

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061920\
 Data File : BF120664.D
 Acq On : 19 Jun 2020 15:27
 Operator : JU/CG
 Sample : L3020-16
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-27(13-15)

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-BF061020.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	2.116	3	5	23	rVB3	24785	71760	1.70%	0.231%
2	4.998	492	495	503	rVB	39230	48915	1.16%	0.158%
3	5.410	560	565	568	rBV	2826105	2619945	62.03%	8.438%
4	6.434	735	739	742	rBV	2708880	2745211	65.00%	8.842%
5	6.628	768	772	785	rVB	93560	99253	2.35%	0.320%
6	6.798	797	801	804	rBV	968312	788834	18.68%	2.541%
7	6.857	808	811	823	rBV2	42687	55670	1.32%	0.179%
8	6.951	823	827	831	rBV	2568504	2401845	56.87%	7.736%
9	7.363	892	897	900	rBV	1869359	1887238	44.68%	6.078%
10	8.081	1015	1019	1022	rBV	1250100	1033654	24.47%	3.329%
11	9.157	1197	1202	1205	rBV	4301945	3586551	84.92%	11.551%
12	9.275	1216	1222	1232	rVB	953130	851417	20.16%	2.742%
13	9.427	1245	1248	1253	rBV	52933	43124	1.02%	0.139%
