397954	86.65%	10.201%
12	9.316	1226	1229	1231	rVB	90556	67177	1.32%	0.156%
13	9.510	1258	1262	1268	rBV	220058	179553	3.54%	0.416%
14	9.633	1279	1283	1286	rBV	473750	421719	8.31%	0.978%
15	9.845	1316	1319	1323	rBV	244494	181097	3.57%	0.420%
16	9.921	1328	1332	1340	rVV	1537093	1457451	28.72%	3.380%
17	10.345	1401	1404	1407	rVB	276326	203275	4.01%	0.471%
18	10.563	1437	1441	1444	rBV	62904	82459	1.62%	0.191%
19	10.715	1463	1467	1477	rVB	2504546	2464621	48.56%	5.716%
20	10.815	1482	1484	1494	rVB	198170	222046	4.37%	0.515%
21	11.268	1558	1561	1563	rBV	77927	66715	1.31%	0.155%
22	11.410	1582	1585	1589	rBV	1305783	1213348	23.91%	2.814%
23	11.927	1669	1673	1682	rBV	182256	213003	4.20%	0.494%
24	12.627	1789	1792	1795	rBV	52872	51954	1.02%	0.121%
25	12.809	1819	1823	1826	rBV	120344	99820	1.97%	0.232%
26	12.998	1850	1855	1858	rBV	3281854	3239466	63.83%	7.514%
27	13.468	1930	1935	1940	rBV	58985	71215	1.40%	0.165%
28	13.515	1940	1943	1946	rVB2	72599	70118	1.38%	0.163%
29	13.880	2002	2005	2017	rBV	708076	682614	13.45%	1.583%
