

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102822\
 Data File : BF130846.D
 Acq On : 29 Oct 2022 02:58
 Operator : CG\JU
 Sample : N5292-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 251032-3

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130846.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.293	28	35	41	rVB	1820457	2395743	61.33%	9.955%
2	5.169	520	524	530	rVB	213902	230782	5.91%	0.959%
3	5.557	585	590	593	rBV	1650888	1434207	36.71%	5.960%
4	6.551	754	759	764	rBV	1019813	894147	22.89%	3.715%
5	6.763	791	795	806	rBV	56320	62085	1.59%	0.258%
6	6.945	822	826	829	rVB	758680	637854	16.33%	2.650%
7	7.510	916	922	925	rBV	2060197	2196386	56.22%	9.127%
8	8.128	1022	1027	1039	rBV	831627	838517	21.46%	3.484%
9	8.228	1039	1044	1047	rVV	903042	816413	20.90%	3.392%
10	9.310	1222	1228	1231	rBV	4101577	3906445	100.00%	16.232%
11	9.416	1242	1246	1250	rBV	602505	553790	14.18%	2.301%
12	9.698	1290	1294	1297	rVB	107913	77273	1.98%	0.321%
13	9.992	1338	1344	1347	rBV	971493	919274	23.53%	3.820%
14	10.780	1471	1478	1481	rBV	2542821	2344971	60.03%	9.744%
15	11.480	1593	1597	1600	rBV	1176135	938180	24.02%	3.898%
16	11.545	1605	1608	1611	rVB2	57203	45113	1.15%	0.187%
17	11.869	1659	1663	1666	rVB	117176	90873	2.33%	0.378%
18	11.998	1681	1685	1690	rBV	37636	41248	1.06%	0.171%
19	12.574	1776	1783	1792	rBV	371100	371991	9.52%	1.546%
20	12.663	1795	1798	1803	rVB	133071	105712	2.71%	0.439%
21	13.074	1863	1868	1871	rBV	3735019	3367154	86.19%	13.991%
22	13.333	1907	1912	1917	rVB3	40137	42415	1.09%	0.176%
23	14.010	2022	2027	2036	rBV9	19678	56200	1.44%	0.234%
24	14.127	2043	2047	2050	rVB	795679	705732	18.07%	2.933%
25	14.221	2058	2063	2069	rBV	228897	252808	6.47%	1.050%
26	14.998	2191	2195	2199	rBV2	221646	224098	5.74%	0.931%
27	15.639	2299	2304	2309	rBV	405750	516403	13.22%	2.146%

