

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
 Data File : BF108154.D
 Acq On : 14 Aug 2018 19:29
 Operator : JU/SJ
 Sample : J4458-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-93

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	2.366	3	5	15	rVB	1349459	1521557	36.84%	5.040%
2	2.502	23	28	39	rVB2	35804	73449	1.78%	0.243%
3	5.249	491	495	503	rVB	150441	143089	3.46%	0.474%
4	5.637	557	561	565	rBV	1208541	1094492	26.50%	3.626%
5	6.625	726	729	734	rBV	789005	708409	17.15%	2.347%
6	6.784	752	756	759	rBV	2477597	2056183	49.78%	6.811%
7	7.019	792	796	799	rBV	1435909	1211644	29.33%	4.014%
8	7.172	818	822	826	rVB	3237814	3020747	73.13%	10.006%
9	7.578	886	891	894	rBV	2677975	2439572	59.06%	8.081%
10	8.301	1009	1014	1017	rBV	1701731	1445955	35.00%	4.790%
11	8.837	1101	1105	1113	rBV2	62000	56789	1.37%	0.188%
12	9.372	1190	1196	1200	rBV	4429188	4130729	100.00%	13.683%
13	9.472	1210	1213	1218	rVB2	44064	48306	1.17%	0.160%
14	9.760	1258	1262	1266	rBV	366759	343928	8.33%	1.139%
15	10.066	1309	1314	1317	rVB	1488762	1376307	33.32%	4.559%