14	9.551	1265	1269	1272	rBV	861819	699932	16.57%	2.254%
15	9.833	1313	1317	1321	rBV	1534085	1221112	28.91%	3.933%
16	10.416	1413	1416	1430	rBV	167616	210163	4.98%	0.677%
17	10.621	1447	1451	1455	rBV	2481866	2392918	56.66%	7.707%
18	11.321	1566	1570	1573	rBV	1420005	1318199	31.21%	4.246%
19	11.557	1604	1610	1619	rBV5	46330	91364	2.16%	0.294%
20	11.851	1656	1660	1663	rBV	228070	207770	4.92%	0.669%
21	12.380	1746	1750	1760	rBV3	67701	141449	3.35%	0.456%
22	12.457	1760	1763	1769	rVB	48815	47243	1.12%	0.152%
23	12.568	1778	1782	1785	rVB	48259	46802	1.11%	0.151%
24	12.910	1835	1840	1843	rBV	4271050	4223532	100.00%	13.603%
25	13.139	1875	1879	1889	rBV2	29255	46203	1.09%	0.149%
26	13.815	1988	1994	2003	rBV2	239436	452613	10.72%	1.458%
27	13.957	2012	2018	2021	rBV	1401916	1362199	32.25%	4.387%
28	14.127	2043	2047	2050	rBV	63469	67885	1.61%	0.219%
29	14.280	2070	2073	2077	rBV	62991	55265	1.31%	0.178%
30	14.427	2095	2098	2101	rBV	75537	69955	1.66%	0.225%
31	14.709	2141	2146	2148	rBV2	134589	167000	3.95%	0.538%
32	14.733	2148	2150	2155	rVB	122573	113726	2.69%	0.366%
