

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
 Data File : BF125422.D
 Acq On : 10 Sep 2021 14:07
 Operator : JU/CG
 Sample : M3681-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WATER-PIT

Integration Parameters: rteint.p

Integrator: RTE

Smoother: 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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125422.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	34	rVB	2108877	2877938	94.68%	12.306%
2	3.004	152	156	164	rVB	25456	42166	1.39%	0.180%
3	3.969	317	320	325	rVB	36934	44860	1.48%	0.192%
4	5.504	578	581	592	rBV	884145	821389	27.02%	3.512%
5	6.510	749	752	766	rVB	449516	483424	15.90%	2.067%
6	6.886	812	816	819	rBV	944230	853547	28.08%	3.650%
7	7.445	906	911	914	rBV	1736566	1511347	49.72%	6.462%
8	8.075	1014	1018	1029	rBV	95508	198441	6.53%	0.849%
9	8.169	1029	1034	1037	rBV	1231757	1098674	36.15%	4.698%
10	9.245	1212	1217	1220	rBV	2825487	2657388	87.43%	11.363%
11	9.845	1316	1319	1323	rVB	99579	75858	2.50%	0.324%
12	9.927	1328	1333	1336	rBV	1285441	1235698	40.65%	5.284%
13	10.122	1361	1366	1371	rBV4	28917	44843	1.48%	0.192%
14	10.345	1401	1404	1407	rVB	207354	155924	5.13%	0.667%
15	10.557	1434	1440	1448	rBV8	19582	40826	1.34%	0.175%
16	10.716	1463	1467	1475	rBV	1969332	1814789	59.71%	7.760%
17	10.822	1481	1485	1489	rBV	234956	208651	6.86%	0.892%
18	11.269	1557	1561	1564	rBV	189584	151352	4.98%	0.647%
19	11.410	1582	1585	1589	rBV	1347876	1271487	41.83%	5.437%
20	11.692	1630	1633	1640	rBV	86141	81512	2.68%	0.349%
21	11.933	1669	1674	1679	rBV	662257	678519	22.32%	2.901%
22	12.104	1697	1703	1706	rBV2	51376	56560	1.86%	0.242%
23	12.627	1788	1792	1801	rBV9	22167	65880	2.17%	0.282%
24	12.716	1803	1807	1820	rBV	272388	359942	11.84%	1.539%
