

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120518\
 Data File : BF111118.D
 Acq On : 5 Dec 2018 20:21
 Operator : JU/SJ
 Sample : J5764-27 2X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JC-02-113018-D

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-BF120518.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	4.998	491	495	502	rVB	324390	380864	5.14%	0.526%
2	5.410	560	565	568	rBV	7107347	6628750	89.45%	9.149%
3	6.428	733	738	746	rBV	7905951	7410567	100.00%	10.228%
4	6.569	758	762	766	rBV	7833688	6877692	92.81%	9.493%
5	6.804	798	802	806	rBV	4253956	3414739	46.08%	4.713%
6	6.963	825	829	832	rVB	6465018	5184188	69.96%	7.156%
7	7.363	892	897	900	rBV	4947955	4328740	58.41%	5.975%
8	8.086	1016	1020	1023	rBV	5733829	4536677	61.22%	6.262%
9	8.522	1090	1094	1099	rBV	82669	98759	1.33%	0.136%
10	9.163	1199	1203	1206	rBV	9062042	7225171	97.50%	9.973%
11	9.257	1213	1219	1223	rBV5	92259	117254	1.58%	0.162%
12	9.504	1254	1261	1263	rBV7	67008	116272	1.57%	0.160%
13	9.551	1267	1269	1272	rBV	450239	383635	5.18%	0.530%