33	15.062	2202	2206	2210	rVB	123362	132209	3.13%	0.426%
34	15.404	2259	2264	2267	rBV	1095992	1347854	31.91%	4.341%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	15.427	2267	2268	2275	rVB	123352	129680	3.07%	0.418%
36	15.851	2336	2340	2346	rBV	86401	126537	3.00%	0.408%
37	16.345	2419	2424	2429	rBV	51017	87944	2.08%	0.283%
38	16.921	2518	2522	2529	rVB2	30121	56095	1.33%	0.181%

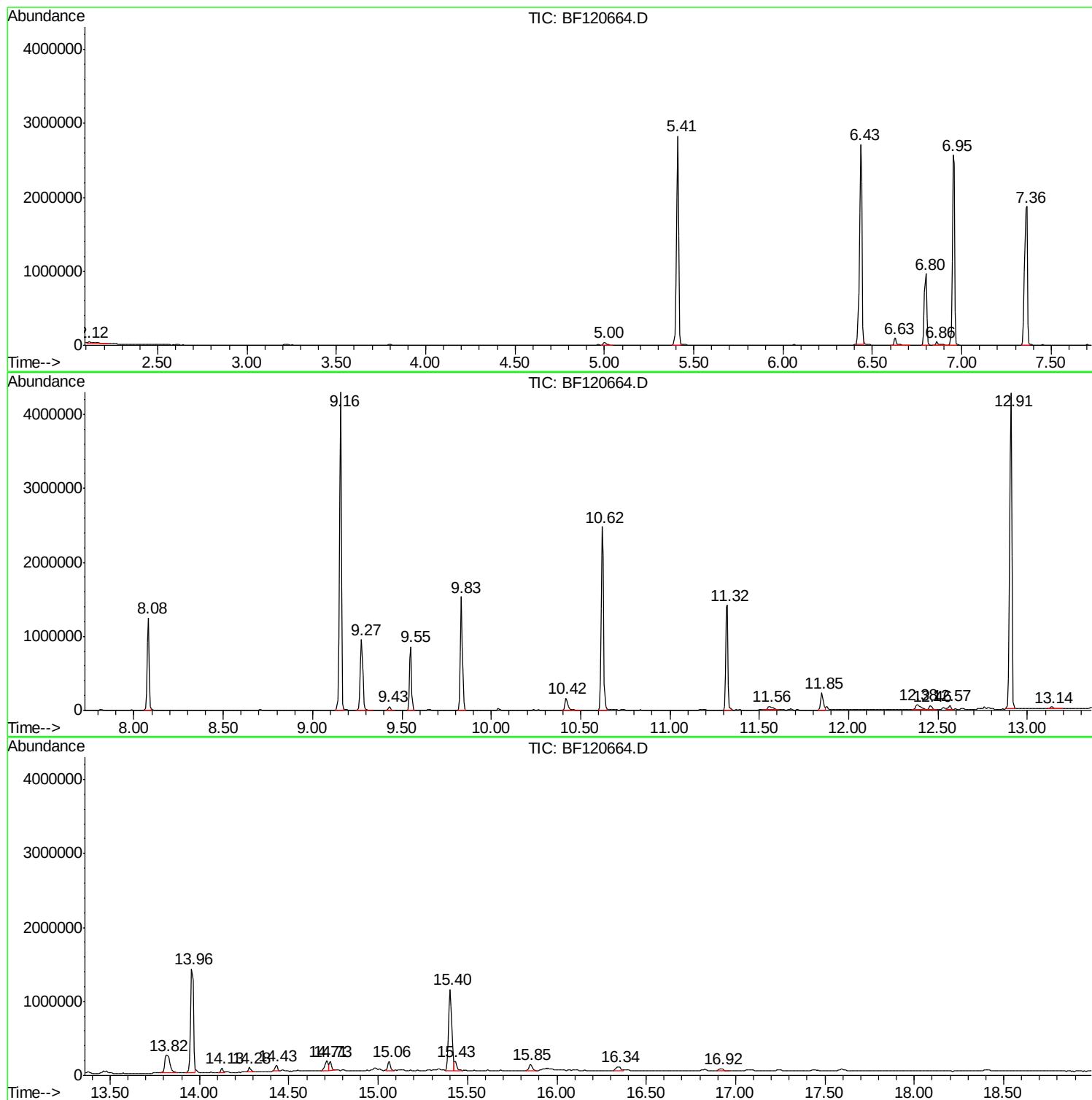
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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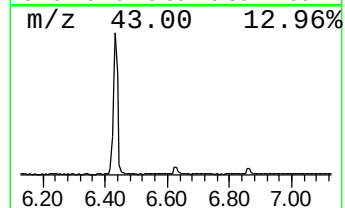
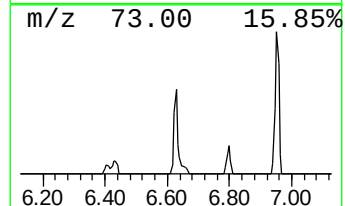
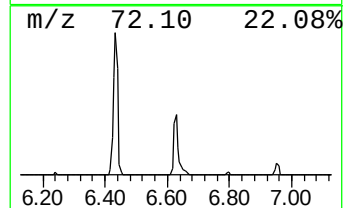
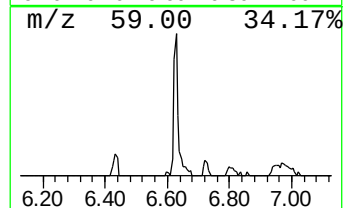
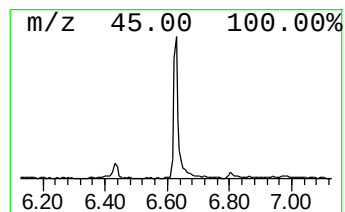
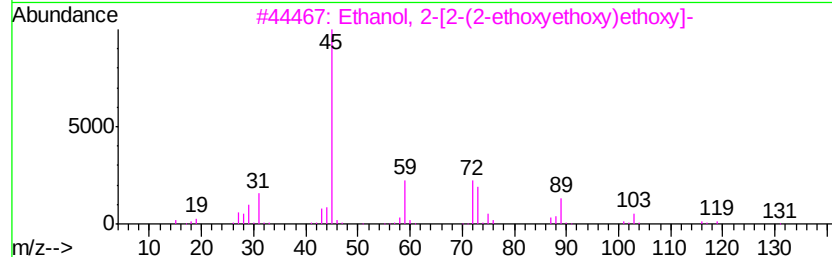
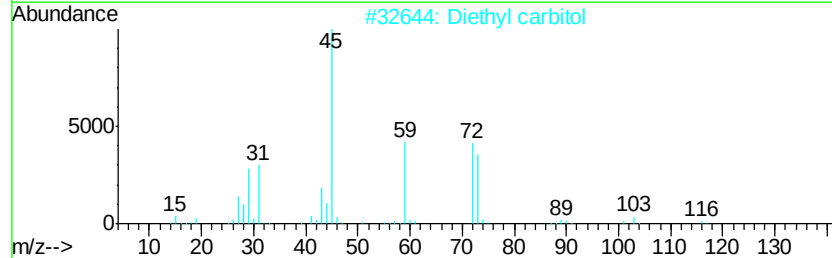
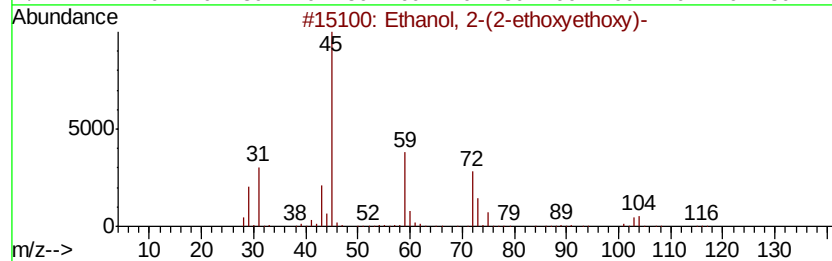
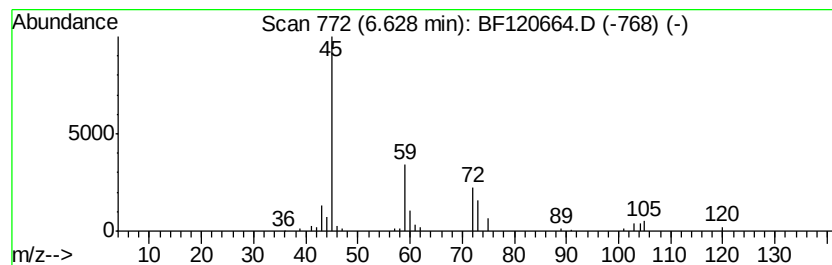
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.63	2.52 ng	99253	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	64