30	14.051	2030	2034	2038	rBV	1063674	1056137	20.81%	2.450%
31	14.515	2109	2113	2120	rBV2	61258	88325	1.74%	0.205%
32	15.539	2281	2287	2296	rBV2	762226	1054501	20.78%	2.446%
33	16.050	2370	2374	2382	rBV2	54294	99678	1.96%	0.231%

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ALS Vial : 21 Sample Multiplier: 1

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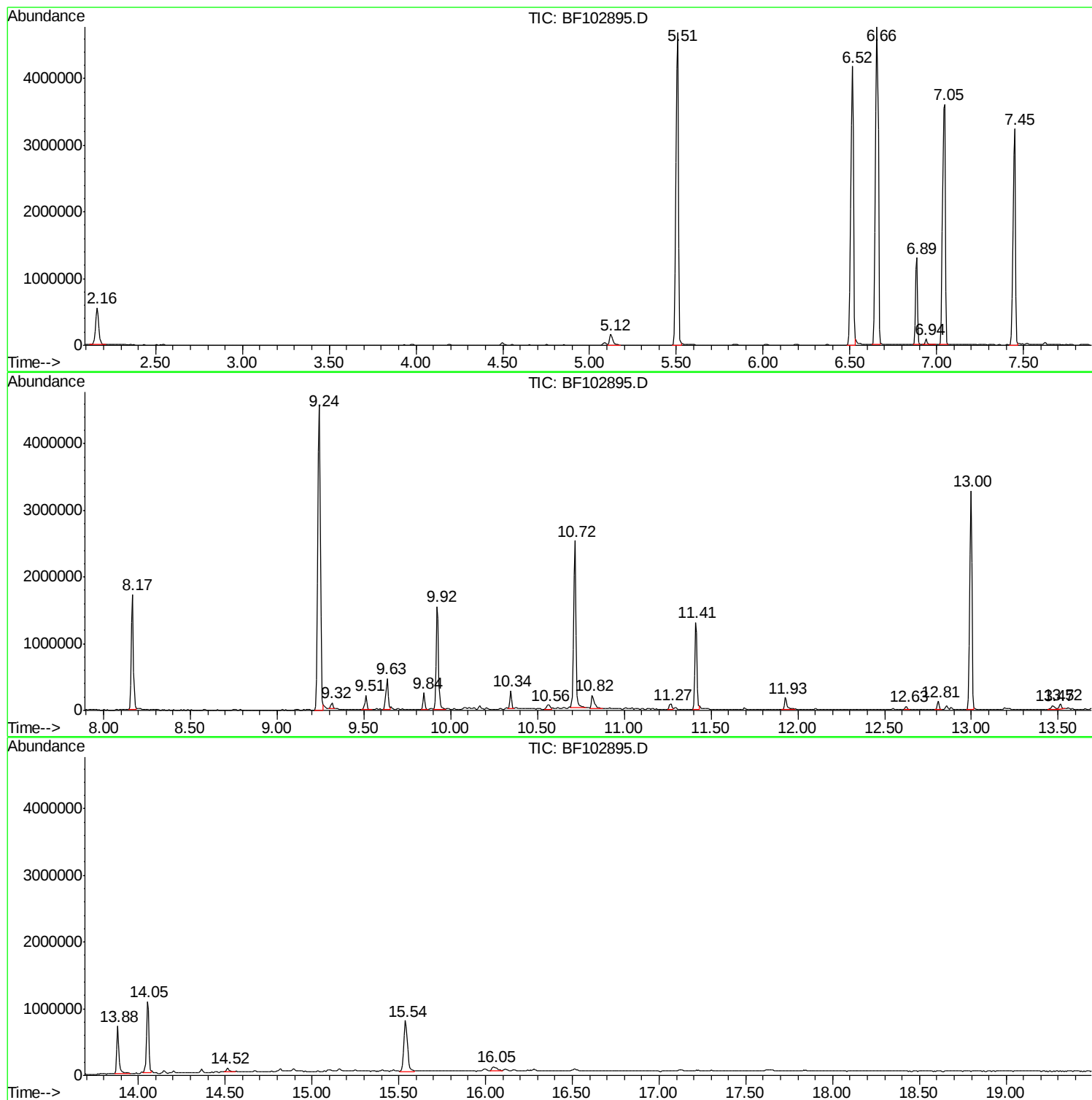
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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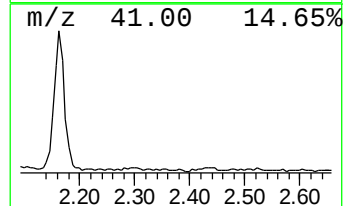
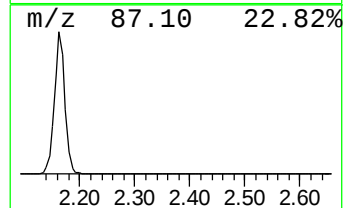
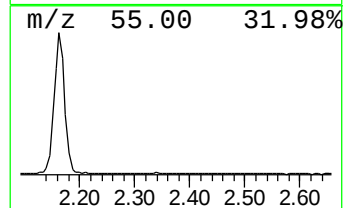
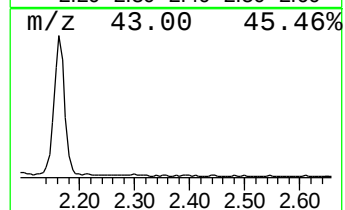
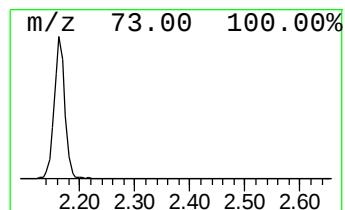
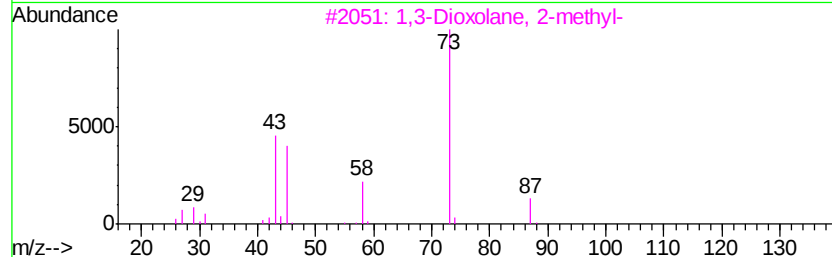
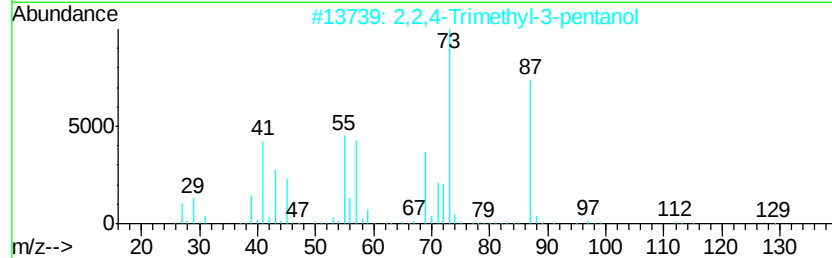
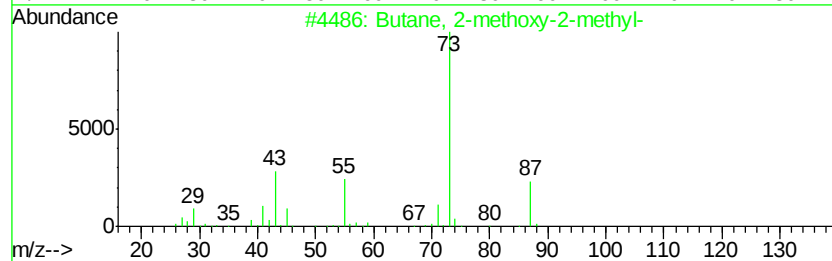
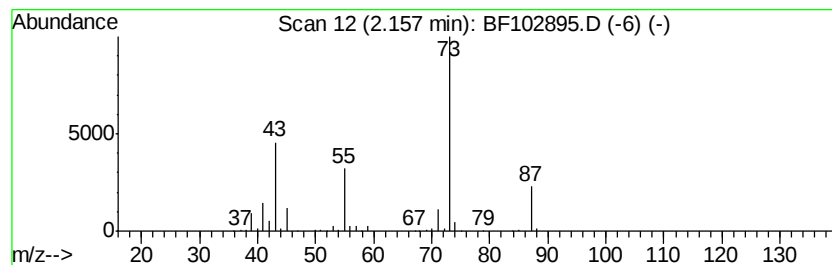