16	10.242	1339	1344	1348	rBV5	42881	55117	1.33%	0.183%
17	10.389	1365	1369	1375	rBV6	30556	61227	1.48%	0.203%
18	10.472	1380	1383	1386	rVB2	67176	57365	1.39%	0.190%
19	10.854	1443	1448	1457	rBV	1618109	1468344	35.55%	4.864%
20	10.948	1461	1464	1466	rBV	76065	80368	1.95%	0.266%
21	11.054	1479	1482	1485	rBV3	47978	44819	1.09%	0.148%
22	11.089	1485	1488	1491	rBV2	48077	53249	1.29%	0.176%
23	11.195	1504	1506	1511	rVB3	50821	66774	1.62%	0.221%
24	11.242	1511	1514	1515	rBV2	54219	55912	1.35%	0.185%
25	11.395	1538	1540	1543	rBV	58172	59404	1.44%	0.197%
26	11.560	1564	1568	1571	rBV	1543371	1267796	30.69%	4.200%
27	11.930	1629	1631	1633	rVB2	66441	48749	1.18%	0.161%
28	12.072	1651	1655	1662	rBV	654871	766147	18.55%	2.538%
29	12.860	1786	1789	1794	rBV	299148	322106	7.80%	1.067%
30	13.148	1834	1838	1841	rBV	3527981	3059117	74.06%	10.133%
31	14.030	1985	1988	1997	rBV	616927	601127	14.55%	1.991%
32	14.219	2016	2020	2023	rVB	1354035	1170473	28.34%	3.877%
33	14.983	2148	2150	2154	rVB	161369	153765	3.72%	0.509%
34	15.354	2210	2213	2218	rVB	160247	182256	4.41%	0.604%