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	33



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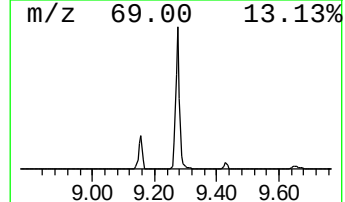
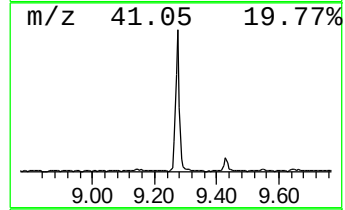
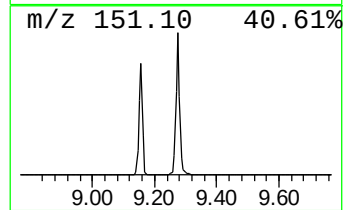
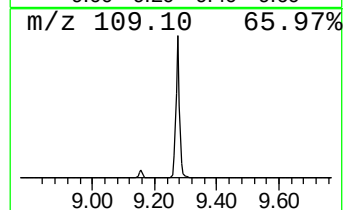
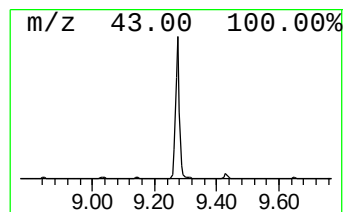
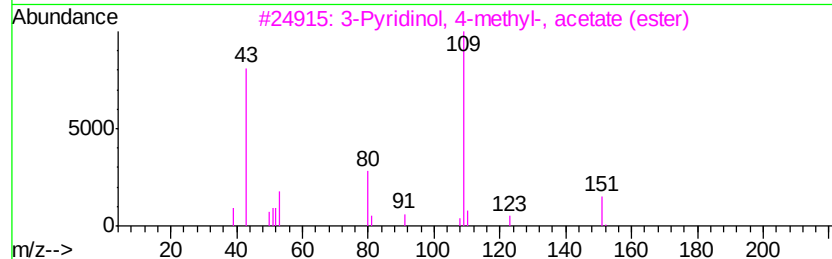
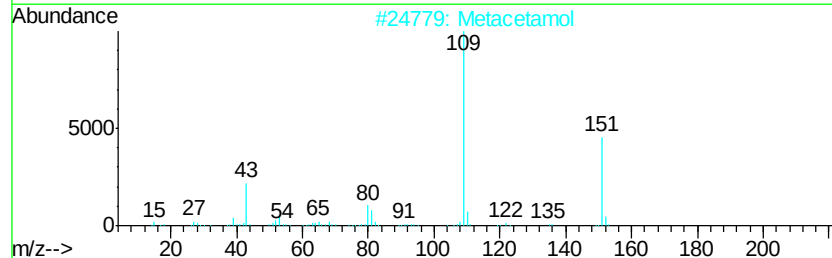
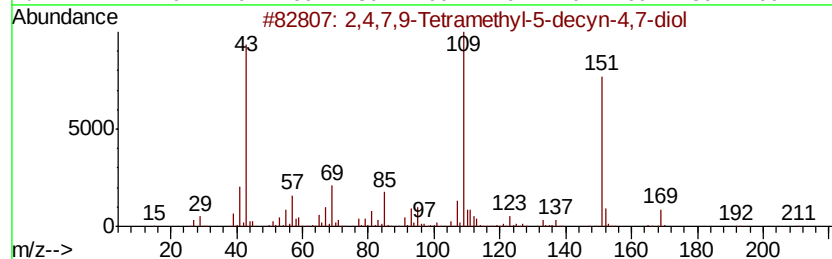
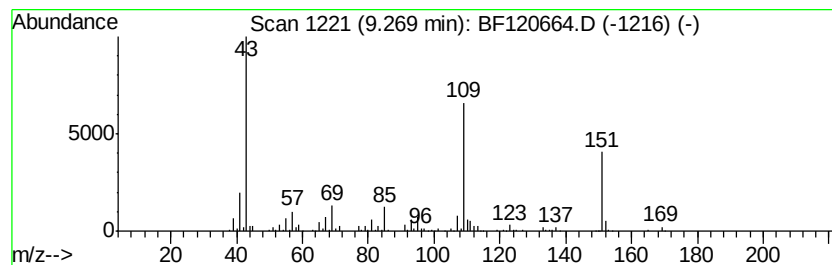
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.27	13.94 ng	851417	Acenaphthene-d10	9.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226 C14H26O2	000126-86-3	91
2	Metacetamol	151 C8H9NO2	000621-42-1	64
3	3-Pyridinol, 4-methyl-, acetate ...	151 C8H9NO2	001006-96-8	59
4	Pyridine, 2-butyl-, 1-oxide	151 C9H13NO	031396-32-4	59
5	Butanamide, N-acetyl-N-(4-hydrox...	221 C12H15NO3	1000107-08-7	45



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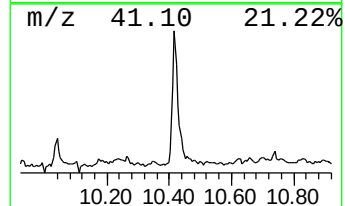
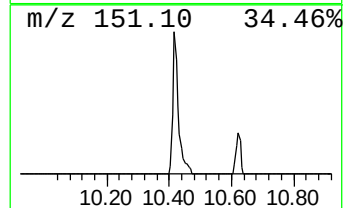
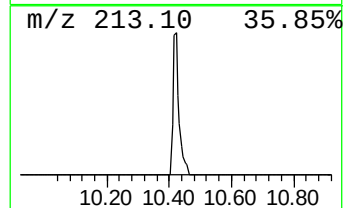