25	12.998	1851	1855	1858	rBV	3386340	3039532	100.00%	12.997%
26	13.345	1911	1914	1917	rBV4	22936	32948	1.08%	0.141%
27	13.557	1947	1950	1953	rBV2	36759	48470	1.59%	0.207%
28	13.845	1996	1999	2002	rBV	43693	52165	1.72%	0.223%
29	13.886	2002	2006	2008	rBV2	102377	116997	3.85%	0.500%
30	13.921	2008	2012	2022	rVB	321941	439704	14.47%	1.880%
31	14.057	2032	2035	2039	rVB	1191329	1027332	33.80%	4.393%
32	14.515	2110	2113	2122	rVB	58955	96458	3.17%	0.412%
33	15.551	2283	2289	2297	rBV	723527	994604	32.72%	4.253%
34	16.004	2362	2366	2372	rVB5	28307	48228	1.59%	0.206%
35	16.180	2392	2396	2406	rVB	66318	105553	3.47%	0.451%
36	17.286	2576	2584	2592	rBV2	142521	321545	10.58%	1.375%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.797	2832	2841	2851	rVB4	77735	232288	7.64%	0.993%
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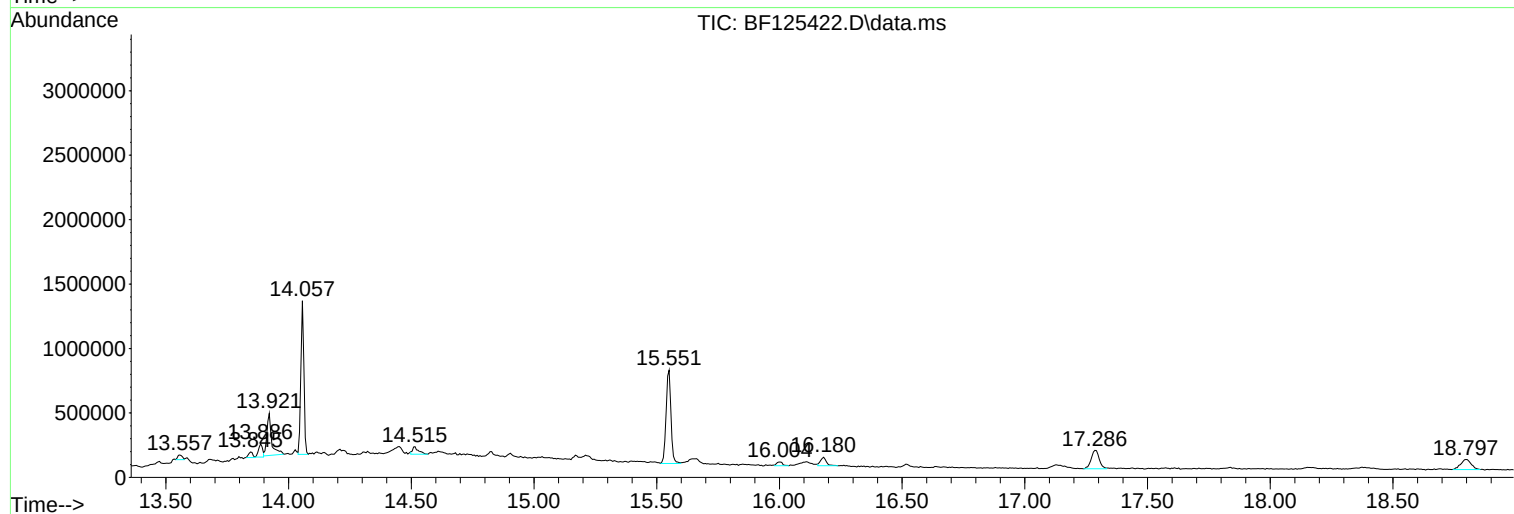
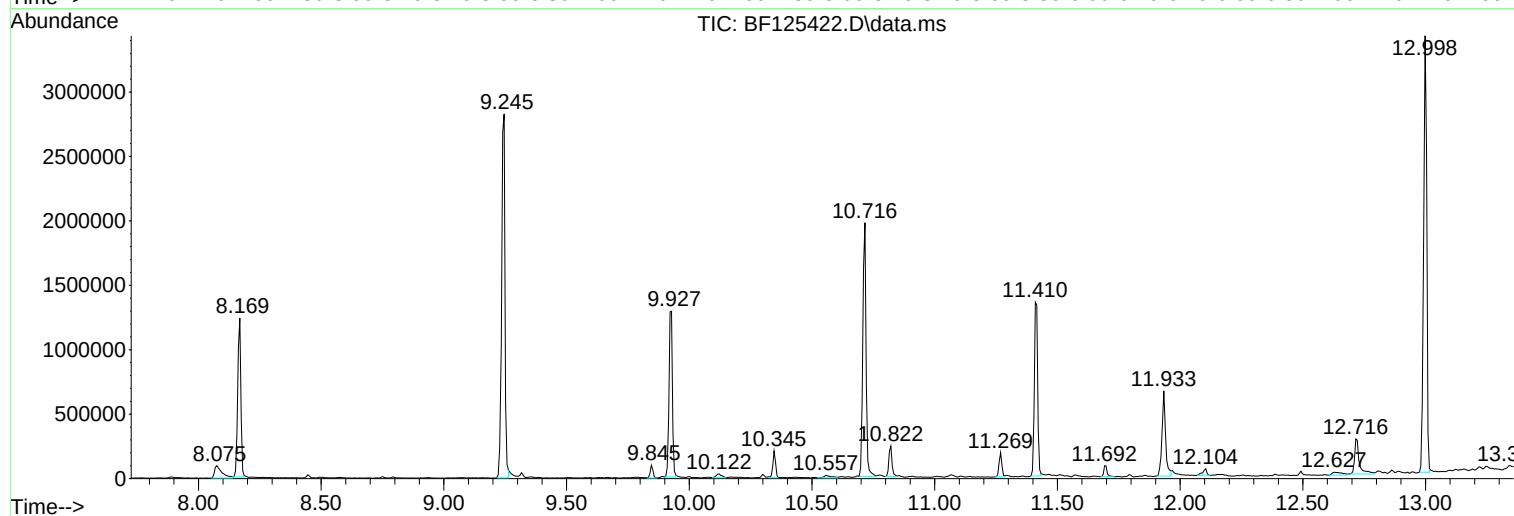
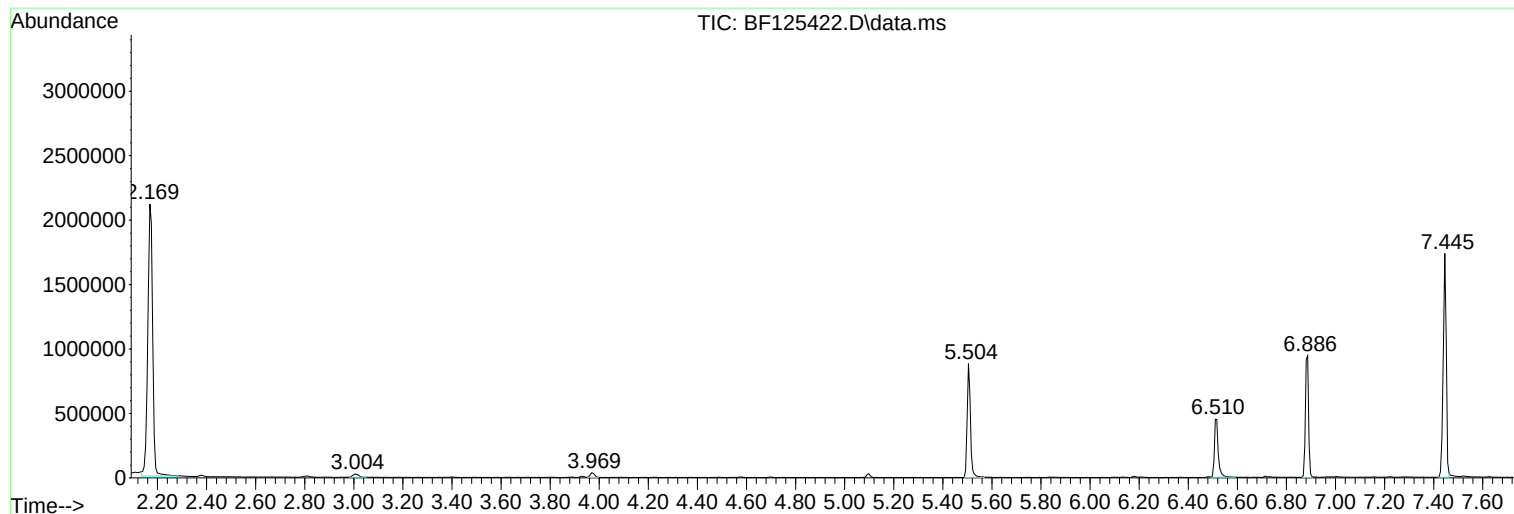
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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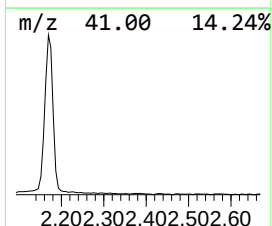
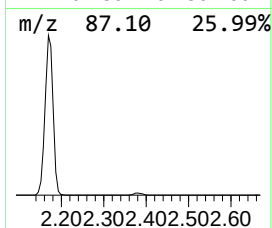
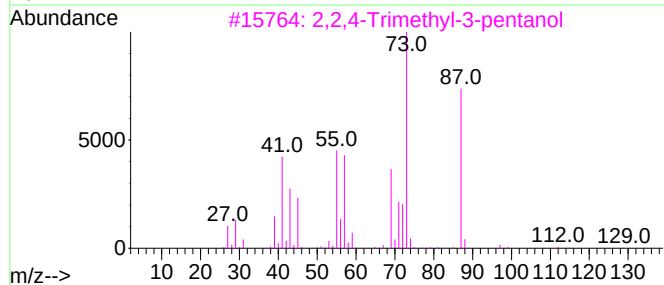
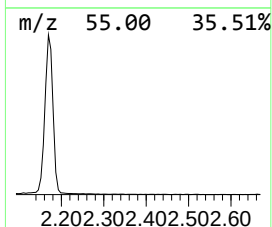
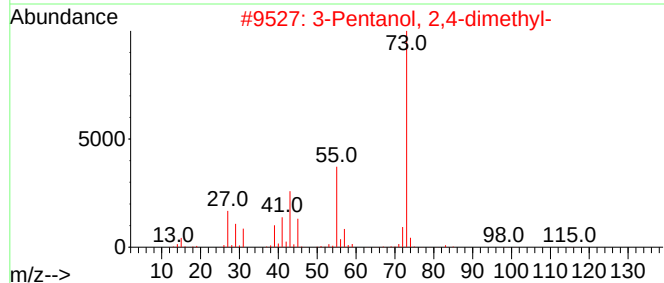
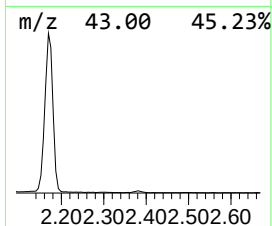
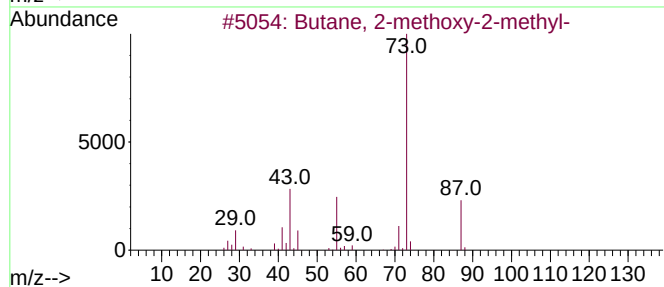
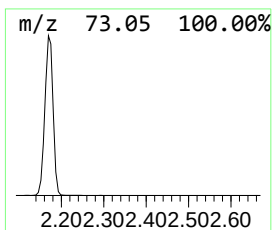
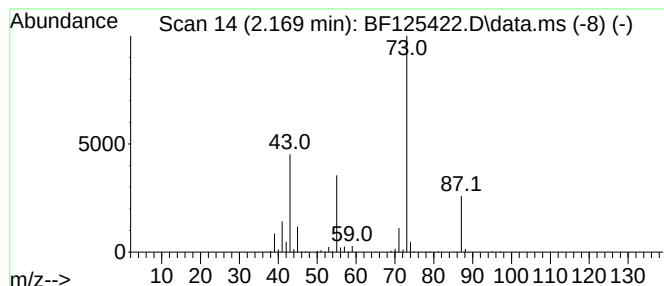
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	67.43 ng	2877940	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
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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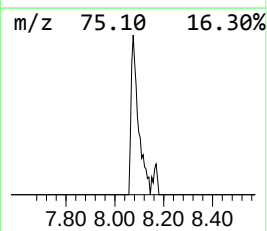
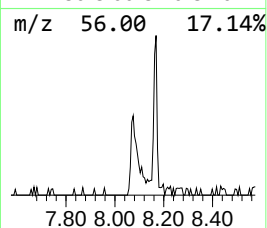
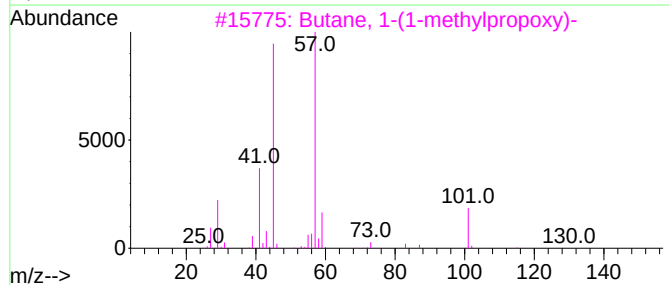