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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 >
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35	15.783	2281	2286	2292	rVB2	600803	942907	22.83%	3.123%
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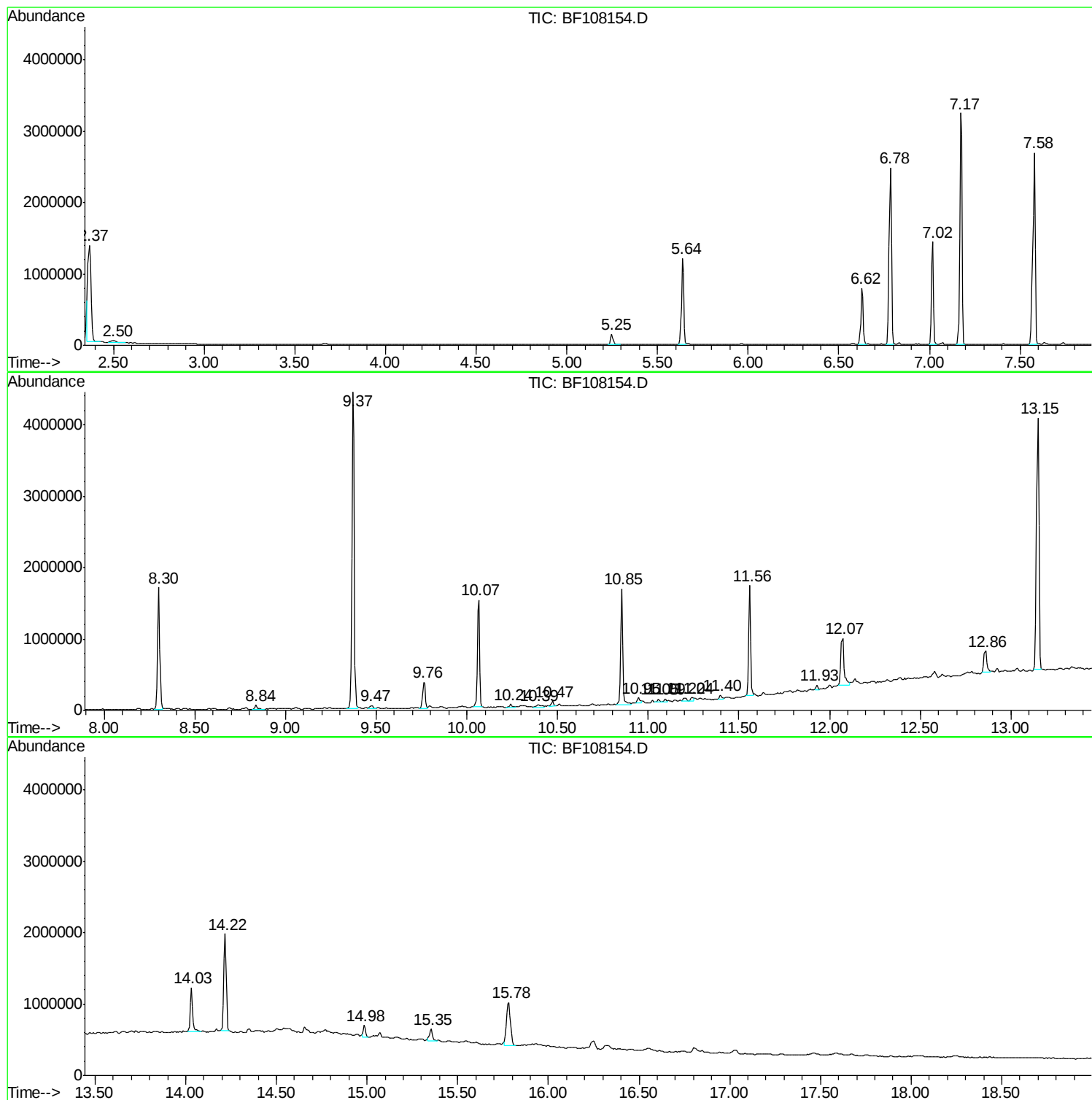
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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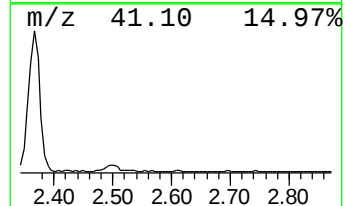
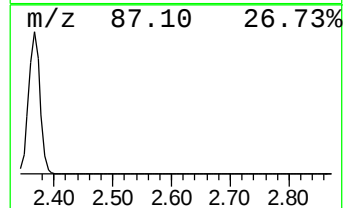
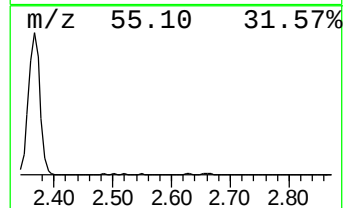
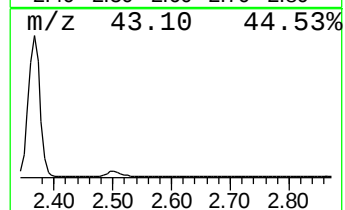
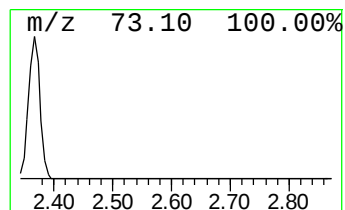
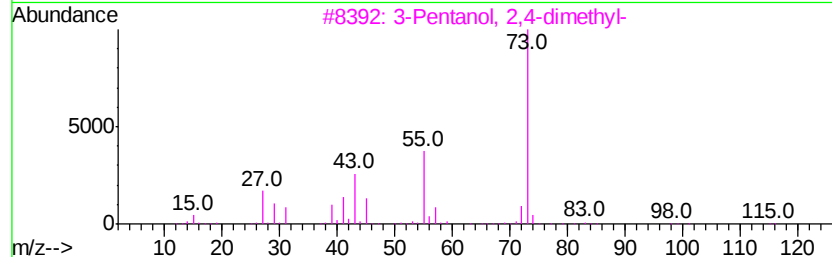
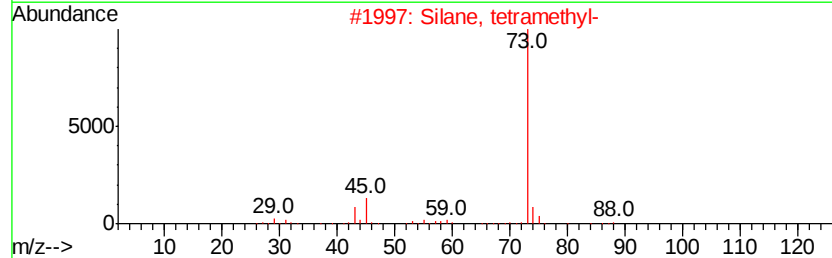
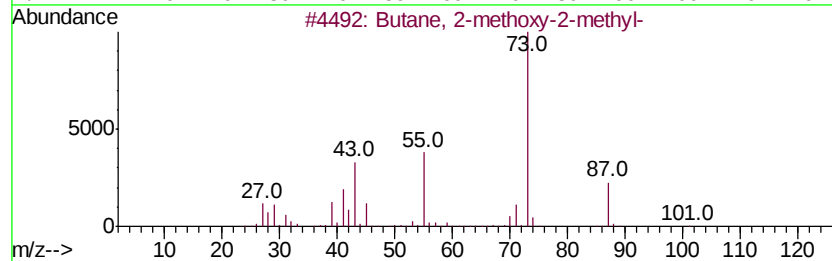
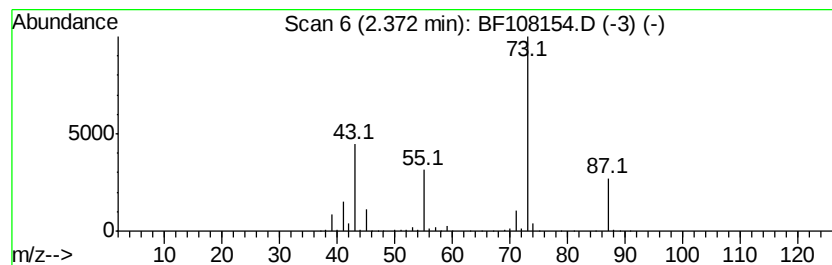
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	25.12 ng	1521560	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
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		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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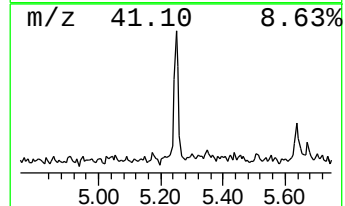