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	13.15 ng	740015	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		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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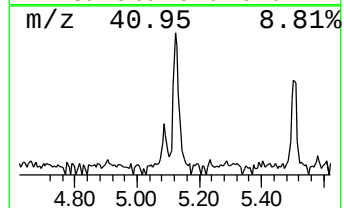
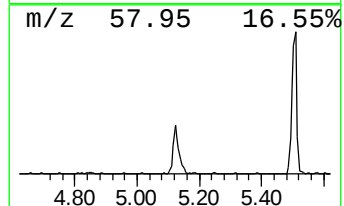
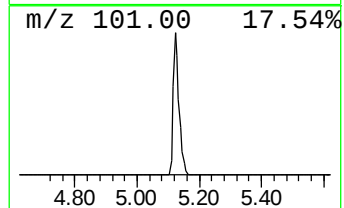
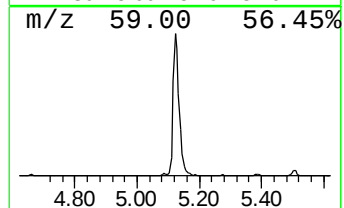
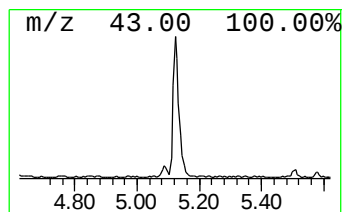
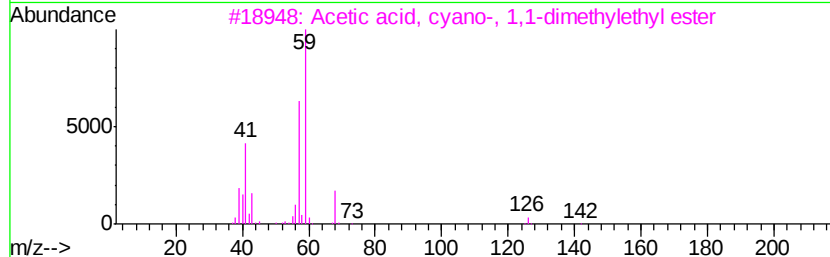
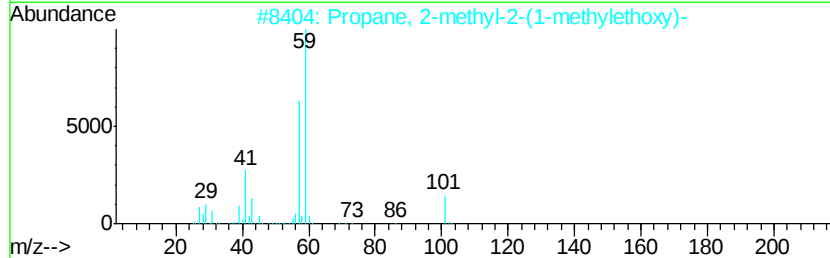
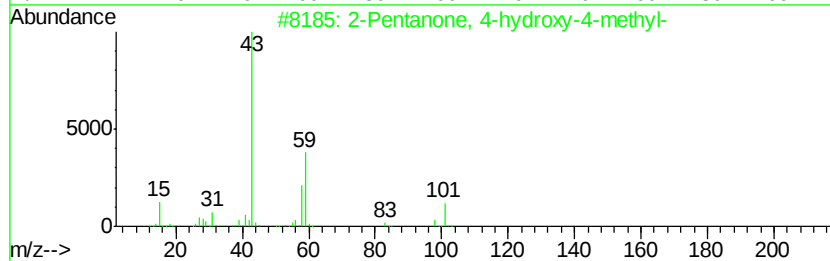
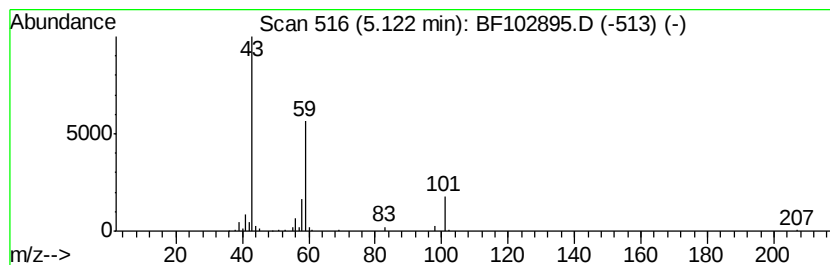
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.78 ng	212528	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	9



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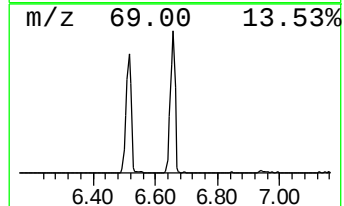
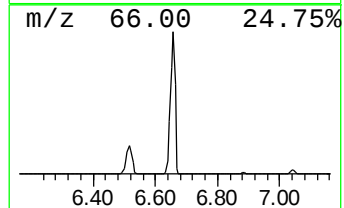
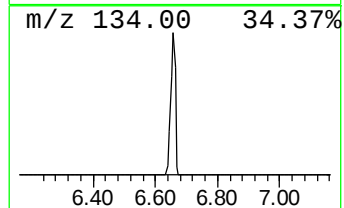
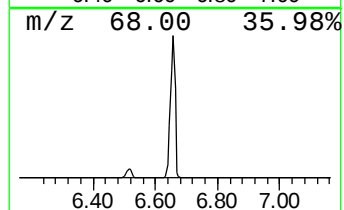
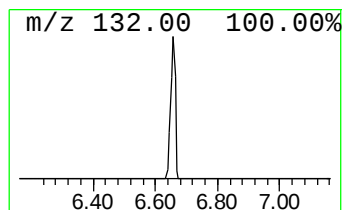
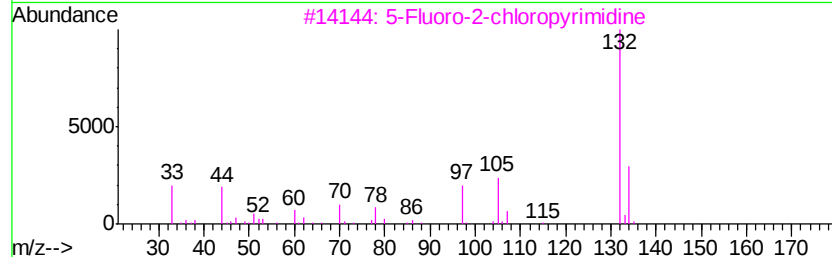
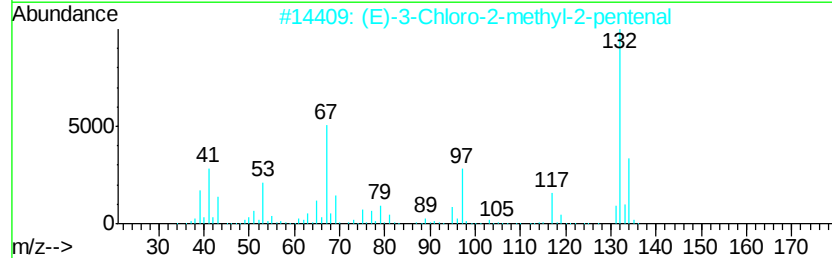
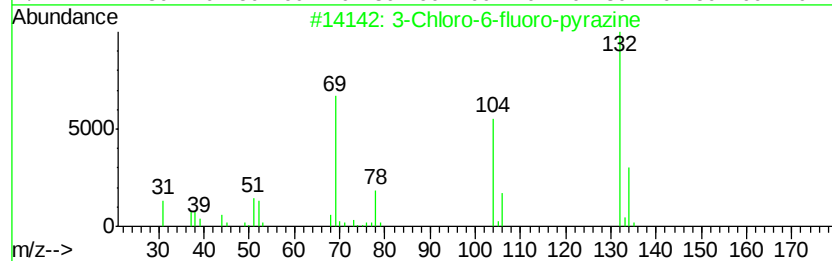
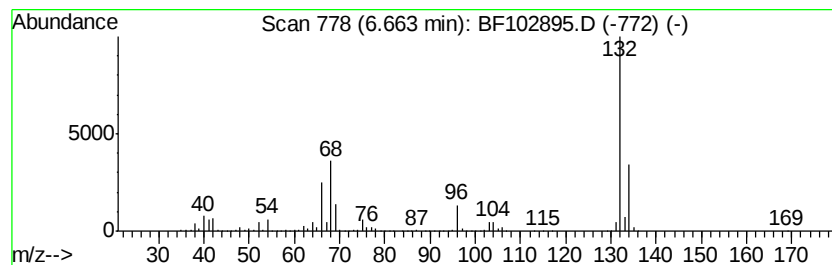