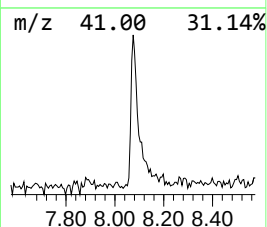
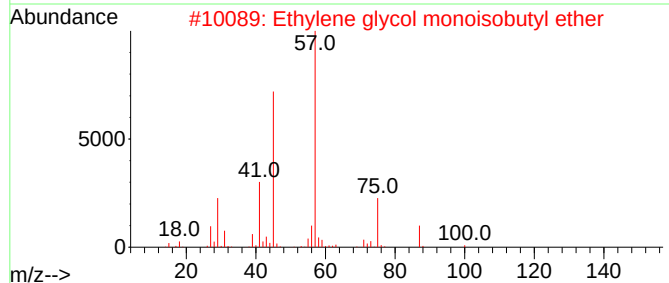
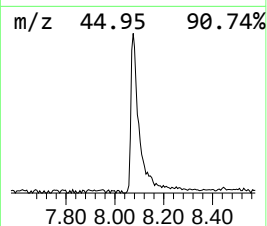
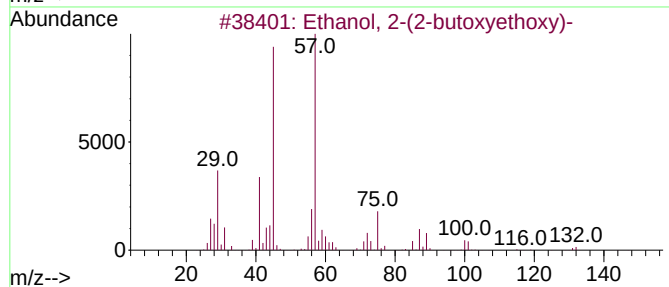
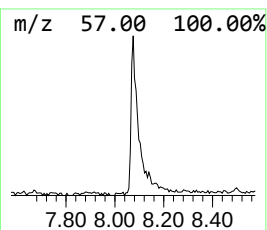
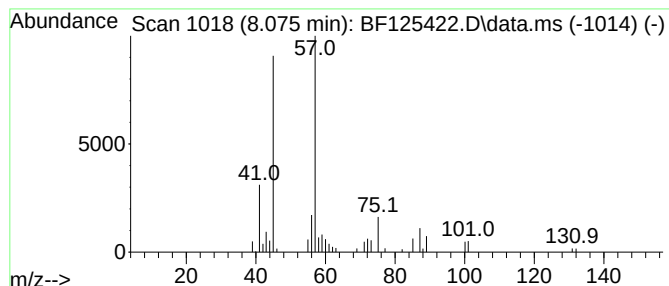
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	3.61 ng	198441	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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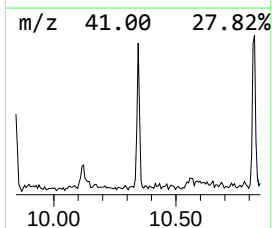
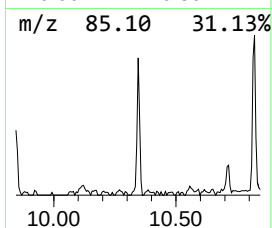
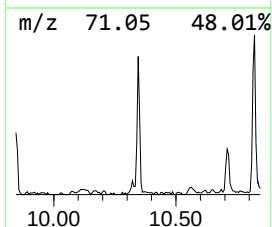
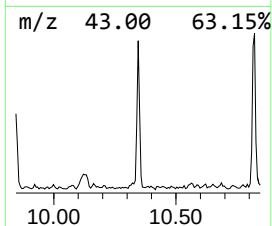
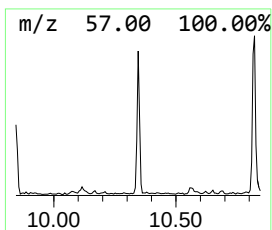
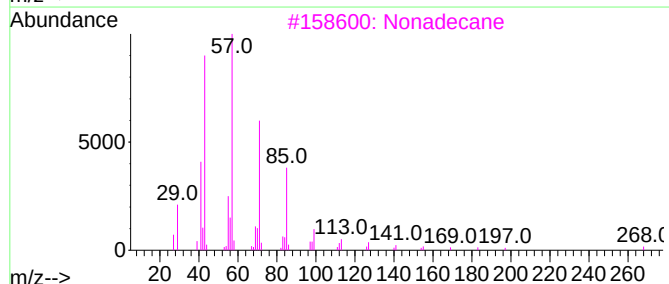
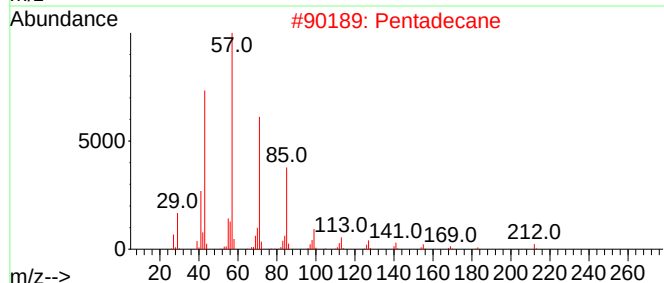
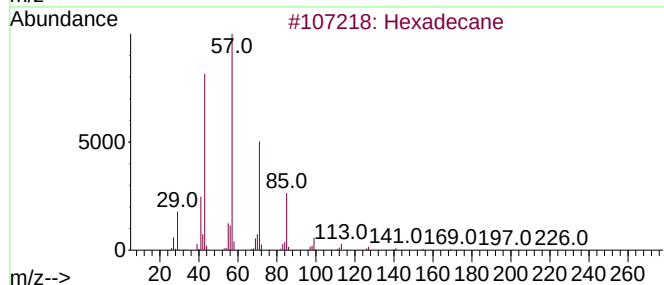
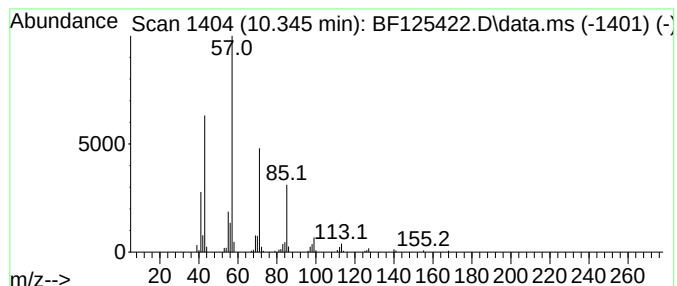
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.345	2.52 ng	155924	Acenaphthene-d10	9.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			Pentadecane	212	C15H32	000629-62-9	90
3			Nonadecane	268	C19H40	000629-92-5	90
4			Tetradecane	198	C14H30	000629-59-4	86
5			Tridecane	184	C13H28	000629-50-5	83



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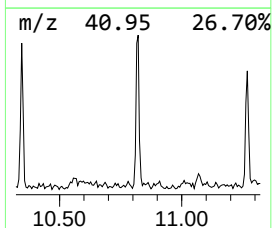
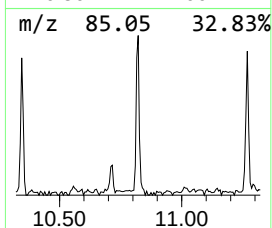
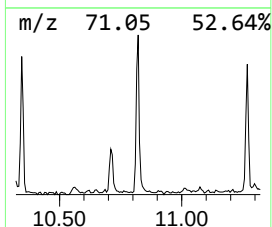
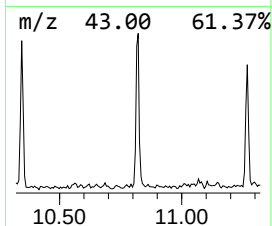
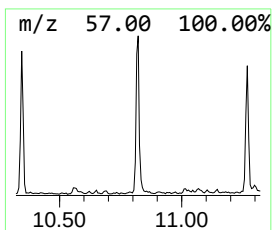
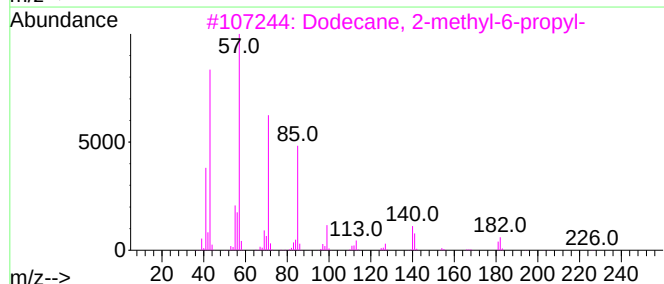
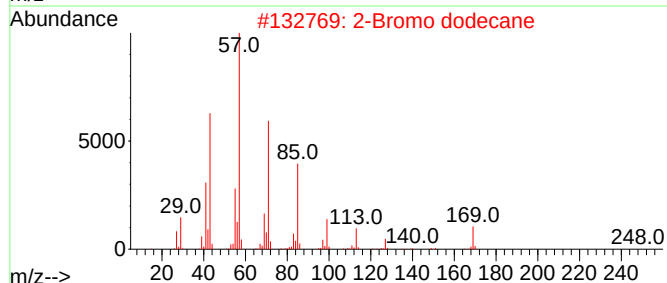
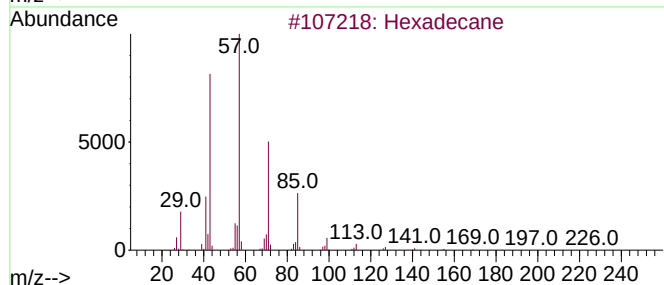
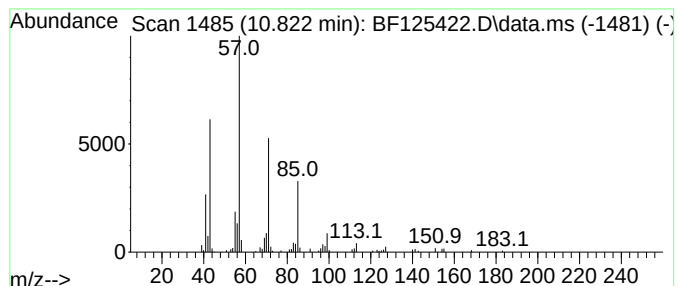
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Bromo dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	3.28 ng	208651	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	86
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	83