14	9.839	1314	1318	1322	rBV2	5333016	4480946	60.47%	6.185%
15	10.039	1349	1352	1356	rVB	104789	104916	1.42%	0.145%
16	10.622	1447	1451	1454	rBV	4149002	3343967	45.12%	4.616%
17	11.204	1547	1550	1554	rBV3	67726	87734	1.18%	0.121%
18	11.322	1566	1570	1572	rBV	4427382	3633034	49.03%	5.015%
19	11.345	1572	1574	1577	rVB	437871	325459	4.39%	0.449%
20	11.392	1577	1582	1586	rBV2	125071	135665	1.83%	0.187%
21	11.857	1657	1661	1664	rBV	527194	533888	7.20%	0.737%
22	11.933	1671	1674	1676	rBV	108619	113624	1.53%	0.157%
23	12.410	1752	1755	1757	rBV2	303940	273134	3.69%	0.377%
24	12.433	1757	1759	1761	rVB	197460	157520	2.13%	0.217%
25	12.527	1772	1775	1778	rBV	485911	425089	5.74%	0.587%
26	12.639	1791	1794	1799	rBV	338524	395524	5.34%	0.546%
27	12.757	1809	1814	1817	rBV	474830	474617	6.40%	0.655%
28	12.904	1836	1839	1843	rBV	5598604	4717684	63.66%	6.512%
29	13.816	1991	1994	2002	rVB2	443705	525086	7.09%	0.725%
30	13.957	2013	2018	2020	rBV	3187487	3136793	42.33%	4.330%
31	13.980	2020	2022	2025	rVB	196515	165653	2.24%	0.229%
32	14.445	2099	2101	2105	rBV	185774	156067	2.11%	0.215%