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	86.62 ng	4876360	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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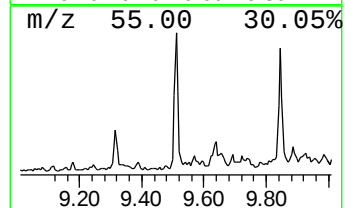
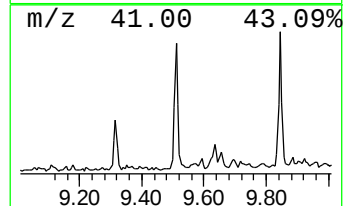
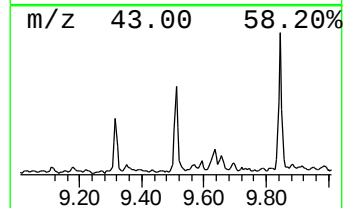
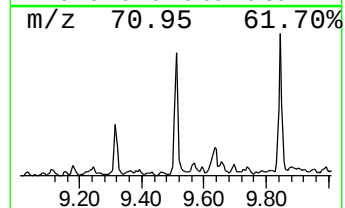
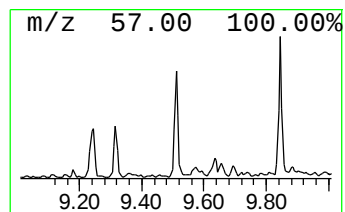
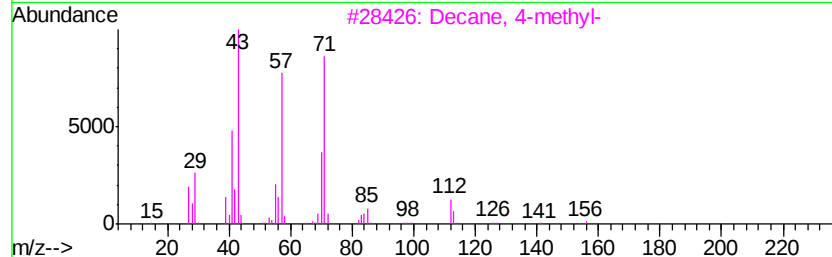
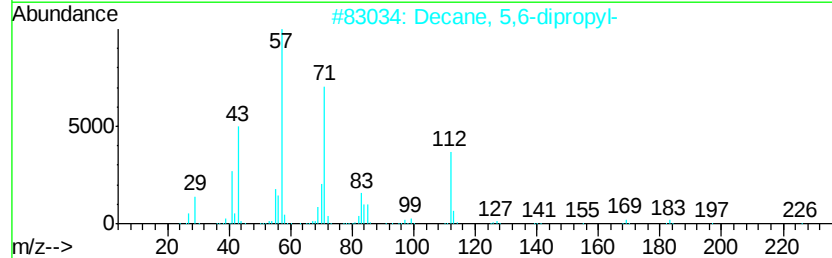
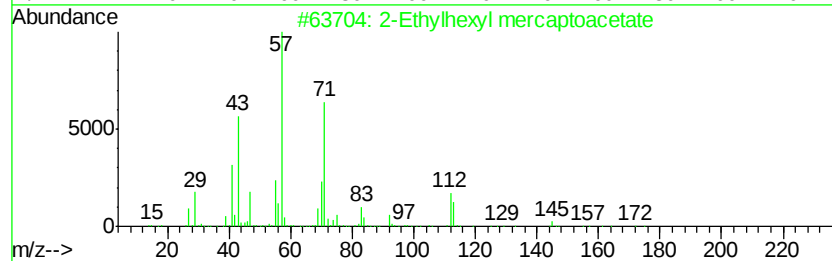
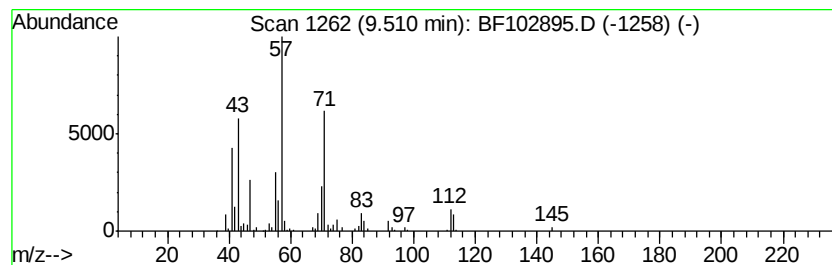
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Ethylhexyl mercaptoacetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.51	2.46 ng	179553	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	80
2		Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	53
3		Decane, 4-methyl-	156	C11H24	002847-72-5	50
4		Octane, 3-ethyl-	142	C10H22	005881-17-4	50
5		4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	50