3			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	64
4			Nonane, 5-butyl-	184	C13H28	017312-63-9	59
5			Nonadecane	268	C19H40	000629-92-5	58



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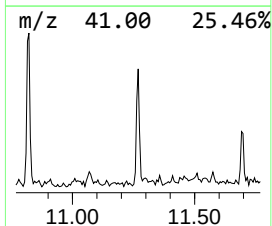
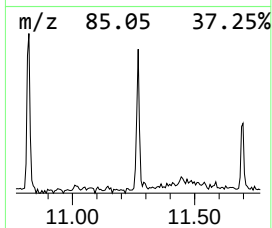
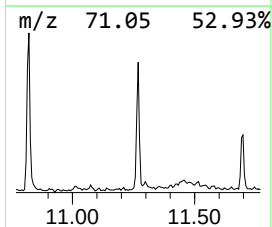
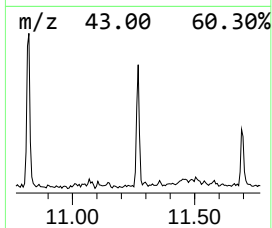
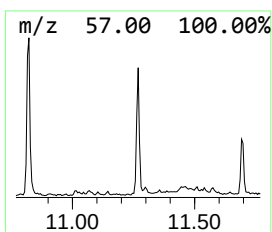
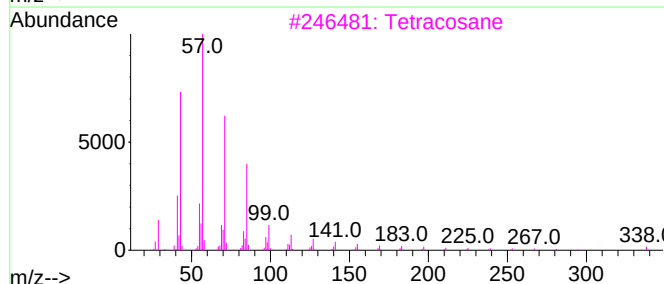
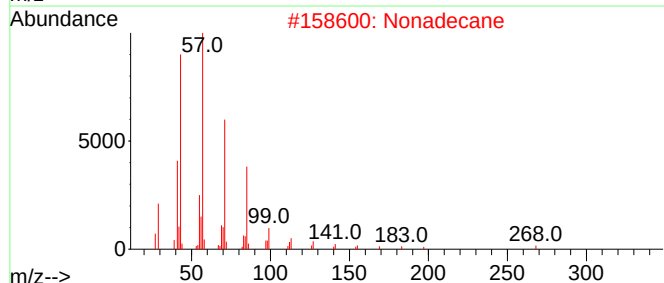
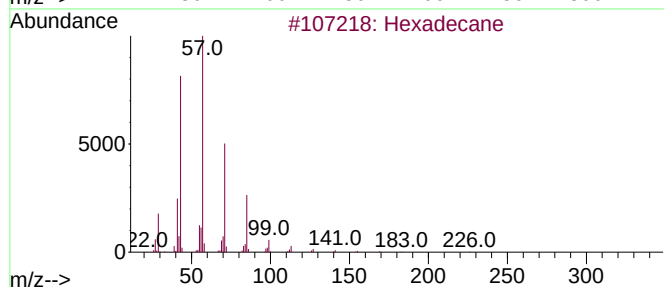
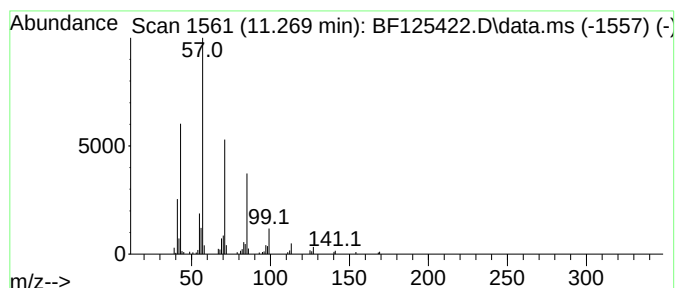
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.269	2.38 ng	151352	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Nonadecane	268	C19H40	000629-92-5	87
3			Tetracosane	338	C24H50	000646-31-1	86
4			2-Bromo dodecane	248	C12H25Br	013187-99-0	83
5			Heptadecane	240	C17H36	000629-78-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
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Operator : JU/CG
Sample : M3681-04
Misc :
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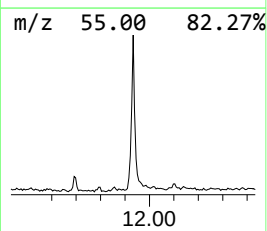
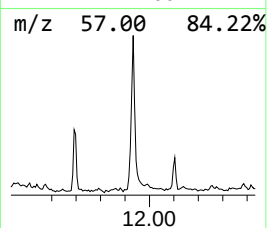
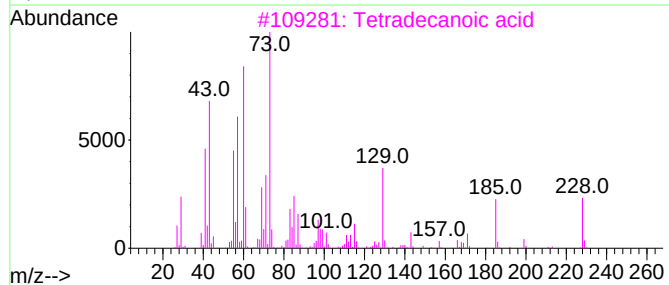
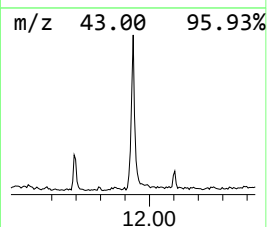
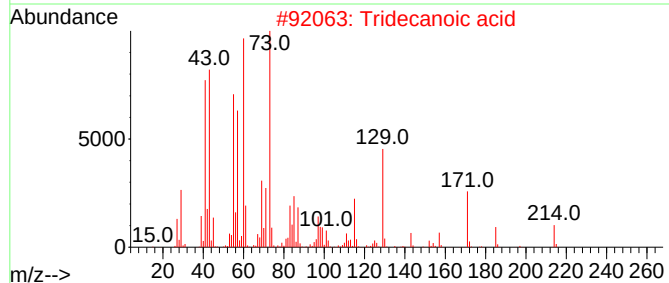
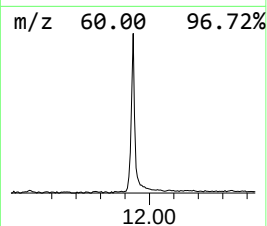
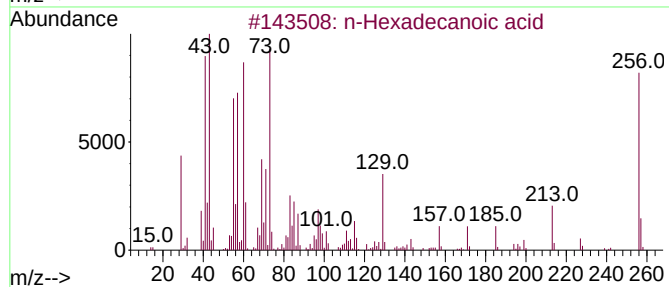
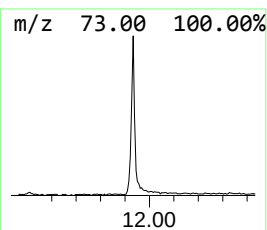
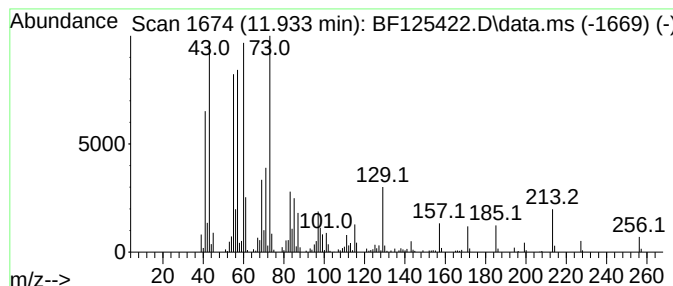
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.933	10.67 ng	678519	Phenanthrene-d10		11.416	
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	91
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	80
5	n-Decanoic acid		172	C10H20O2	000334-48-5	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