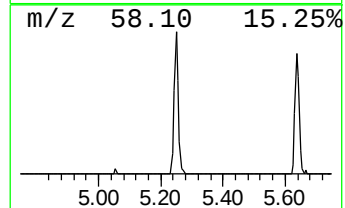
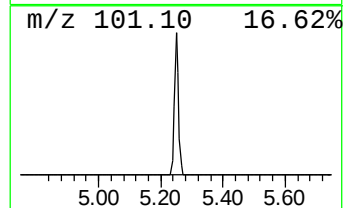
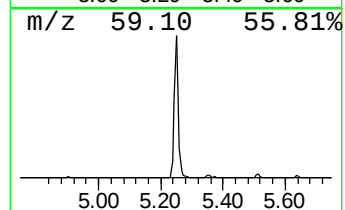
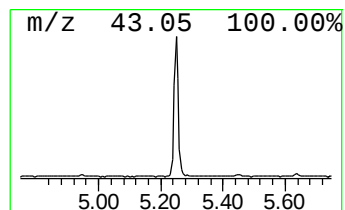
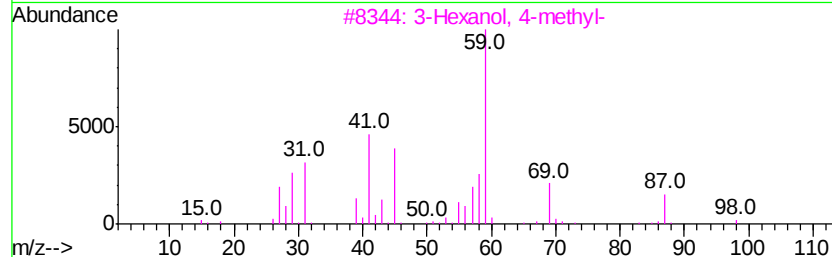
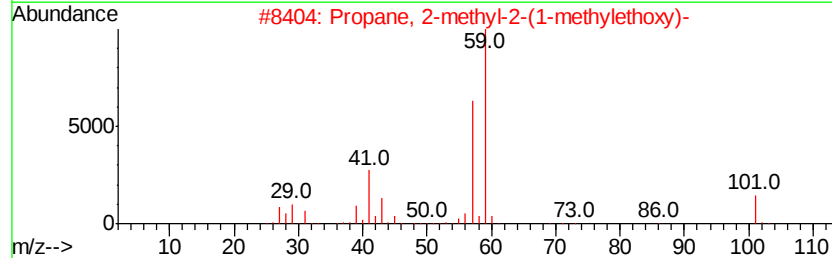
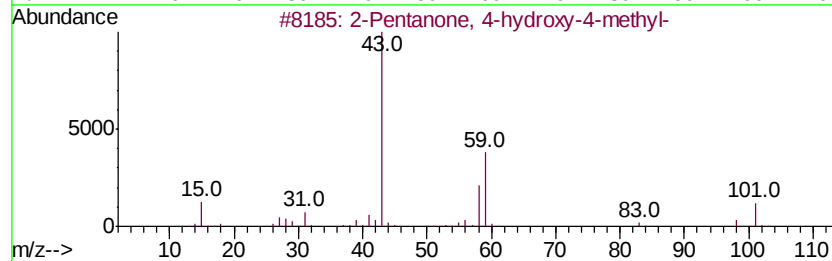
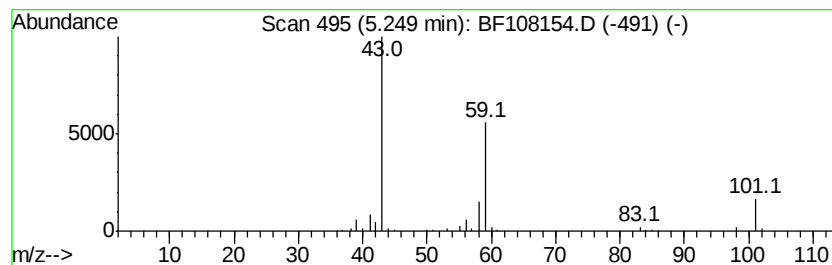
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	2.36 ng	143089	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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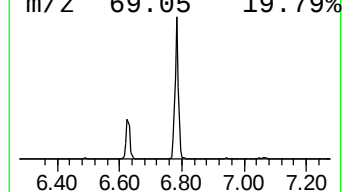
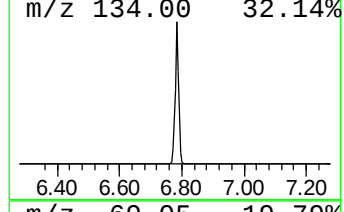
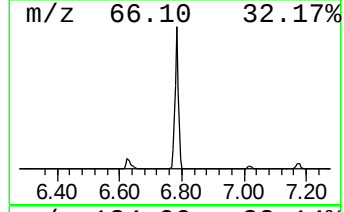
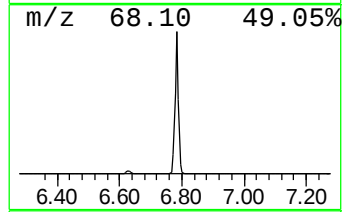
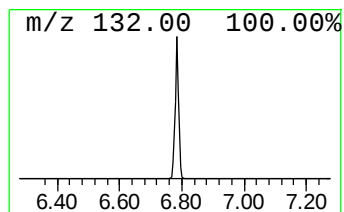
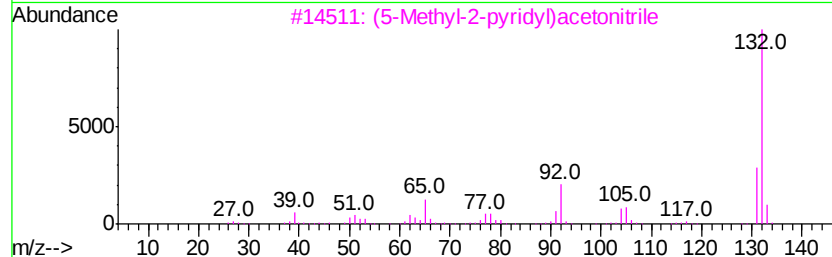
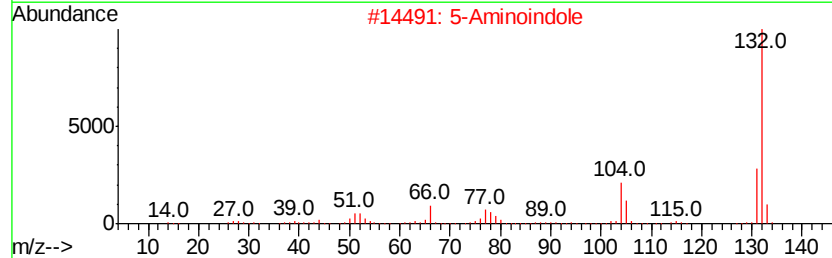
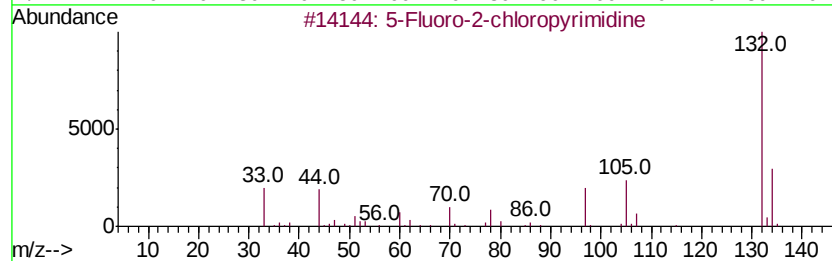
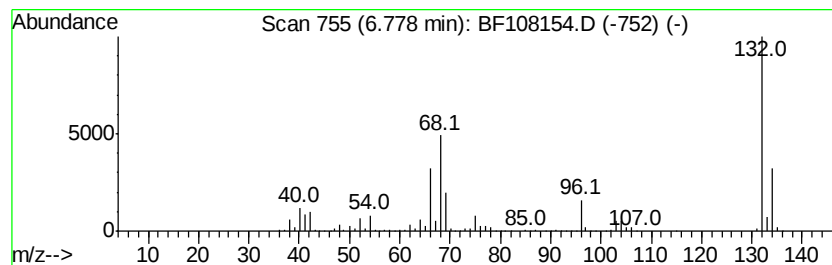
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.78 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	33.94 ng	2056180	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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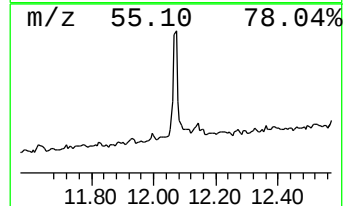