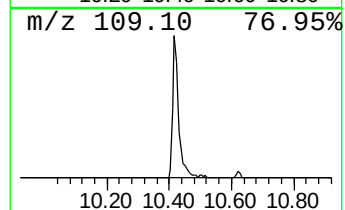
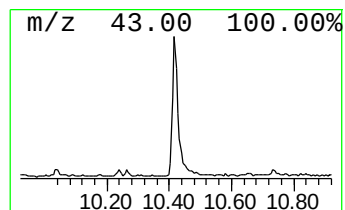
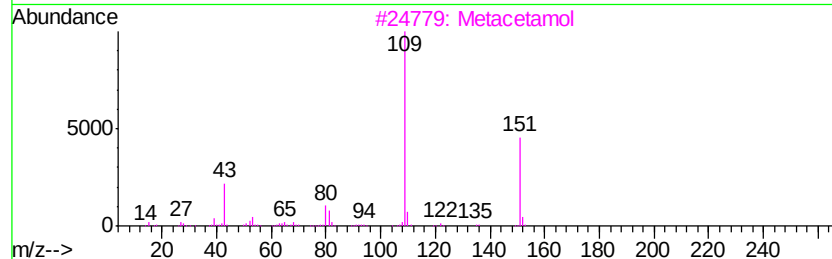
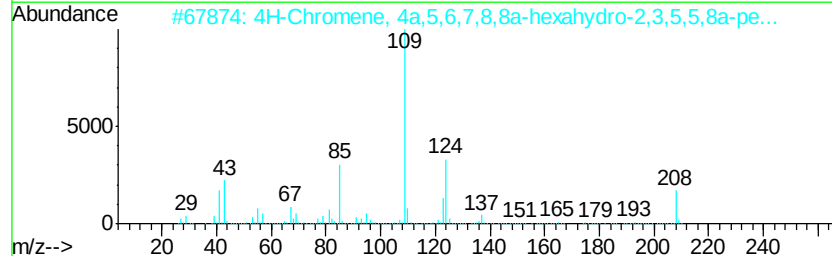
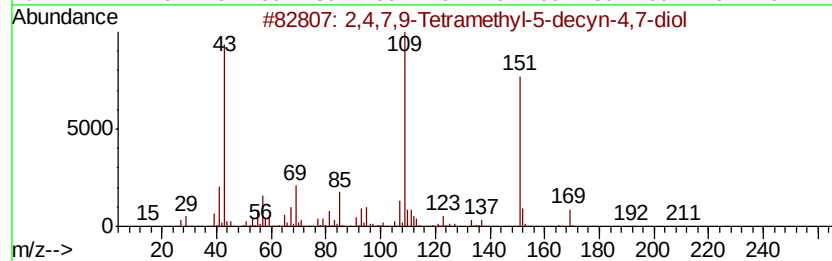
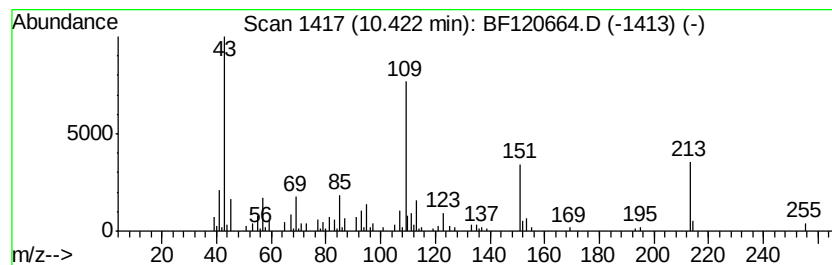
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 4 unknown10.42 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.42	3.44 ng	210163	Acenaphthene-d10	9.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	47
2		4H-Chromene, 4a,5,6,7,8,8a-hexah...	208	C14H24O	1000196-77-4	35
3		Metacetamol	151	C8H9NO2	000621-42-1	30
4		Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	27
5		4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	27



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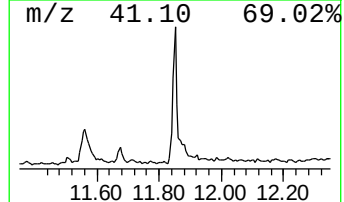
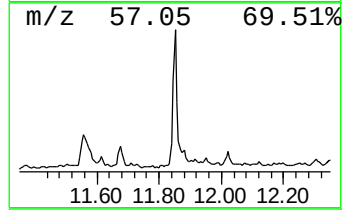
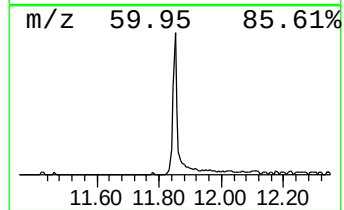
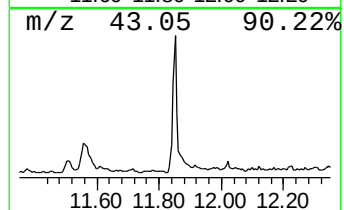
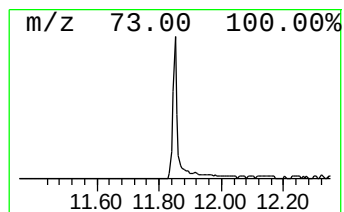
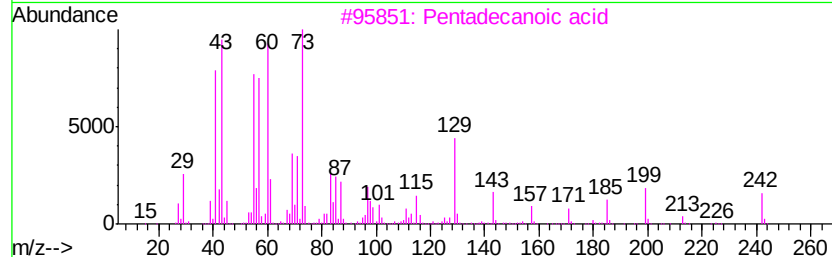
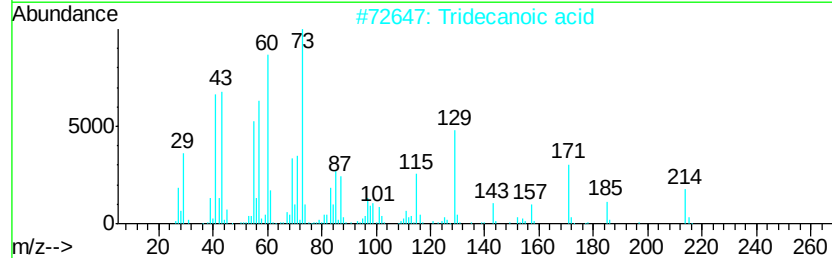