33	14.745	2150	2152	2159	rVB2	270916	321582	4.34%	0.444%
34	15.080	2206	2209	2212	rVB3	324240	362864	4.90%	0.501%

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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 >
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35	15.392	2258	2262	2266	rBV	1676561	1876134	25.32%	2.590%
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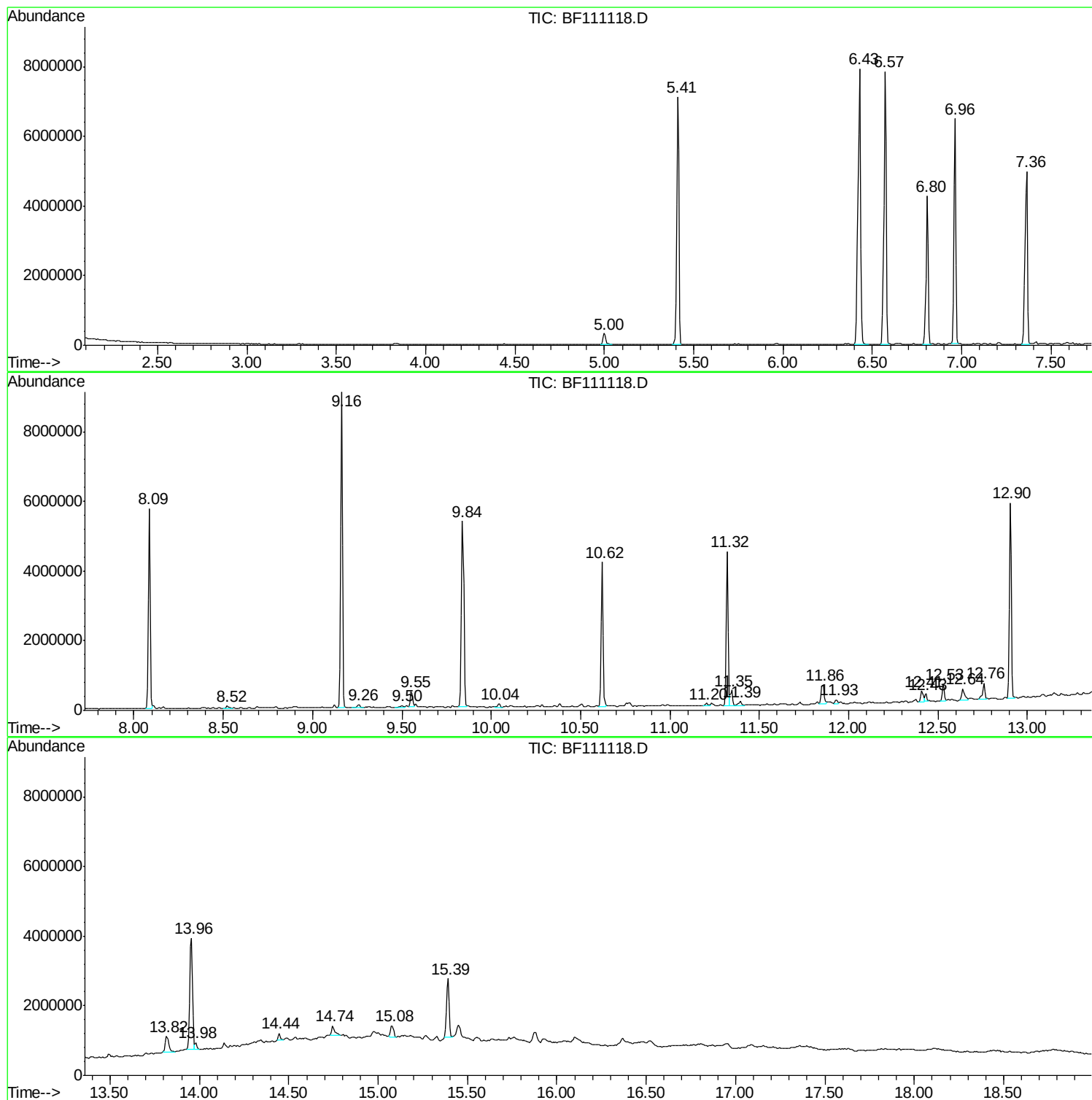
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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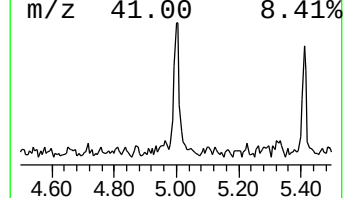
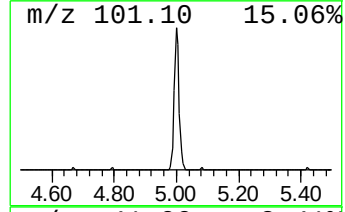
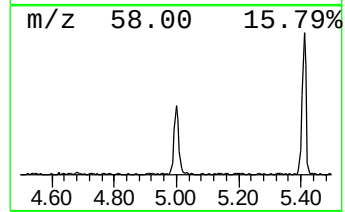
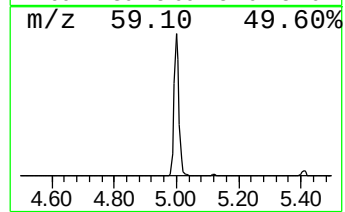
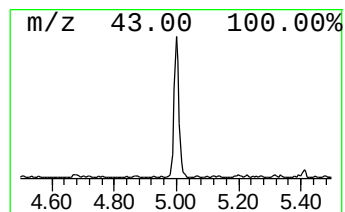
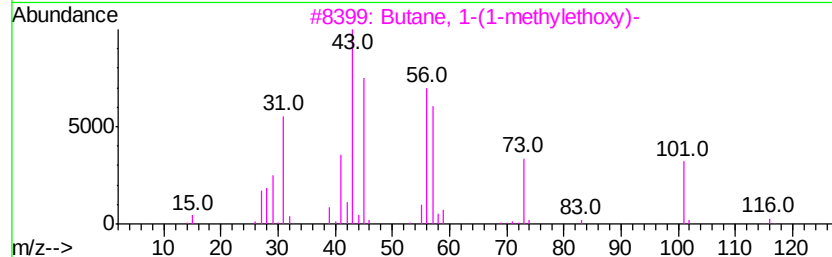
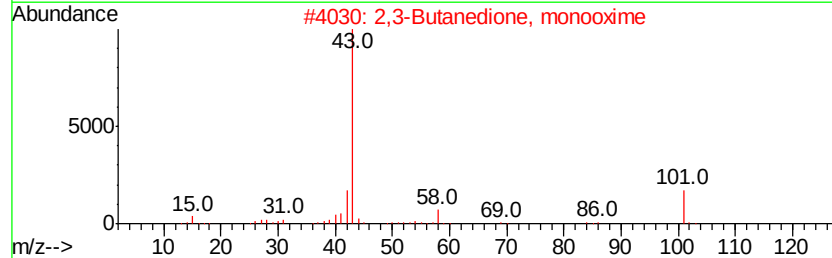
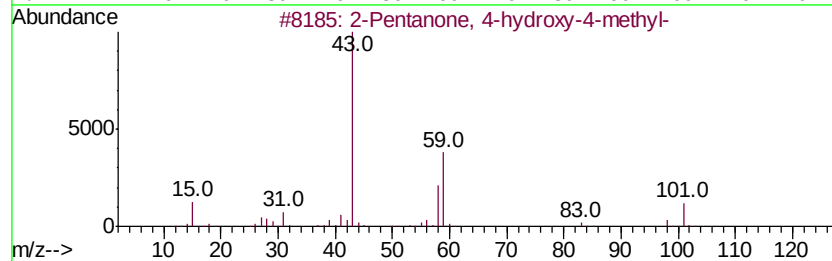
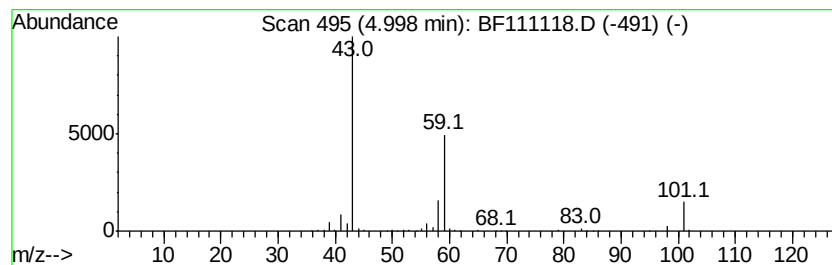
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.23 ng	380864	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	7