Data File : BF125422.D
Acq On : 10 Sep 2021 14:07
Operator : JU/CG
Sample : M3681-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-PIT

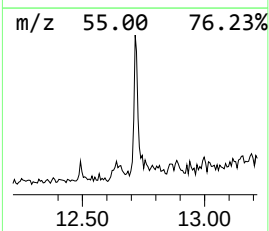
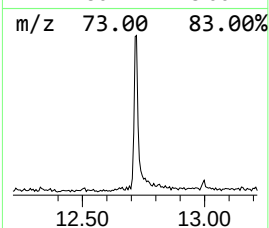
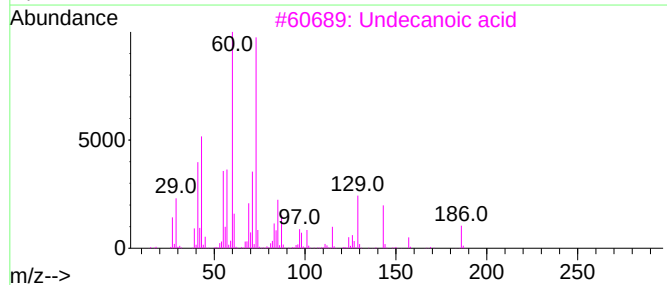
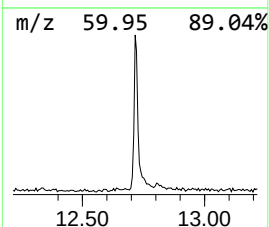
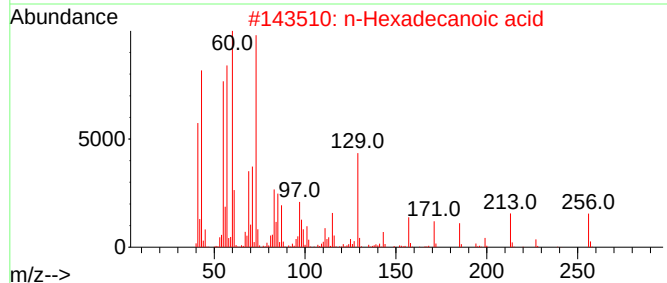
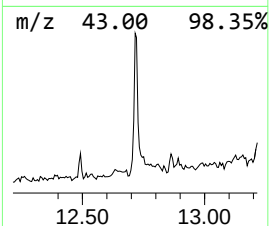
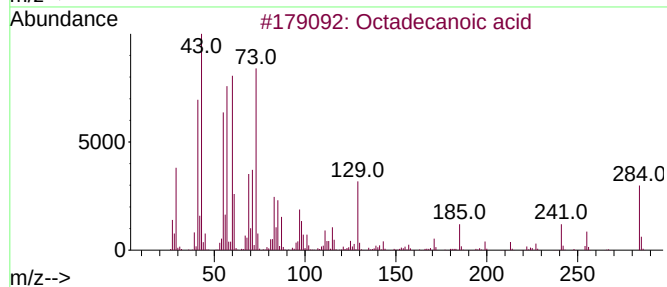
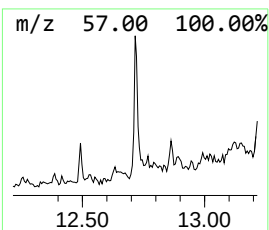
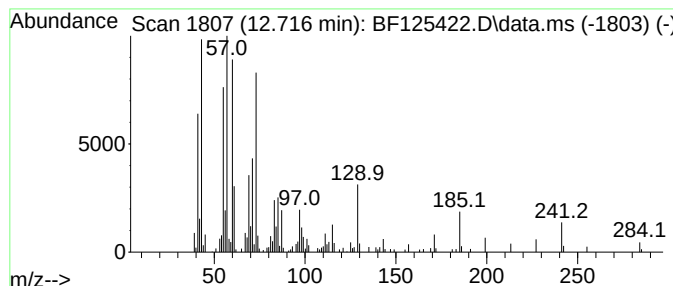
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	5.66 ng	359942	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Undecanoic acid	186	C11H22O2	000112-37-8	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
Data File : BF125422.D
Acq On : 10 Sep 2021 14:07
Operator : JU/CG
Sample : M3681-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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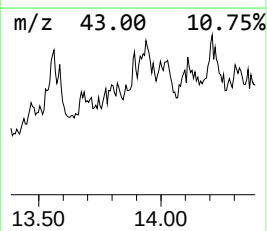
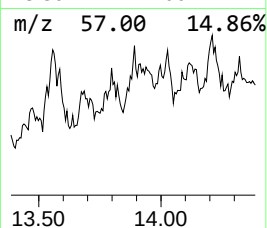
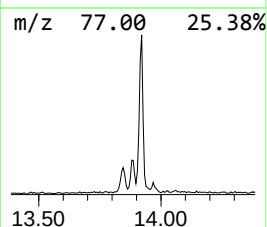
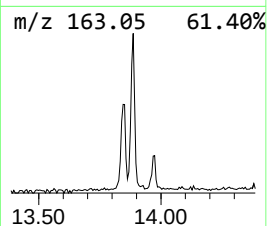
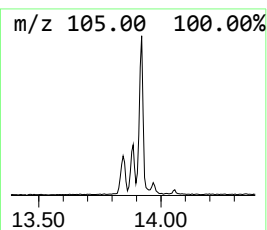
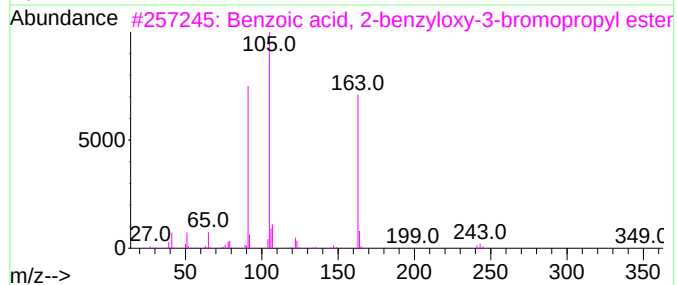
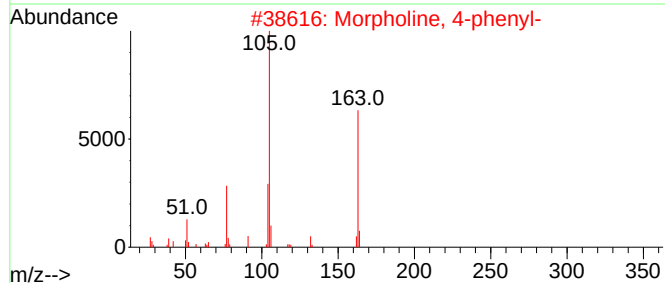
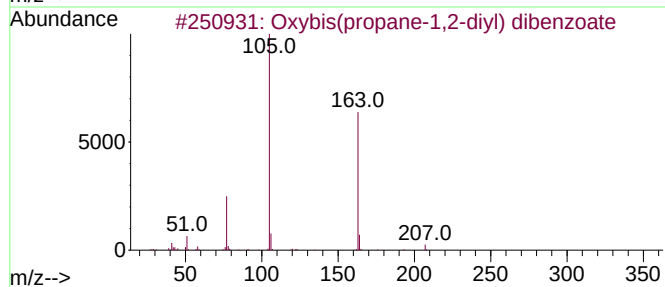
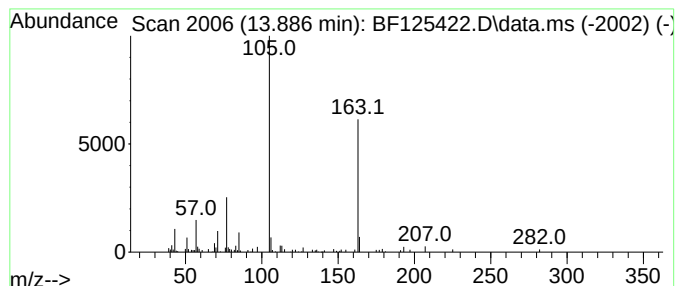
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Oxybis(propene-1,2-diyl) di... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	2.28 ng	116997	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	58
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
3			Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	43
4			.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	27
5			Pentanediamide, N,N'-di-benzoyloxy-	370	C19H18N2O6	1000253-26-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