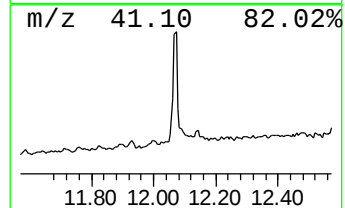
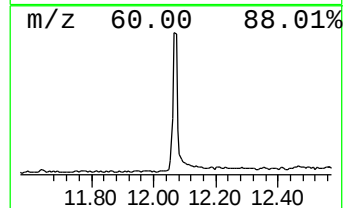
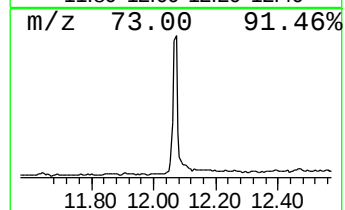
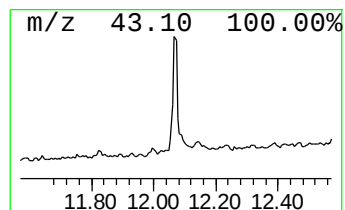
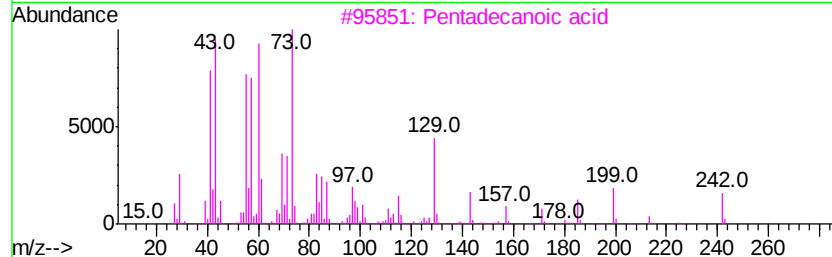
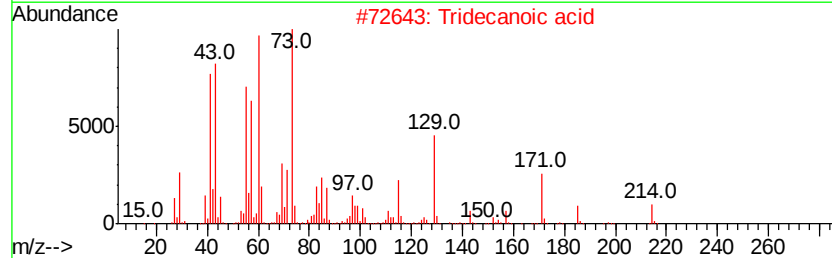
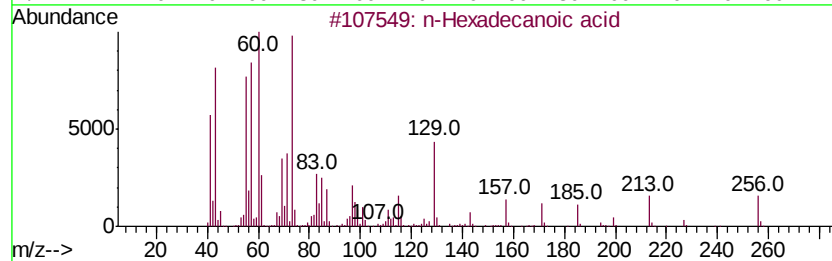
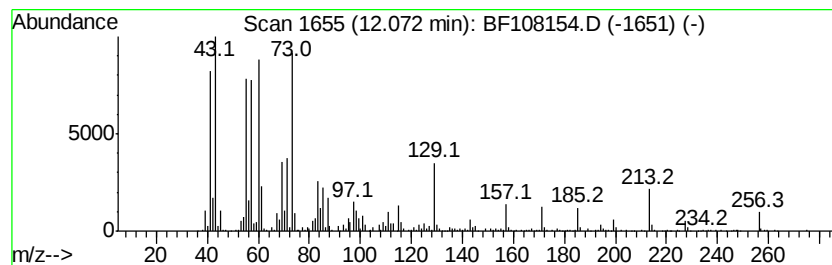
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	12.09 ng	766147	Phenanthrene-d10	11.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Undecanoic acid	186	C11H22O2	000112-37-8	70
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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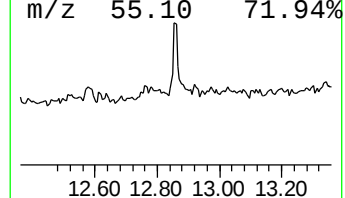
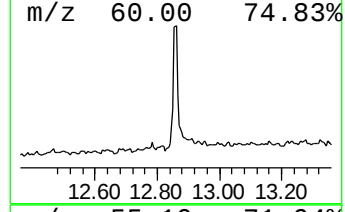
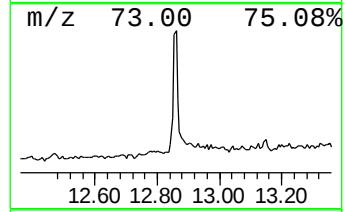
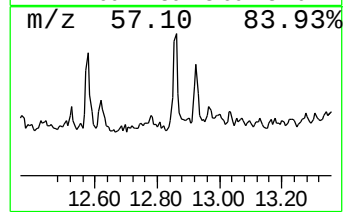
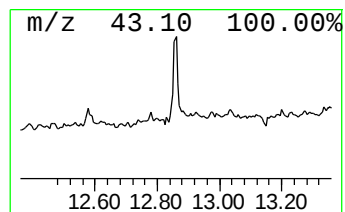
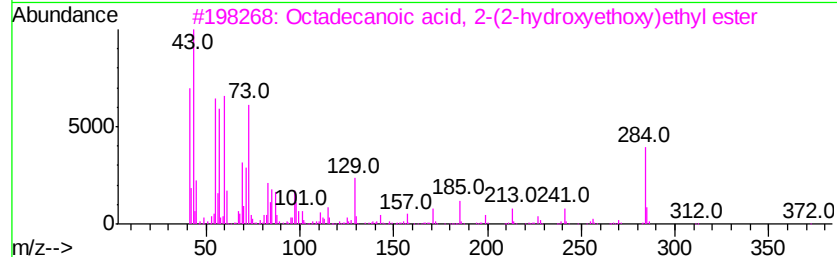
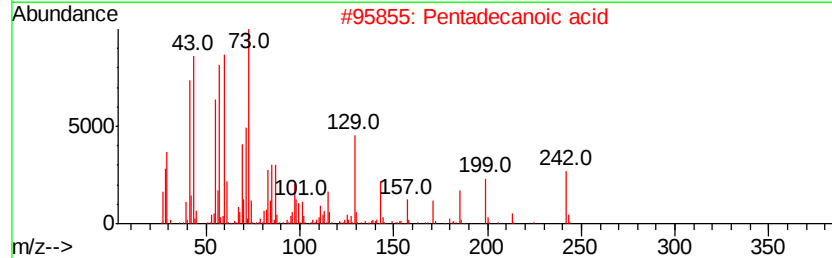
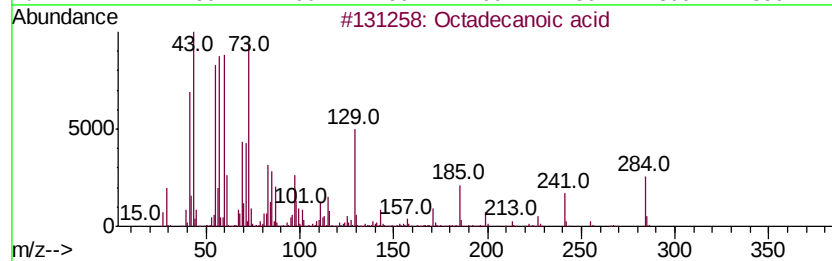
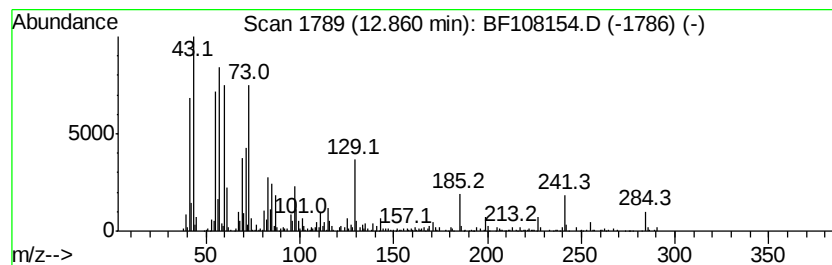