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7
5		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7



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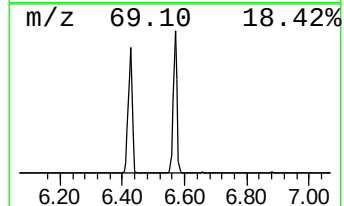
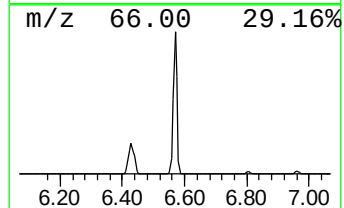
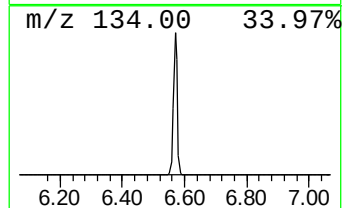
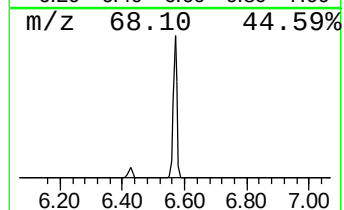
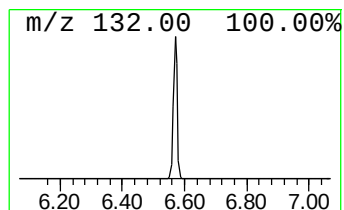
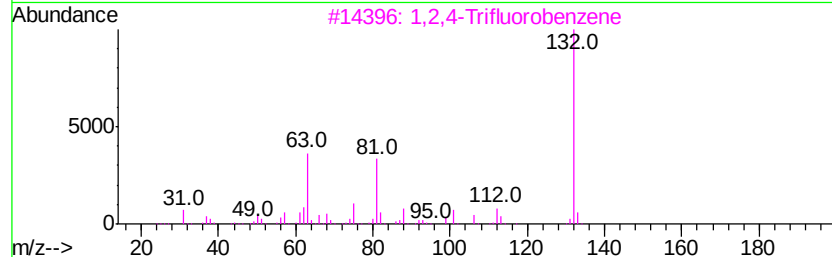
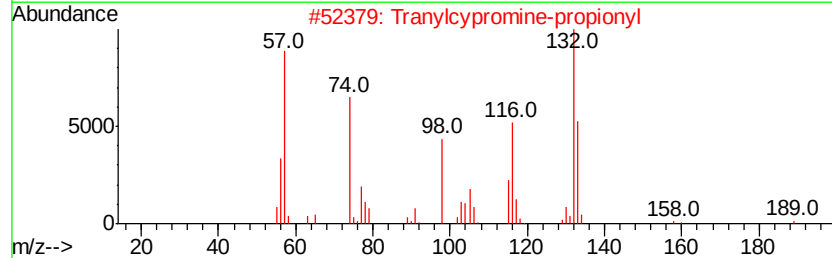
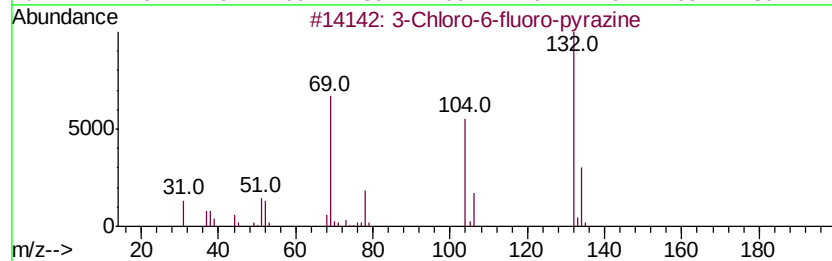
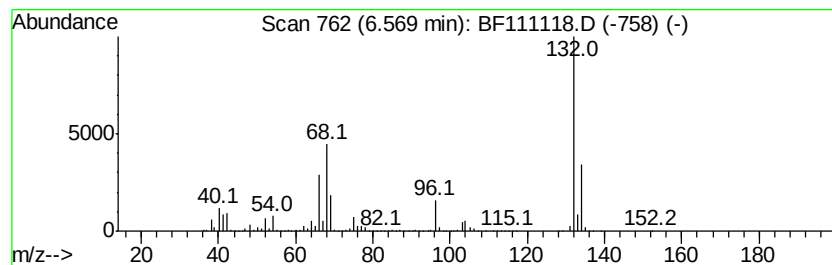
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	40.28 ng	6877690	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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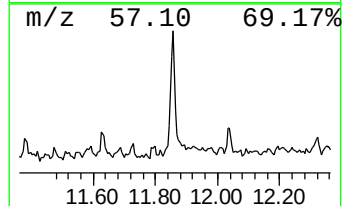
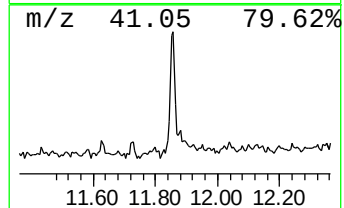
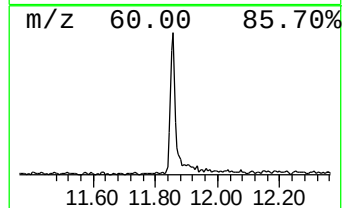
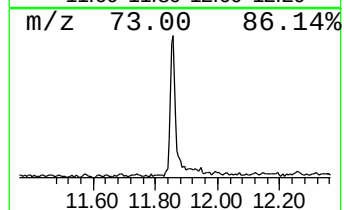
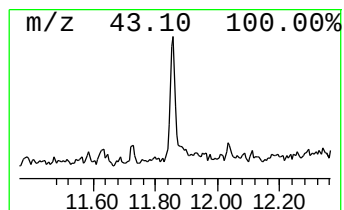
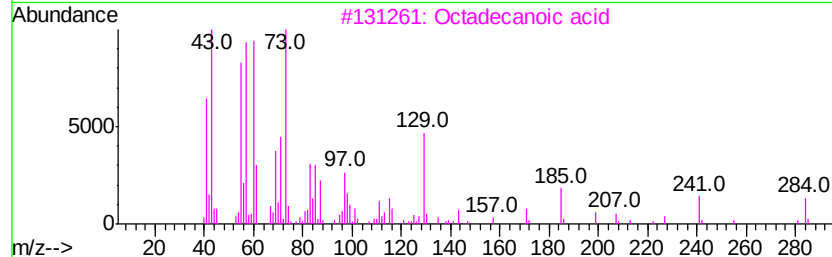
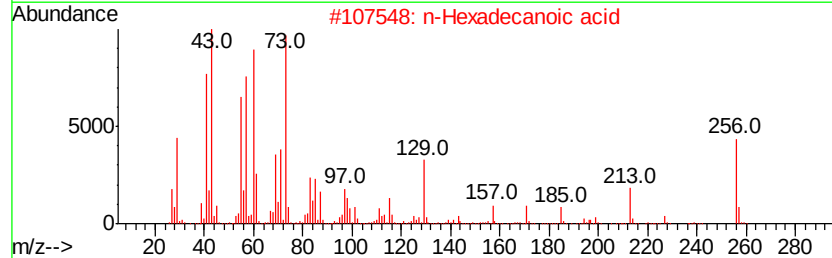
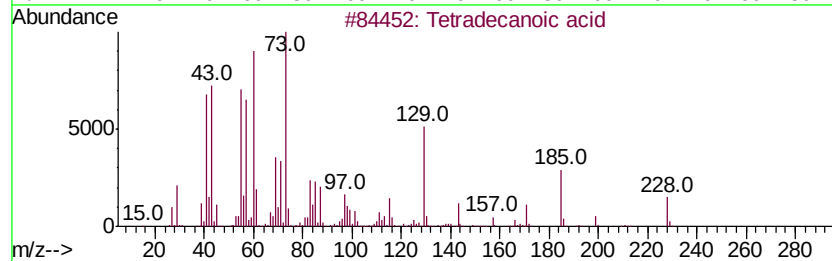