Data File : BF125422.D
Acq On : 10 Sep 2021 14:07
Operator : JU/CG
Sample : M3681-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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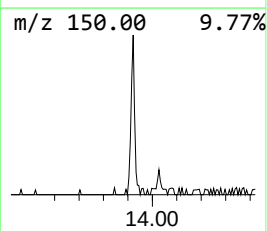
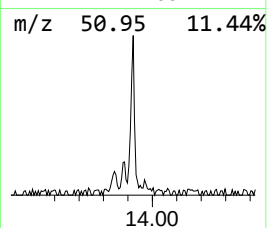
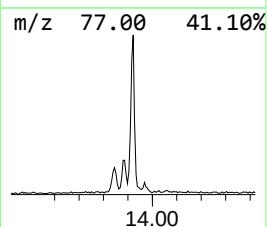
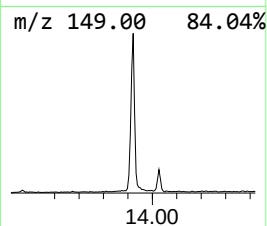
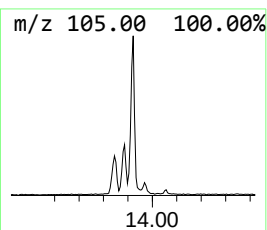
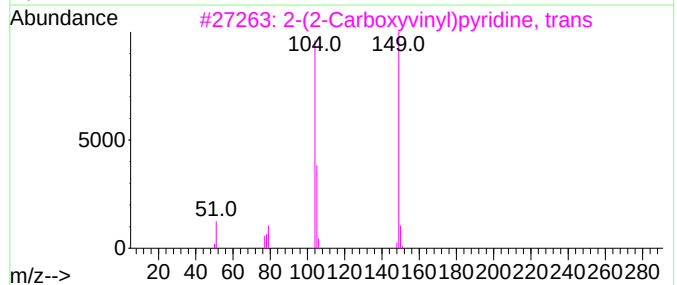
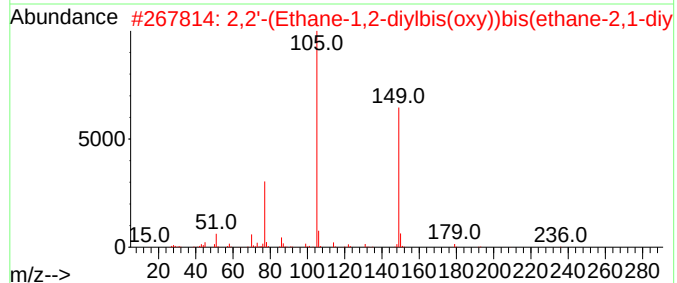
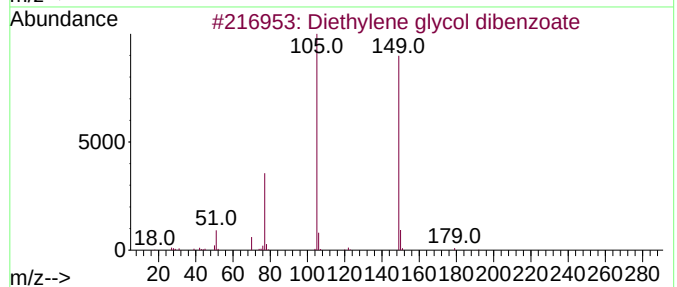
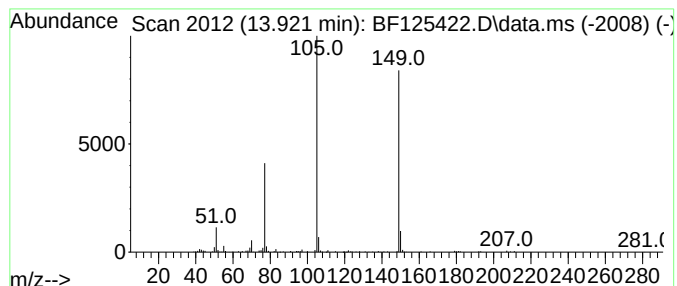
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	8.56 ng	439704	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	91
2			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
4			Phthalic acid, dodecyl ethyl ester	362	C22H34O4	1000308-93-4	43
5			2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
Data File : BF125422.D
Acq On : 10 Sep 2021 14:07
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Sample : M3681-04
Misc :
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Instrument :
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ClientSampleId :
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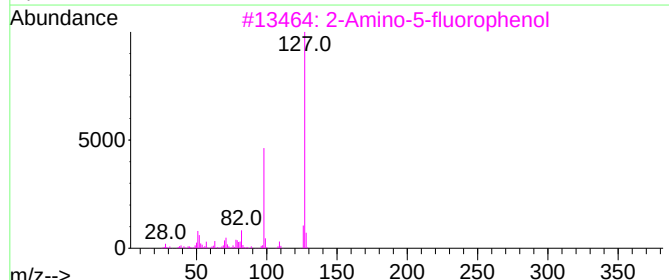
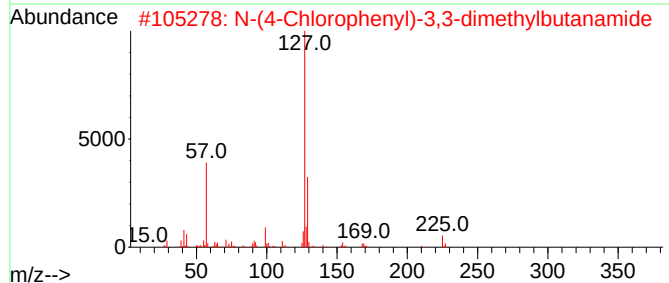
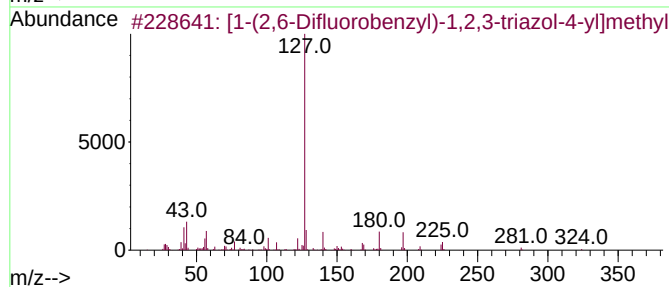
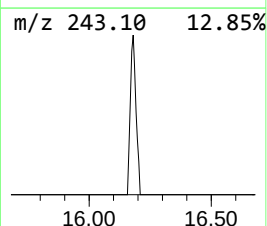
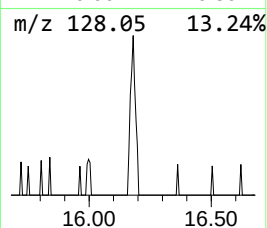
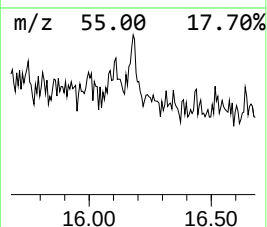
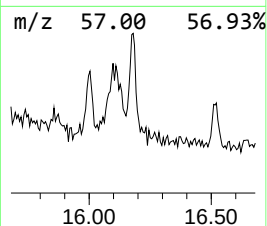
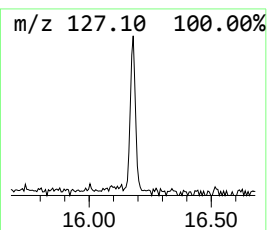
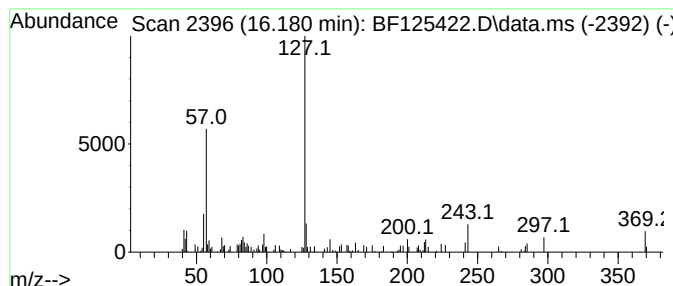
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 [1-(2,6-Difluorobenzyl)-1,2... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.180	2.12 ng	105553	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[1-(2,6-Difluorobenzyl)-1,2,3-tr...	324	C15H18F2N4O2	1000481-77-3	53