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	5.08 ng	322106	Phenanthrene-d10	11.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108154.D
Acq On : 14 Aug 2018 19:29
Operator : JU/SJ
Sample : J4458-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-93

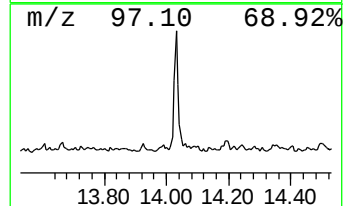
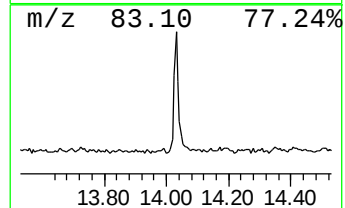
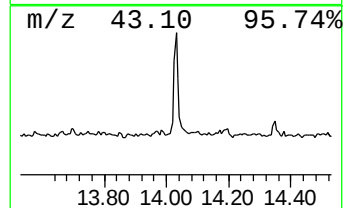
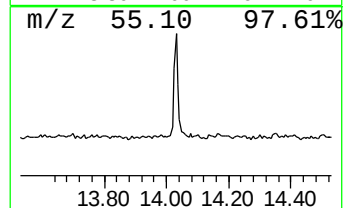
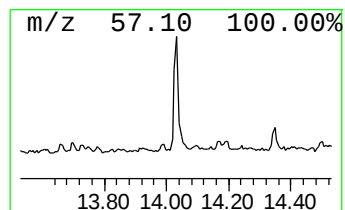
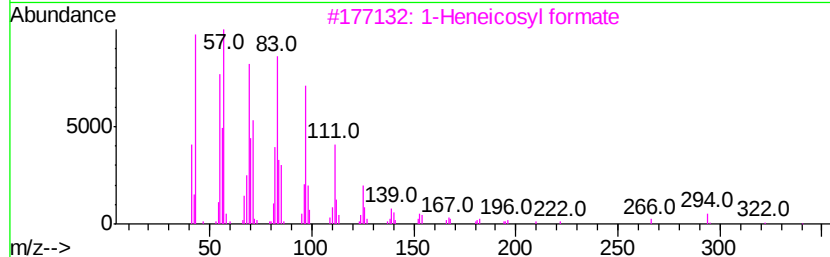
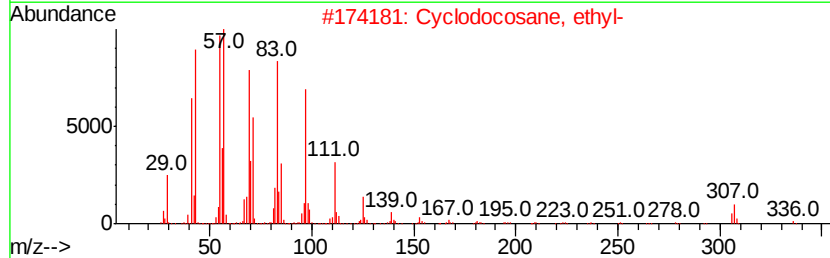
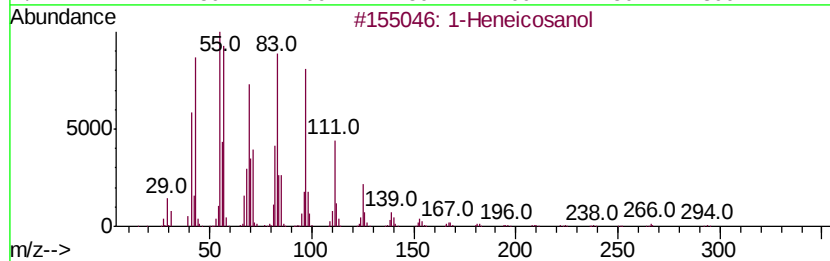
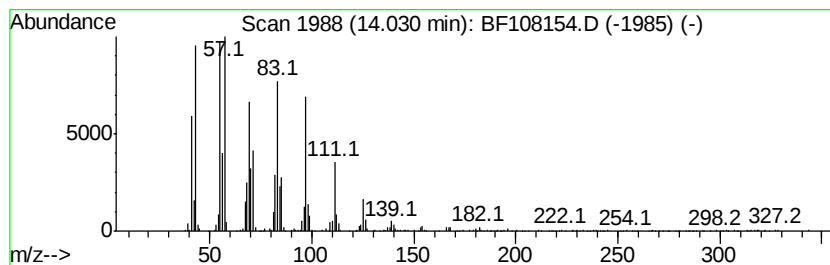
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	10.27 ng	601127	Chrysene-d12	14.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108154.D
Acq On : 14 Aug 2018 19:29
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Sample : J4458-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

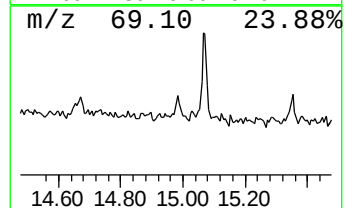
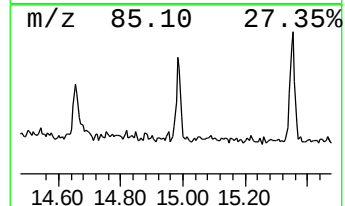
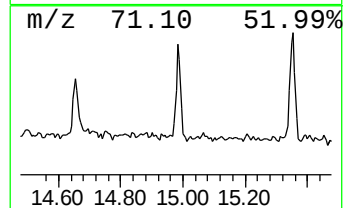