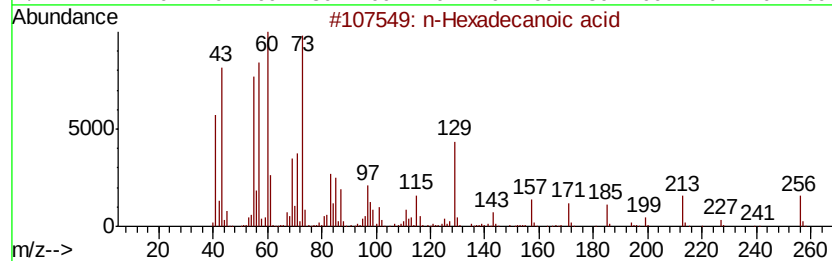
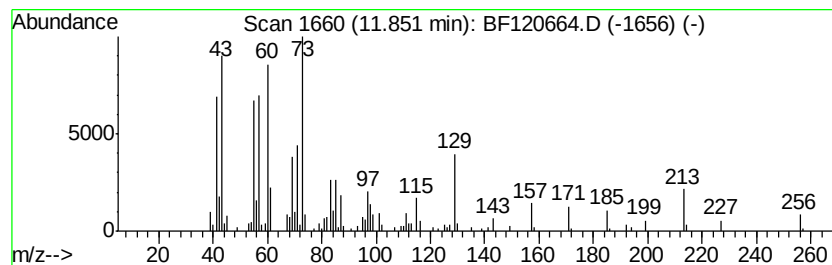
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.85	3.15 ng	207770	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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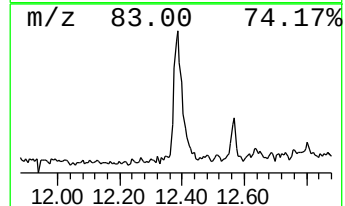
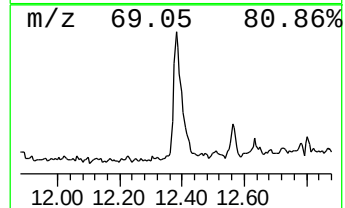
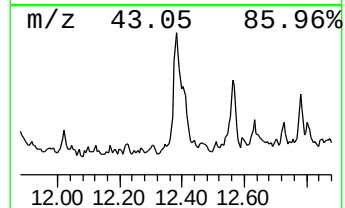
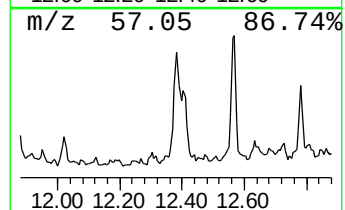
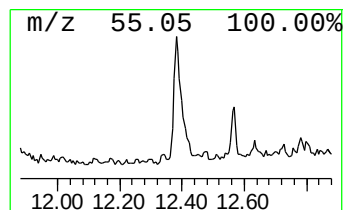
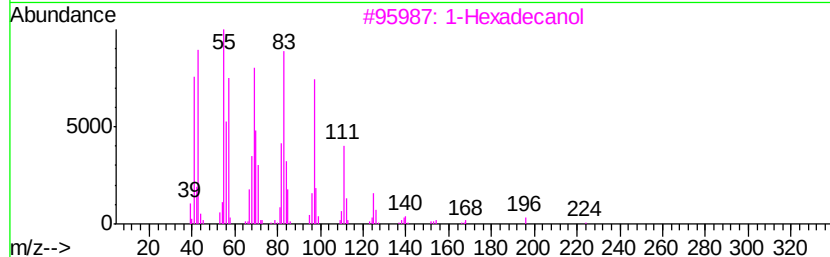
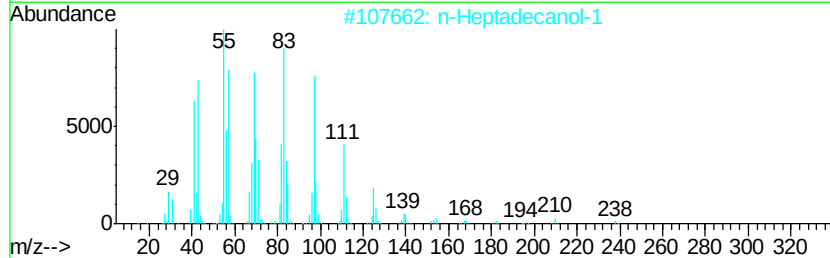
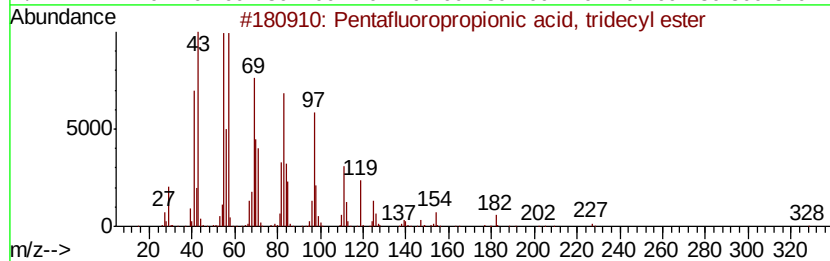
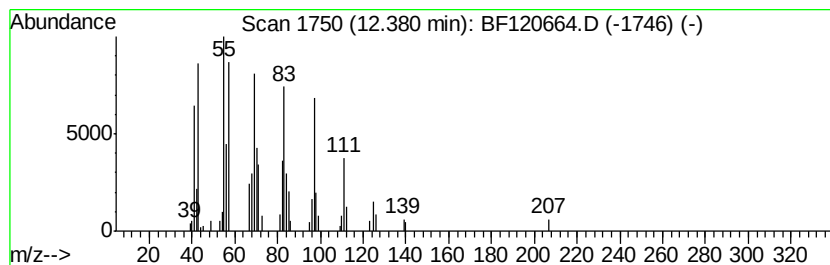
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	2.15 ng	141449	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, tridec...	346	C16H27F5O2	959261-22-4	95
2		n-Heptadecanol-1	256	C17H36O	001454-85-9	95
3		1-Hexadecanol	242	C16H34O	036653-82-4	95
4		n-Pentadecanol	228	C15H32O	000629-76-5	94
5		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061920\
Data File : BF120664.D