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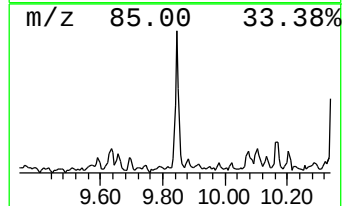
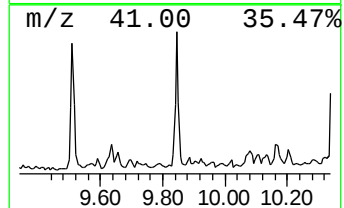
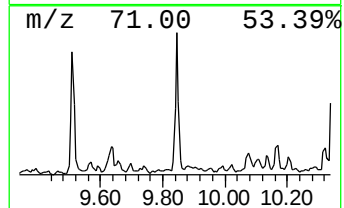
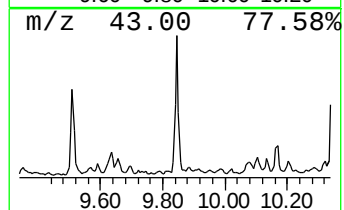
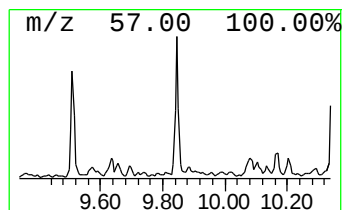
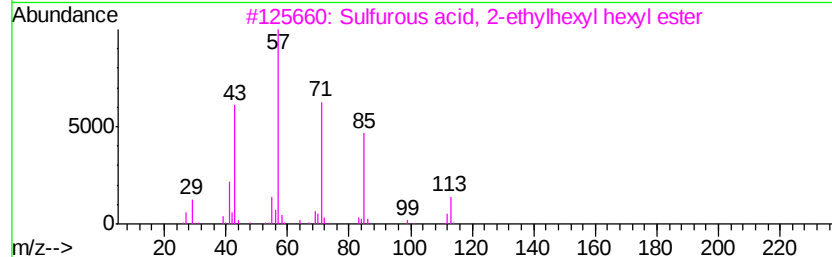
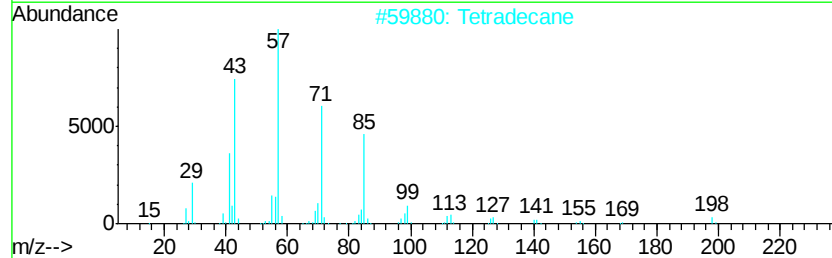
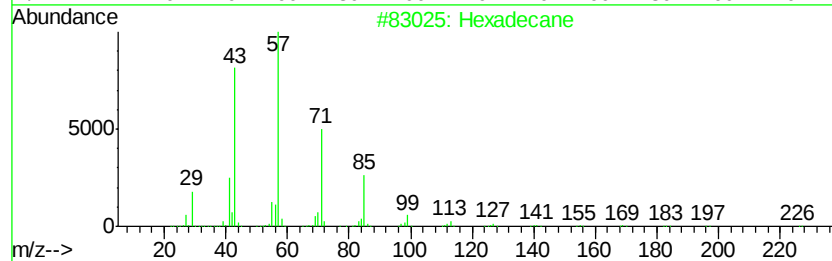
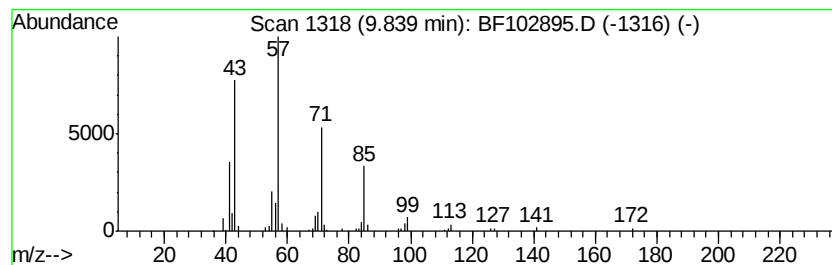
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.84	2.49 ng	181097	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Tetradecane		198	C14H30	000629-59-4	90
3	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	80
4	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	72
5	Pentadecane		212	C15H32	000629-62-9	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
Data File : BF102895.D
Acq On : 9 Feb 2018 18:10
Operator : SJ/JU
Sample : J1506-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-22(8-10)

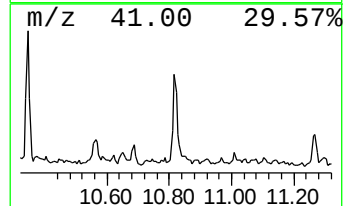
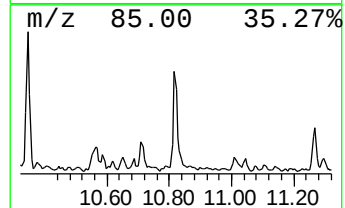
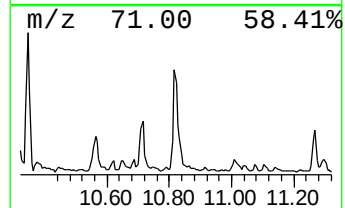