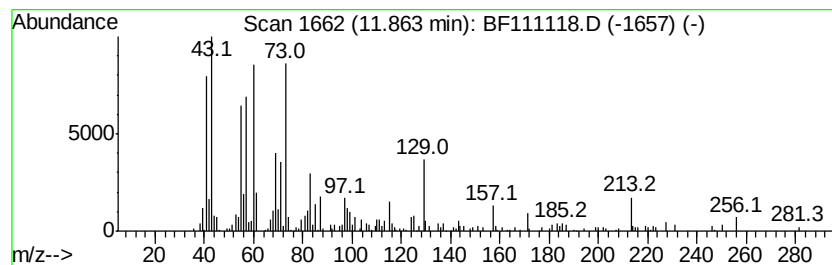
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.86	2.94 ng	533888	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72



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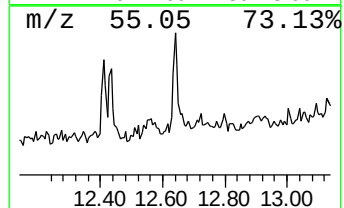
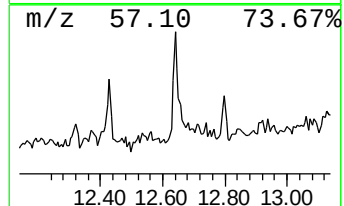
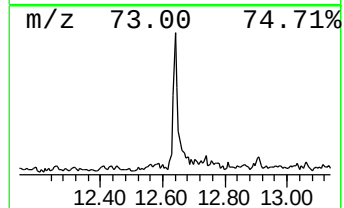
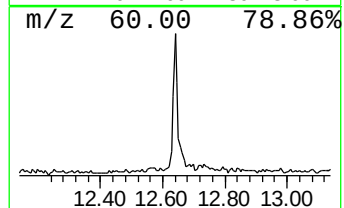
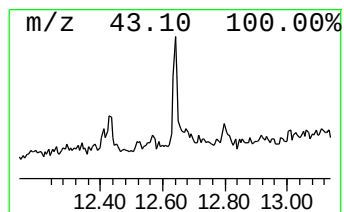
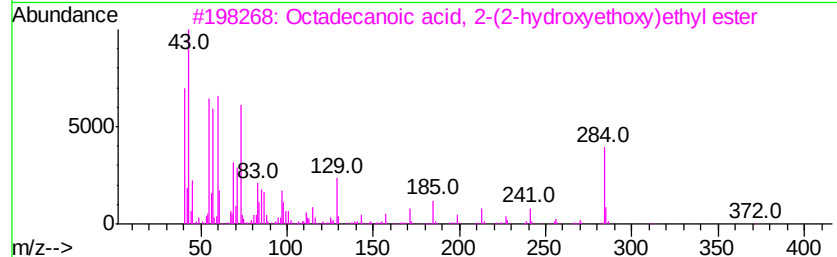
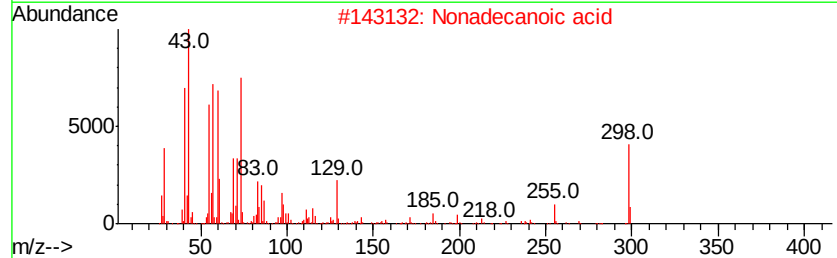
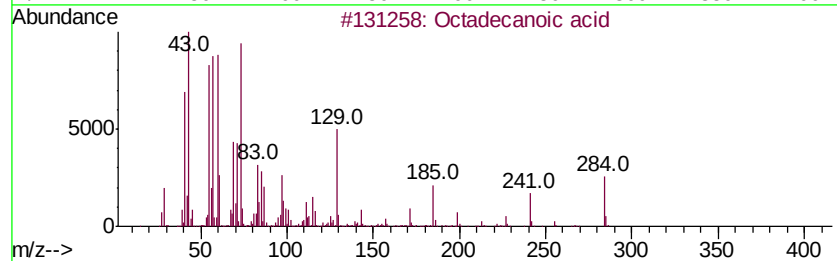
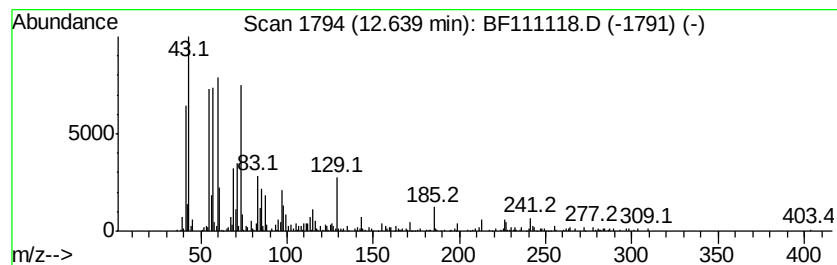
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.64	2.52 ng	395524	Chrysene-d12	13.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Nonadecanoic acid	298	C19H38O2	000646-30-0	93
3	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83



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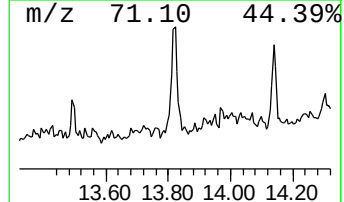
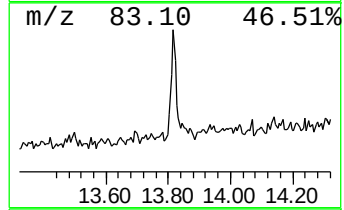
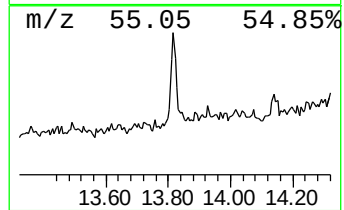
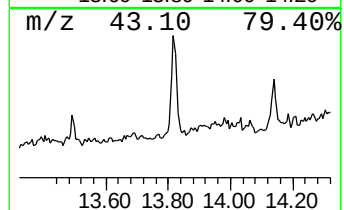