Acq On : 19 Jun 2020 15:27
Operator : JU/CG
Sample : L3020-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-27(13-15)

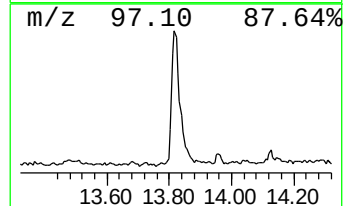
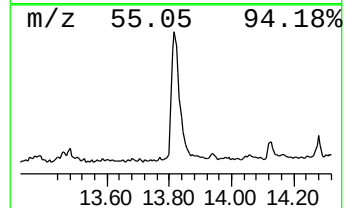
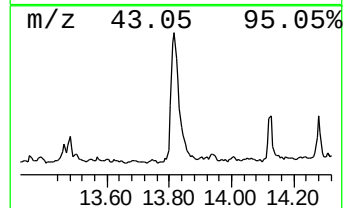
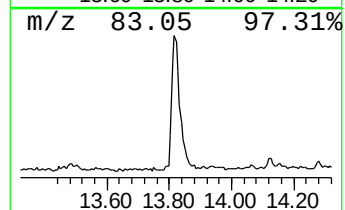
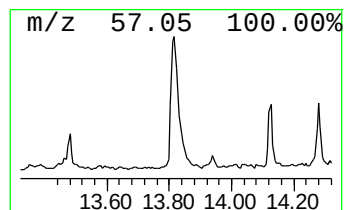
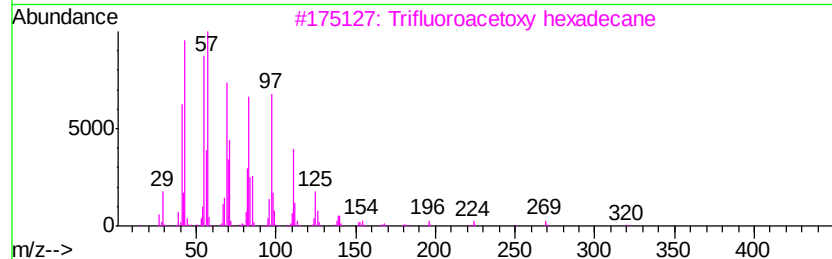
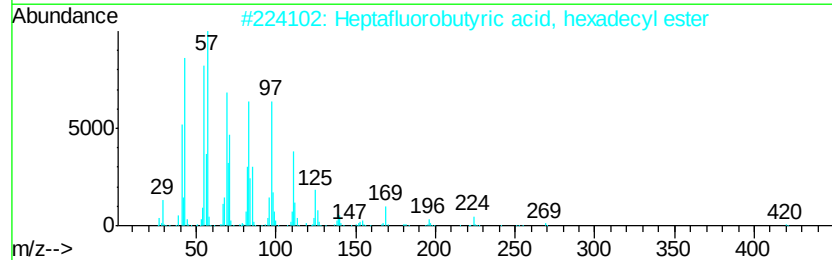
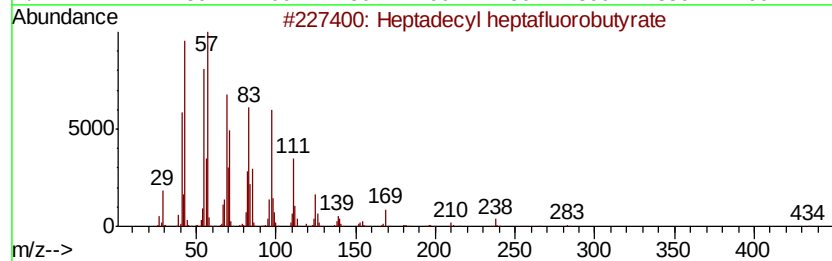
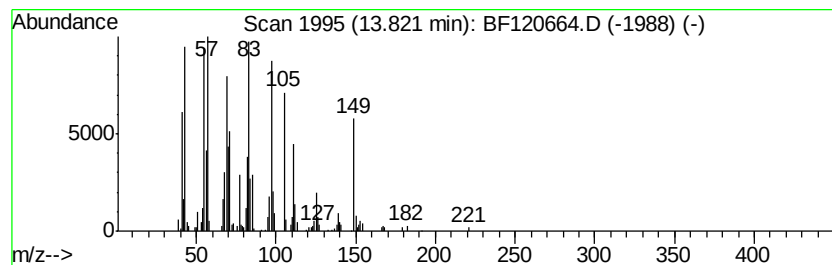
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	6.65 ng	452613	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061920\
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Sample : L3020-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-27(13-15)

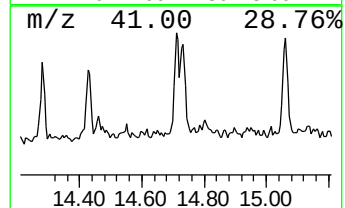
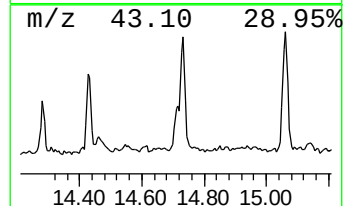
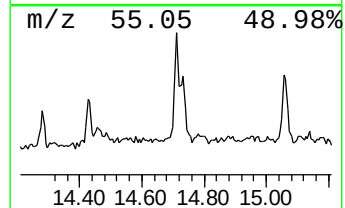
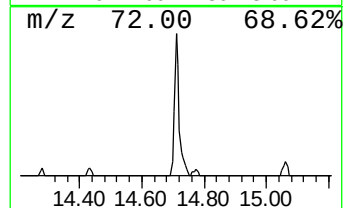
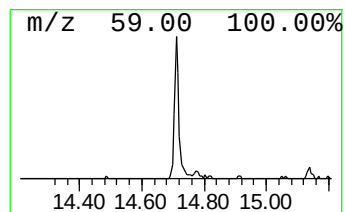
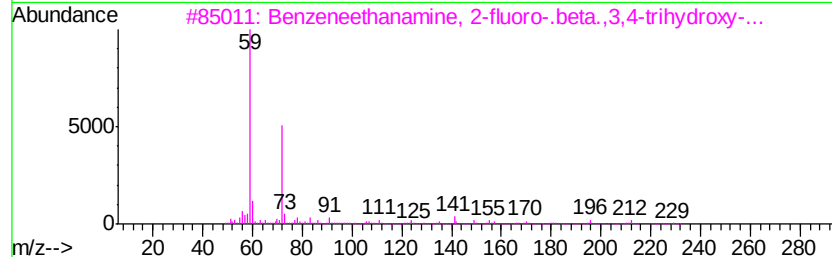
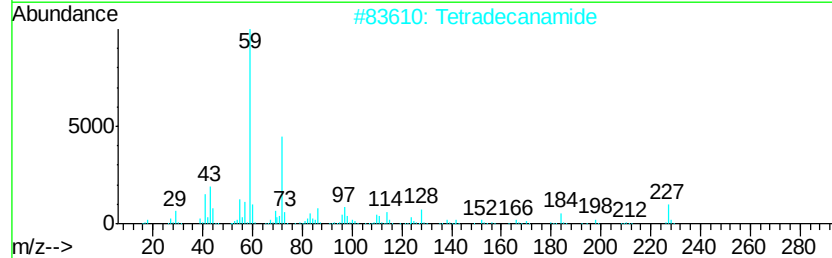