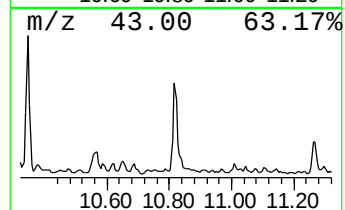
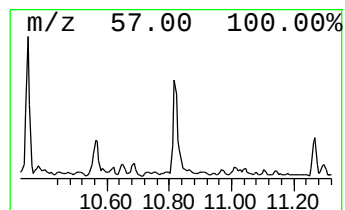
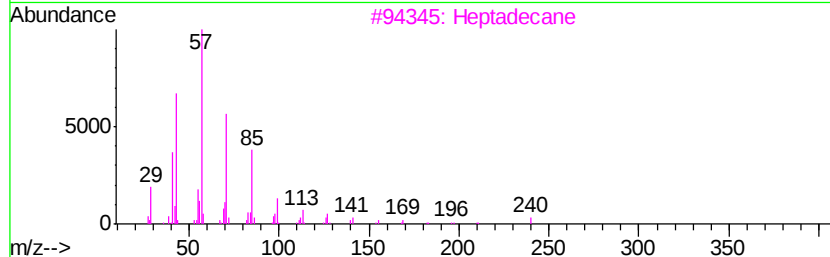
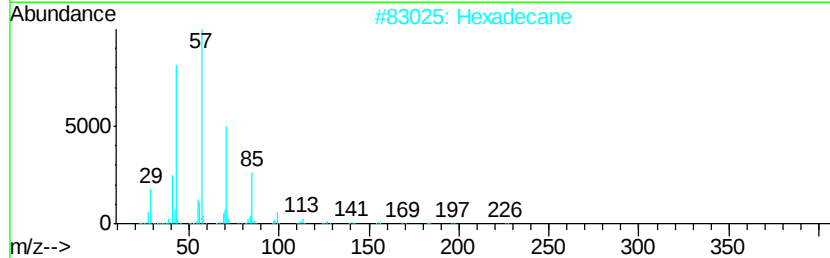
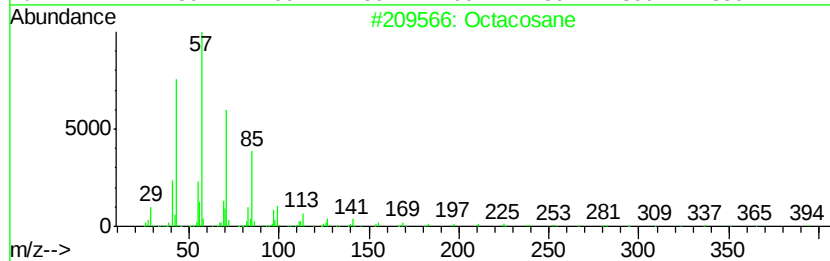
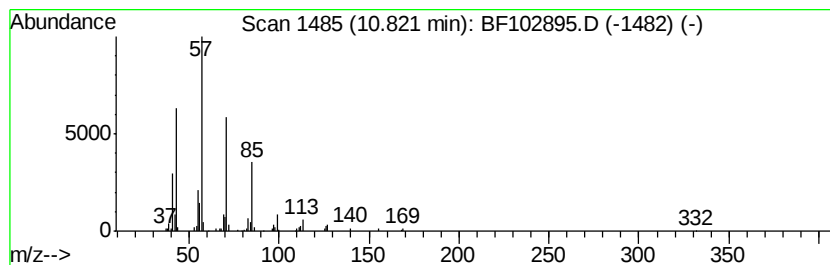
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.66 ng	222046	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexadecane	226	C16H34	000544-76-3	90
3		Heptadecane	240	C17H36	000629-78-7	80
4		Eicosane	282	C20H42	000112-95-8	80
5		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
Data File : BF102895.D
Acq On : 9 Feb 2018 18:10
Operator : SJ/JU
Sample : J1506-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

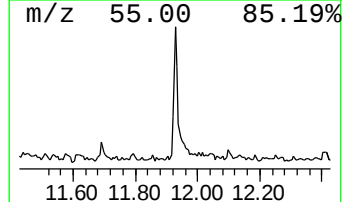
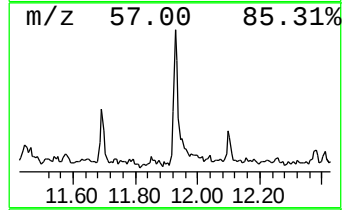
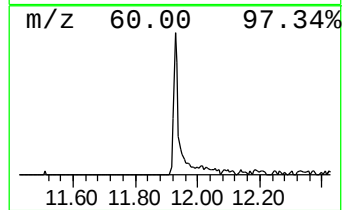
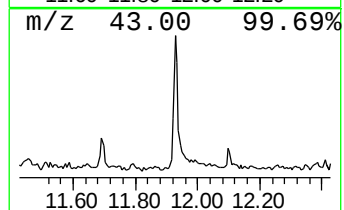
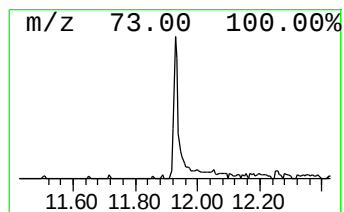
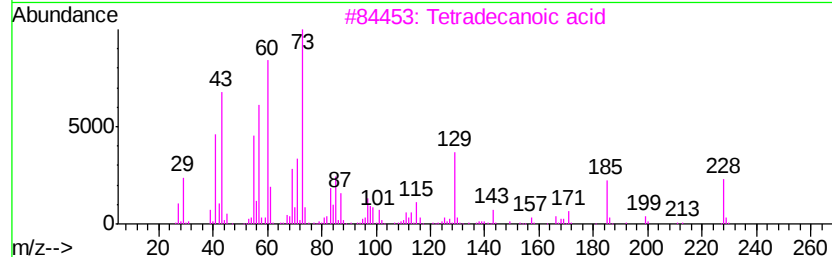
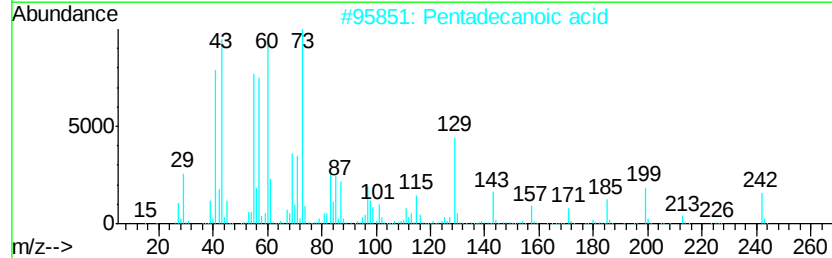
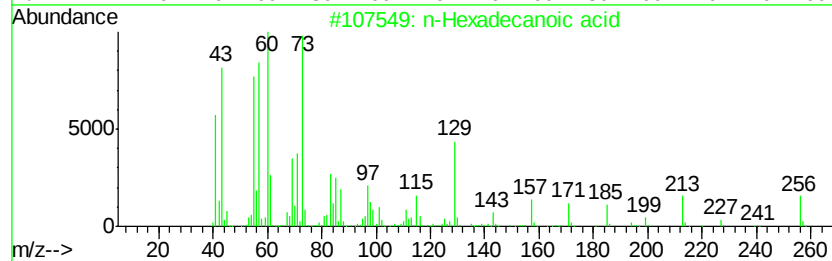