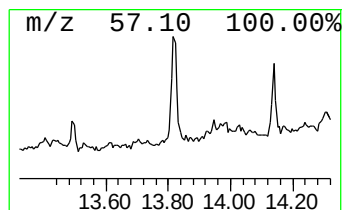
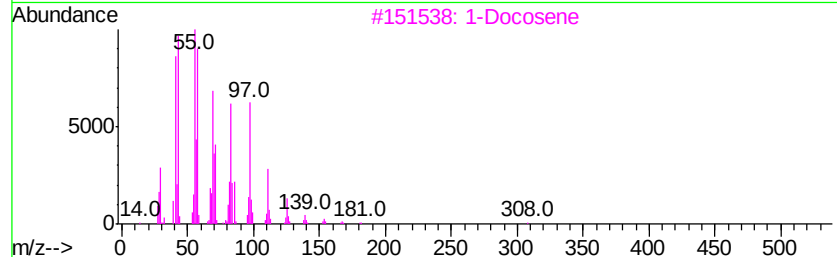
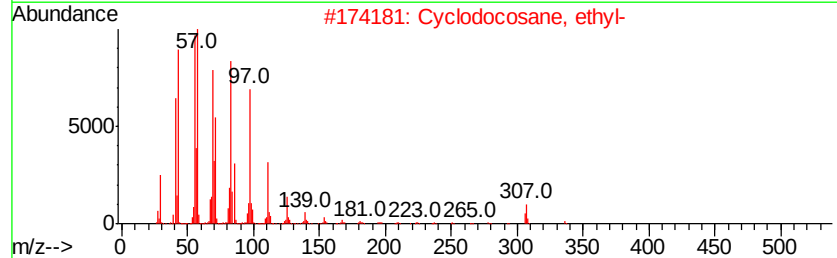
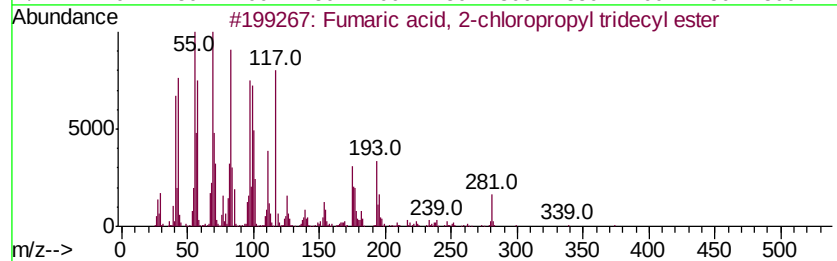
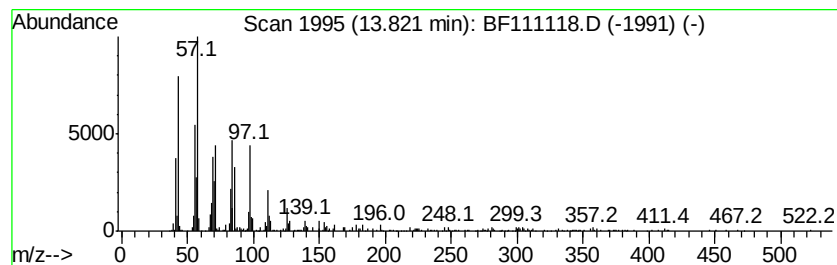
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Fumaric acid, 2-chloropropyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.35 ng	525086	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	97
2		Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	96
3		1-Docosene	308	C22H44	001599-67-3	94
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5		Fumaric acid, hexadecyl 2,2,3,3,...	554	C25H38F8O4	1000348-79-2	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
Data File : BF111118.D
Acq On : 5 Dec 2018 20:21
Operator : JU/SJ
Sample : J5764-27 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

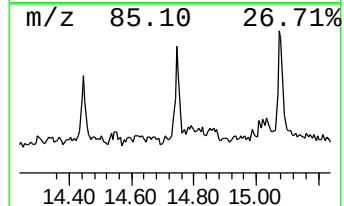
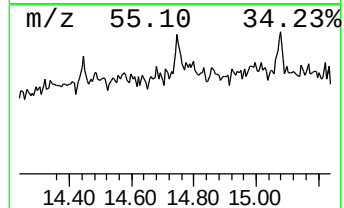
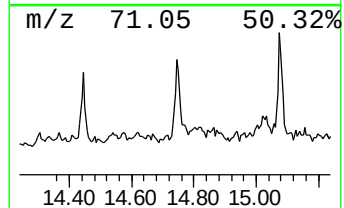
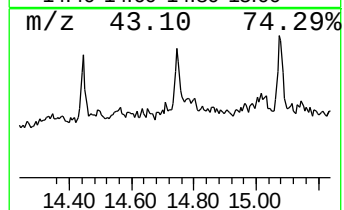
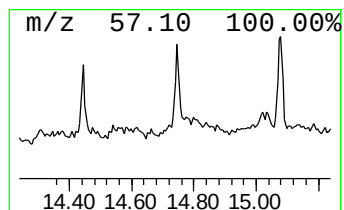
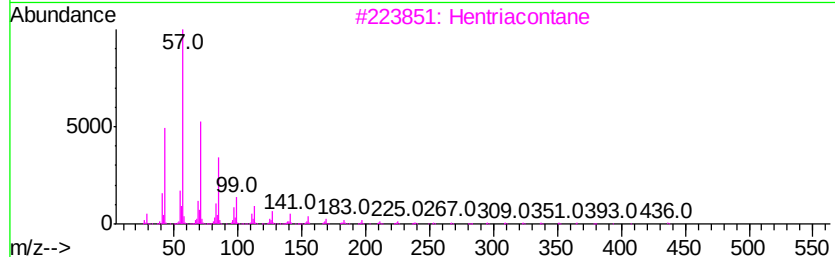