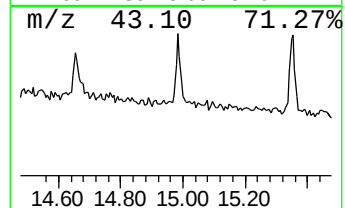
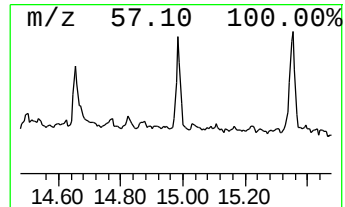
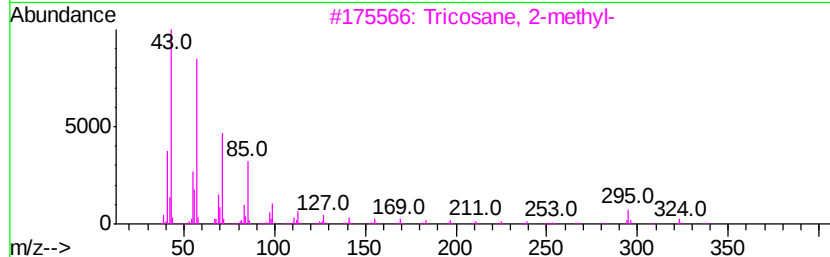
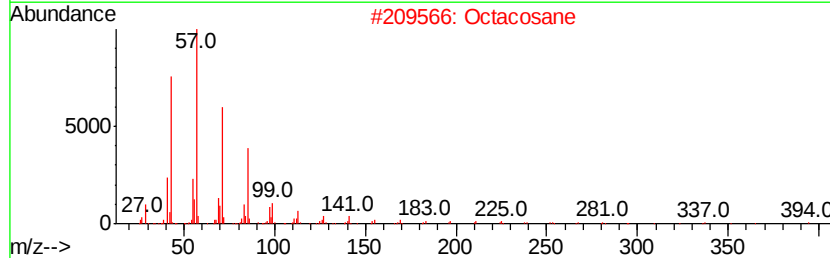
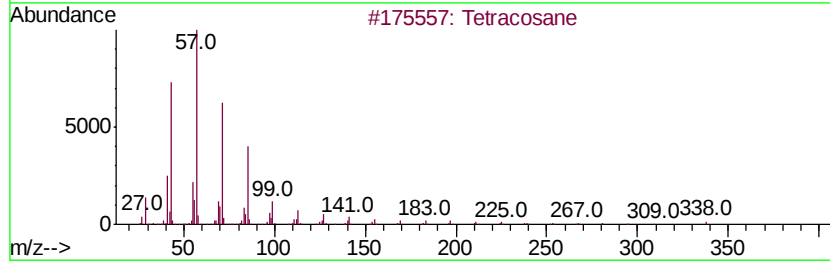
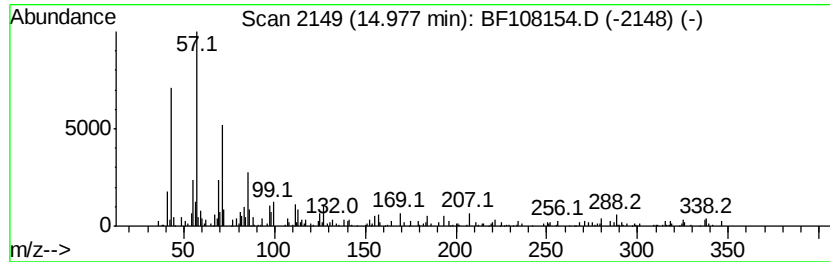
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.63 ng	153765	Chrysene-d12	14.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetracosane	338 C24H50	000646-31-1 96
2		Octacosane	394 C28H58	000630-02-4 87
3		Tricosane, 2-methyl-	338 C24H50	001928-30-9 87
4		Eicosane, 7-hexyl-	366 C26H54	055333-99-8 83
5		Eicosane, 10-methyl-	296 C21H44	054833-23-7 80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108154.D
Acq On : 14 Aug 2018 19:29
Operator : JU/SJ
Sample : J4458-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-93

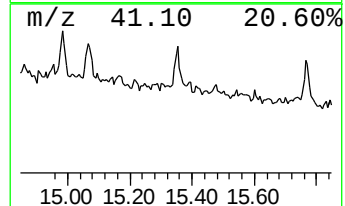
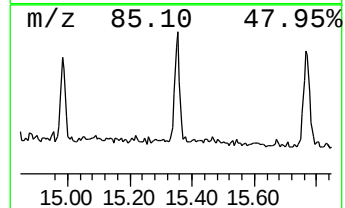
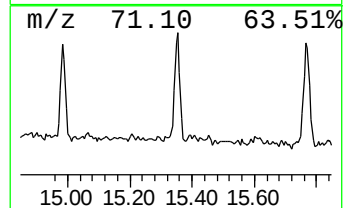
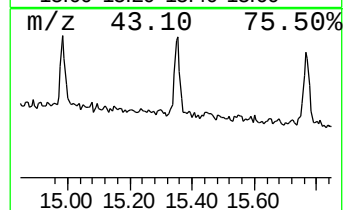
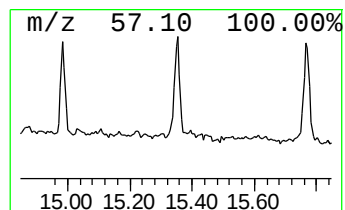
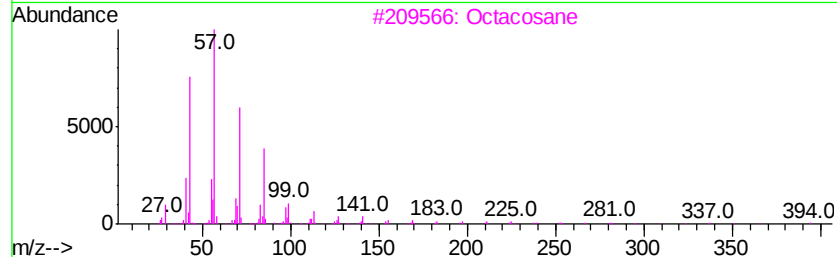
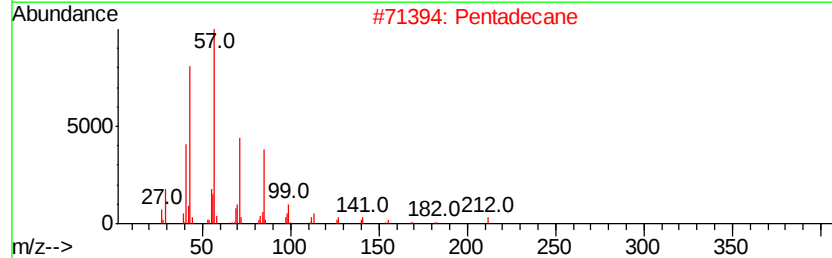