2			N-(4-Chlorophenyl)-3,3-dimethylb...	225	C12H16ClNO	142810-47-7	50
3			2-Amino-5-fluorophenol	127	C6H6FNO	053981-24-1	50
4			2-Amino-3-fluorophenol	127	C6H6FNO	053981-23-0	50
5			Caprylic anhydride	270	C16H30O3	000623-66-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
Data File : BF125422.D
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ClientSampleId :
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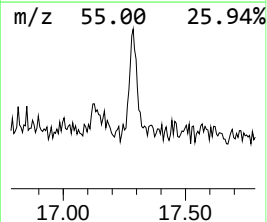
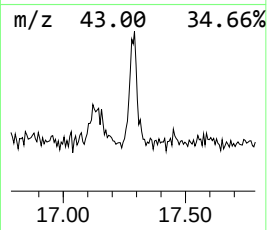
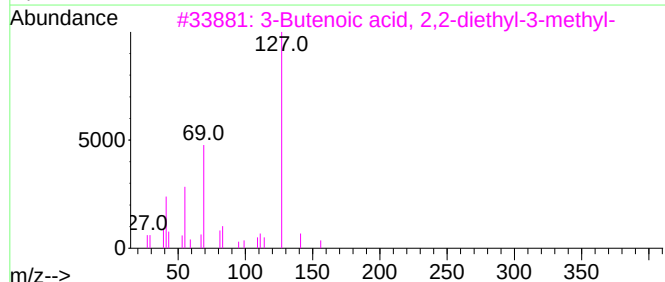
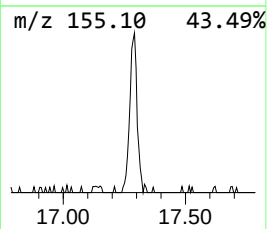
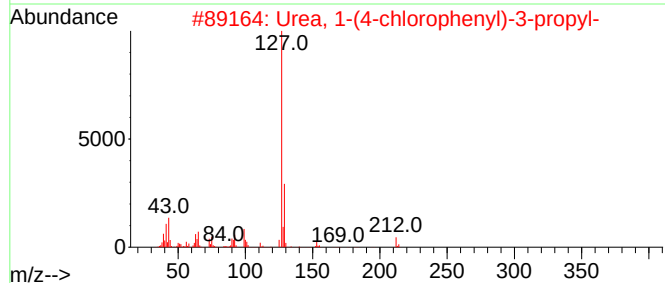
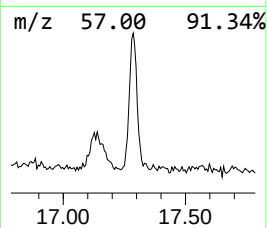
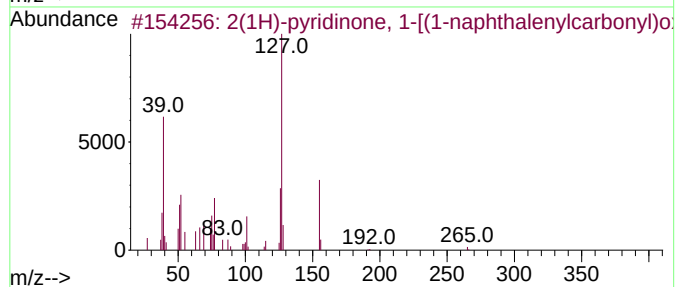
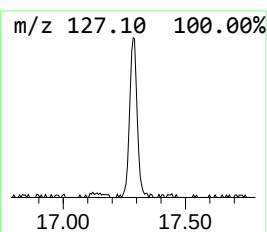
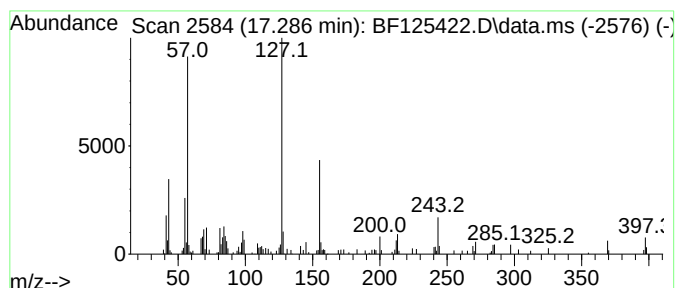
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2(1H)-pyridinone, 1-[(1-nap... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	6.47 ng	321545	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-pyridinone, 1-[(1-naphthal...	265	C16H11N03	1010396-89-3	53		
2	Urea, 1-(4-chlorophenyl)-3-propyl-	212	C10H13ClN2O	013208-64-5	38		
3	3-Butenoic acid, 2,2-diethyl-3-m...	156	C9H16O2	038477-06-4	38		
4	1H-Imidazole, 1-methyl-4-nitro-	127	C4H5N3O2	003034-41-1	38		
5	2-Hydroxy-4-hydroxylaminopyrimidine	127	C4H5N3O2	020555-88-8	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
Data File : BF125422.D
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ALS Vial : 6 Sample Multiplier: 1

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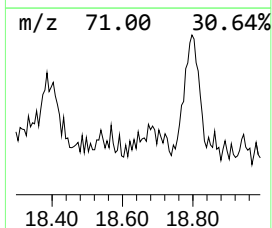
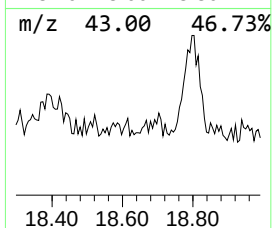