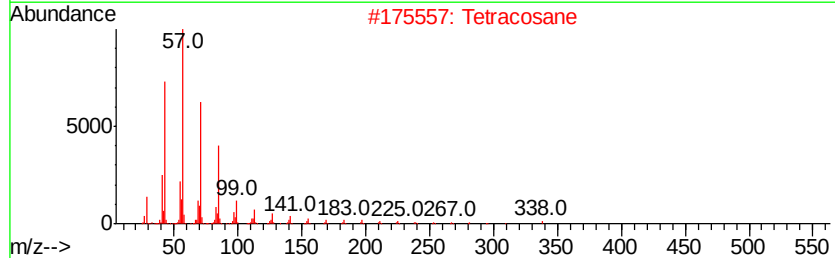
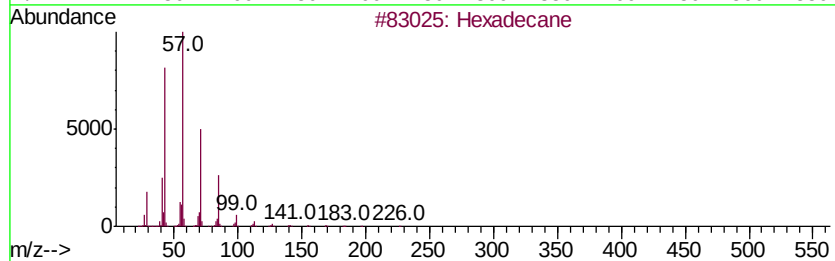
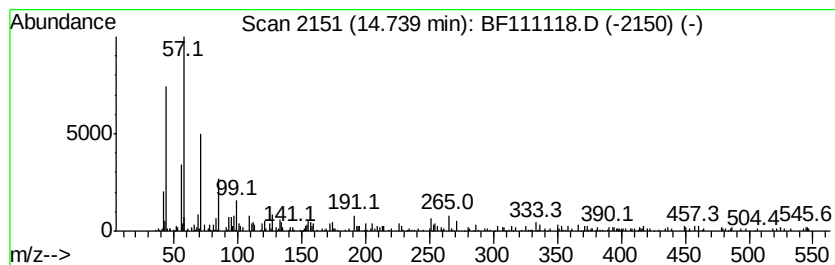
Instrument :
BNA_F
ClientSampleId :
JC-02-113018-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.74	3.43 ng	321582	Perylene-d12		15.39
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hentriacontane	437	C31H64	000630-04-6	74
4	Hexacosane	366	C26H54	000630-01-3	74
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
Data File : BF111118.D
Acq On : 5 Dec 2018 20:21
Operator : JU/SJ
Sample : J5764-27 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

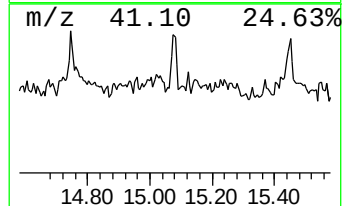
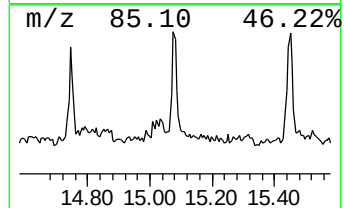
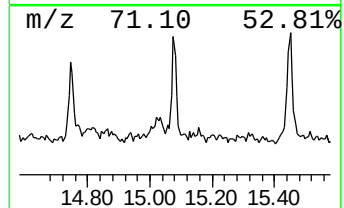
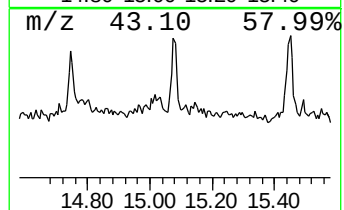
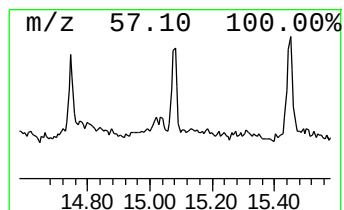
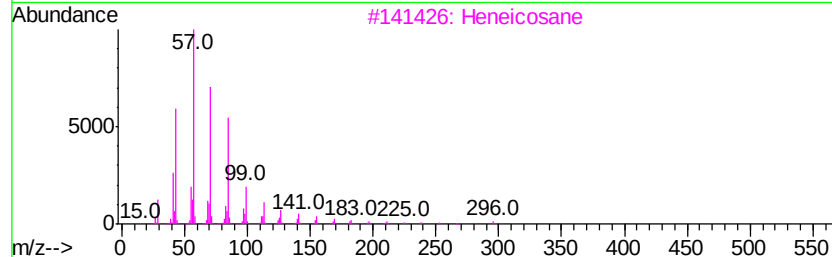
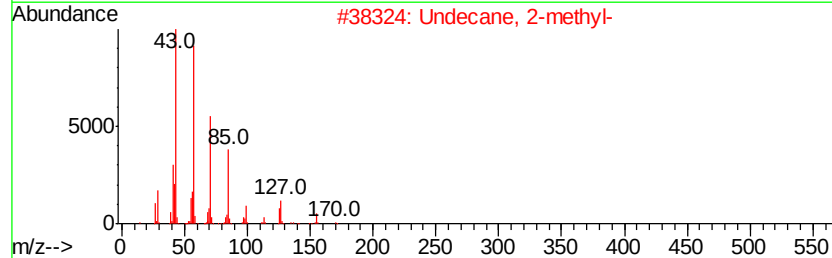
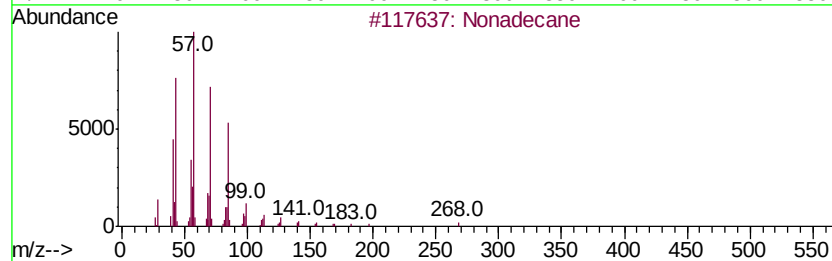
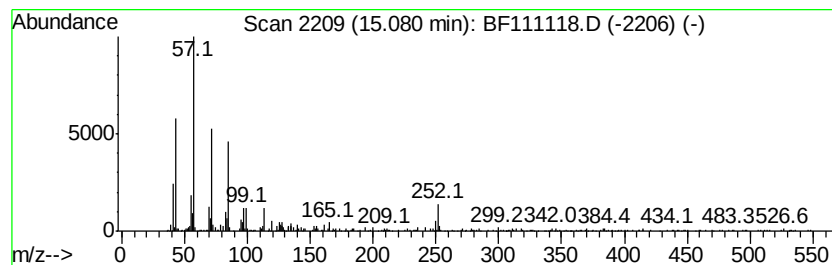
Instrument :
BNA_F
ClientSampleId :
JC-02-113018-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	3.87 ng	362864	Perylene-d12	15.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonadecane		268 C19H40	000629-92-5 64
2	Undecane, 2-methyl-		170 C12H26	007045-71-8 59
3	Heneicosane		296 C21H44	000629-94-7 59
4	Octadecane, 1-iodo-		380 C18H37I	000629-93-6 59
5	Octadecane		254 C18H38	000593-45-3 59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120518\
Data File : BF111118.D
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Operator : JU/SJ
Sample : J5764-27 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-02-113018-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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...	5.00	2.2	ng	380864	1	6.80	3414740	20.0
unknown6.57	6.57	40.3	ng	6877690	1	6.80	3414740	20.0
Tetradecanoic acid	11.86	2.9	ng	533888	4	11.32	3633030	20.0
Octadecanoic acid	12.64	2.5	ng	395524	5	13.96	3136790	20.0
Fumaric acid, 2-c...	13.82	3.4	ng	525086	5	13.96	3136790	20.0
Hexadecane	14.74	3.4	ng	321582	6	15.39	1876130	20.0
Nonadecane	15.08	3.9	ng	362864	6	15.39	1876130	20.0