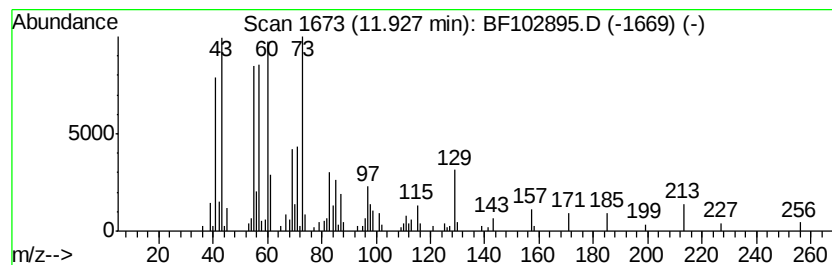
Instrument :
BNA_F
ClientSampleId :
B-22(8-10)

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 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.93	3.51 ng	213003	Phenanthrene-d10	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Oxalic acid, allvl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5	Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
Data File : BF102895.D
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Sample : J1506-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

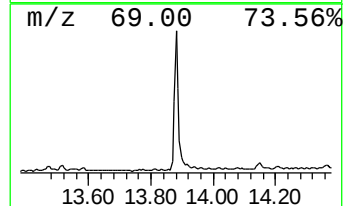
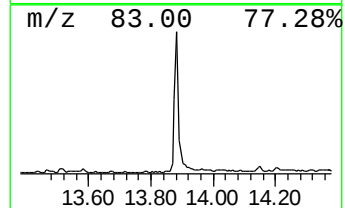
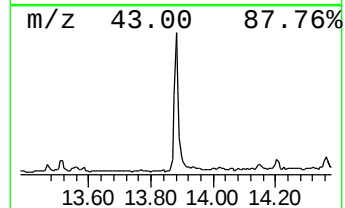
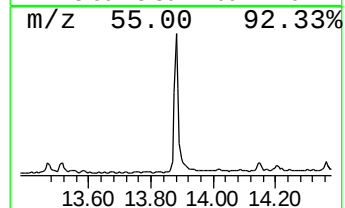
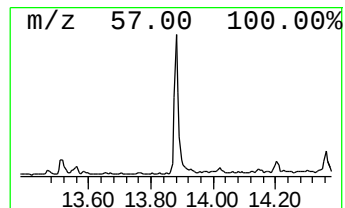
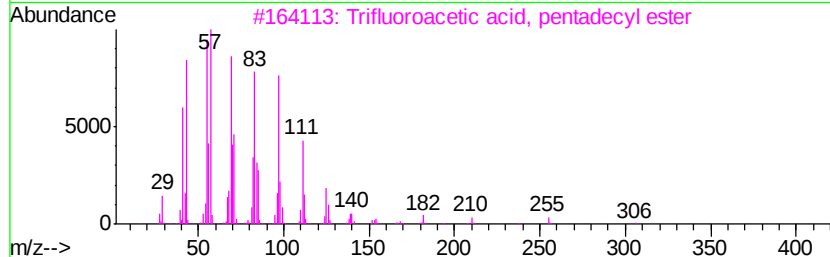
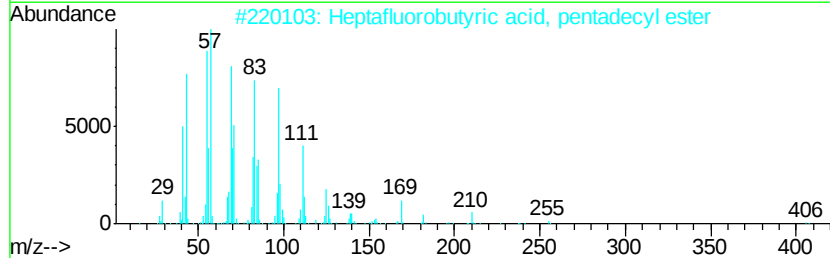
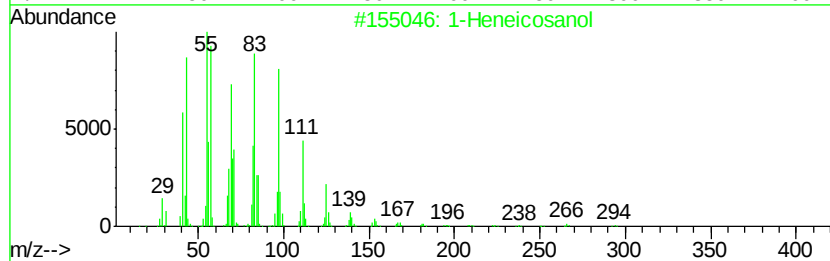
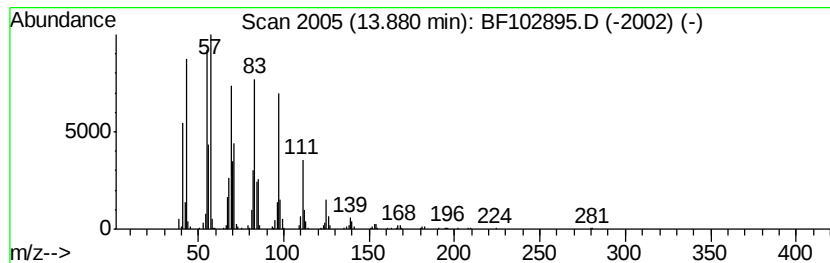
Instrument :
BNA_F
ClientSampleId :
B-22(8-10)

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 10 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	12.93 ng	682614	Chrysene-d12	14.05
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	95
2	Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5	94
3	Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2	94
4	Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0	94
5	n-Nonadecanol-1	284 C19H40O	001454-84-8	94



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Operator : SJ/JU
Sample : J1506-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-22(8-10)

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.16	13.2	ng	740015	1	6.89	1125870	20.0
2-Pentanone, 4-hy...	5.12	3.8	ng	212528	1	6.89	1125870	20.0
unknown6.66	6.66	86.6	ng	4876360	1	6.89	1125870	20.0
2-Ethylhexyl merc...	9.51	2.5	ng	179553	3	9.92	1457450	20.0
Hexadecane	9.84	2.5	ng	181097	3	9.92	1457450	20.0
Octacosane	10.82	3.7	ng	222046	4	11.41	1213350	20.0
n-Hexadecanoic acid	11.93	3.5	ng	213003	4	11.41	1213350	20.0
1-Heneicosanol	13.88	12.9	ng	682614	5	14.05	1056140	20.0