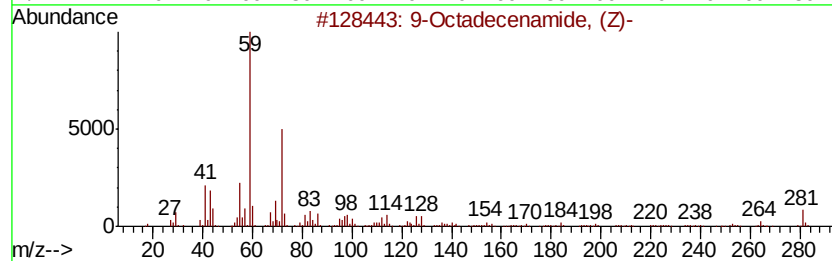
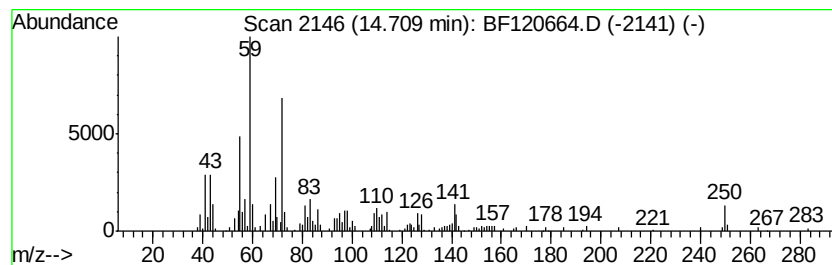
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.48 ng	167000	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
2		Tetradecanamide	227	C14H29NO	000638-58-4	59
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50
4		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	47
5		Decanamide-	171	C10H21NO	002319-29-1	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061920\
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-27(13-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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
Ethanol, 2-(2-eth...	6.63	2.5	ng	99253	1	6.80	788834	20.0
2,4,7,9-Tetrameth...	9.27	13.9	ng	851417	3	9.83	1221110	20.0
unknown10.42	10.42	3.4	ng	210163	3	9.83	1221110	20.0
n-Hexadecanoic acid	11.85	3.1	ng	207770	4	11.32	1318200	20.0
Pentafluoropropio...	12.38	2.1	ng	141449	4	11.32	1318200	20.0
Heptadecyl hepta...	13.82	6.7	ng	452613	5	13.96	1362200	20.0
9-Octadecenamide,...	14.71	2.5	ng	167000	6	15.40	1347850	20.0