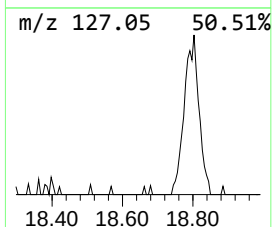
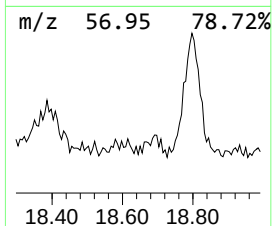
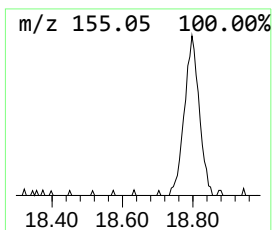
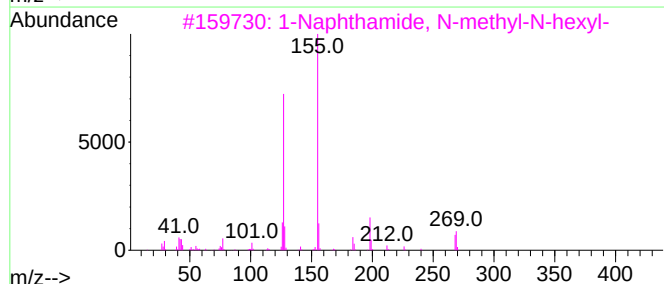
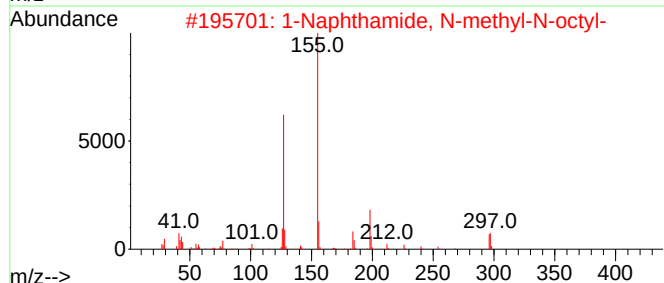
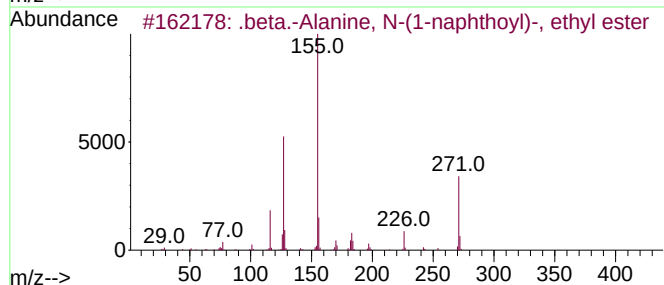
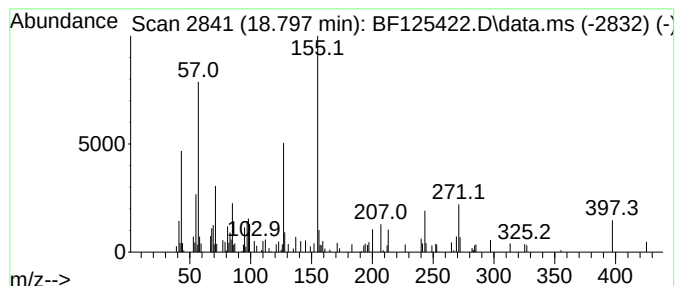
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 .beta.-Alanine, N-(1-naphth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.797	4.67 ng	232288	Perylene-d12	15.551

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Alanine, N-(1-naphthoyl)-...	271	C16H17NO3	1000321-94-4	50
2		1-Naphthamide, N-methyl-N-octyl-	297	C20H27NO	1000421-43-7	49
3		1-Naphthamide, N-methyl-N-hexyl-	269	C18H23NO	1000421-43-4	49
4		1-Naphthamide, N-methyl-N-(2-eth...	297	C20H27NO	1000421-43-5	49
5		Imidazole, 4-amino-5-ethoxycarbo...	155	C6H9N3O2	021190-16-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
Data File : BF125422.D
Acq On : 10 Sep 2021 14:07
Operator : JU/CG
Sample : M3681-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-PIT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	67.4	ng	2877940	1	6.886	853547	20.0
Ethanol, 2-(2-b...	8.075	3.6	ng	198441	2	8.169	1098670	20.0
Hexadecane	10.345	2.5	ng	155924	3	9.927	1235700	20.0
2-Bromo dodecane	10.822	3.3	ng	208651	4	11.416	1271490	20.0
Nonadecane	11.269	2.4	ng	151352	4	11.416	1271490	20.0
n-Hexadecanoic ...	11.933	10.7	ng	678519	4	11.416	1271490	20.0
Octadecanoic acid	12.716	5.7	ng	359942	4	11.416	1271490	20.0
Oxybis(propane-...	13.886	2.3	ng	116997	5	14.057	1027330	20.0
Diethylene glyc...	13.921	8.6	ng	439704	5	14.057	1027330	20.0
[1-(2,6-Difluor...	16.180	2.1	ng	105553	6	15.551	994604	20.0
2(1H)-pyridinon...	17.286	6.5	ng	321545	6	15.551	994604	20.0
.beta.-Alanine,...	18.797	4.7	ng	232288	6	15.551	994604	20.0