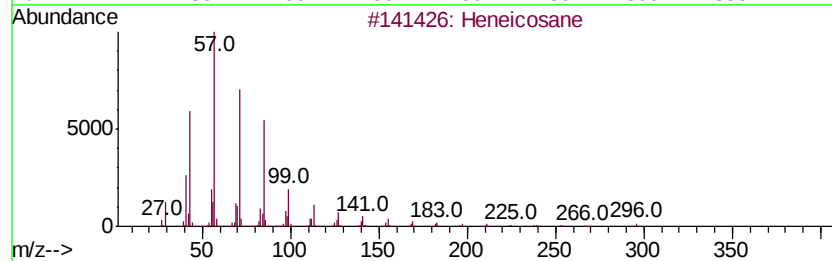
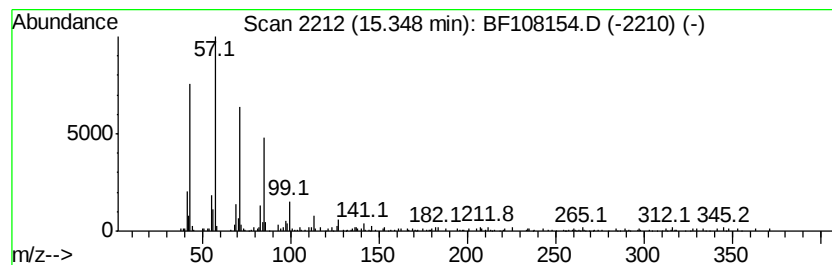
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.35	3.87 ng	182256	Perylene-d12	15.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Pentadecane		212	C15H32	000629-62-9	87
3	Octacosane		394	C28H58	000630-02-4	87
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	80
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081418\
Data File : BF108154.D
Acq On : 14 Aug 2018 19:29
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Sample : J4458-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-93

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	2.37	25.1	ng	1521560	1	7.02	1211640	20.0
2-Pentanone, 4-hy...	5.25	2.4	ng	143089	1	7.02	1211640	20.0
unknown6.78	6.78	33.9	ng	2056180	1	7.02	1211640	20.0
n-Hexadecanoic acid	12.07	12.1	ng	766147	4	11.56	1267800	20.0
Octadecanoic acid	12.86	5.1	ng	322106	4	11.56	1267800	20.0
1-Heneicosanol	14.03	10.3	ng	601127	5	14.22	1170470	20.0
Tetracosane	14.98	2.6	ng	153765	5	14.22	1170470	20.0
Heneicosane	15.35	3.9	ng	182256	6	15.78	942907	20.0