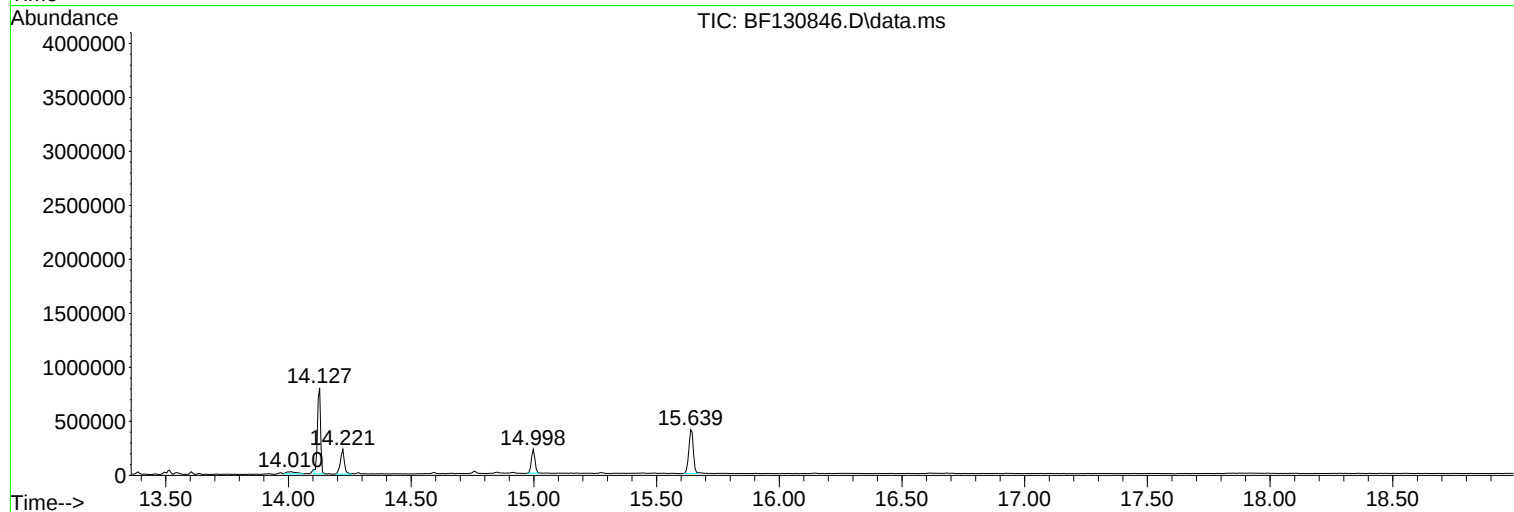
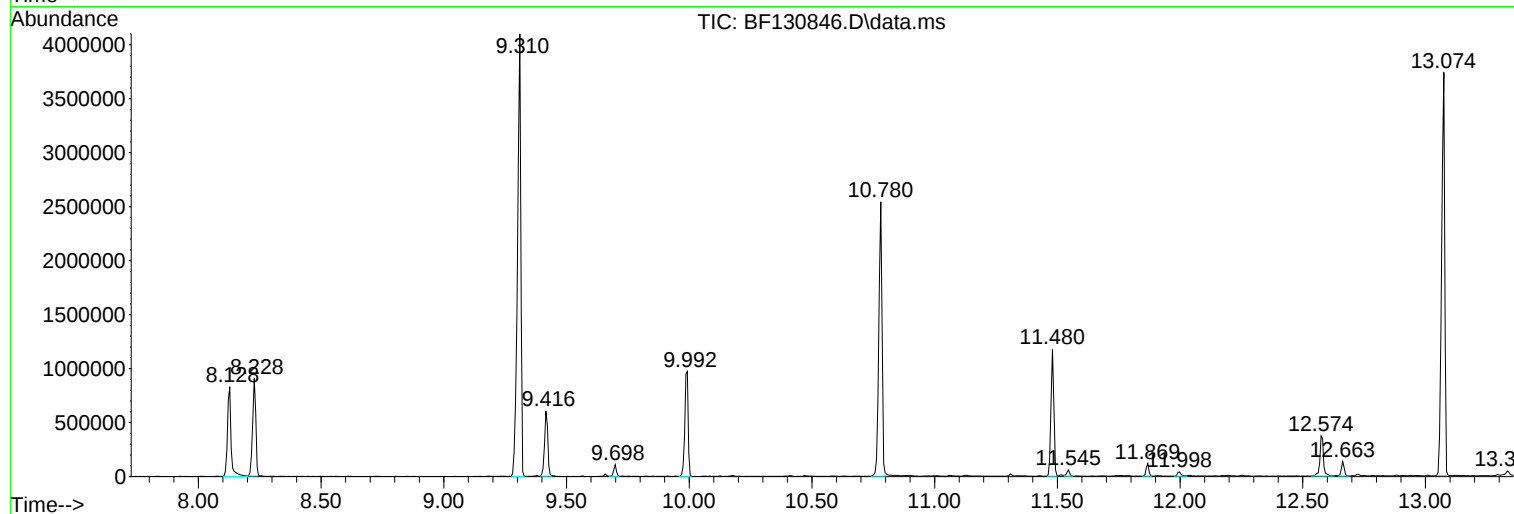
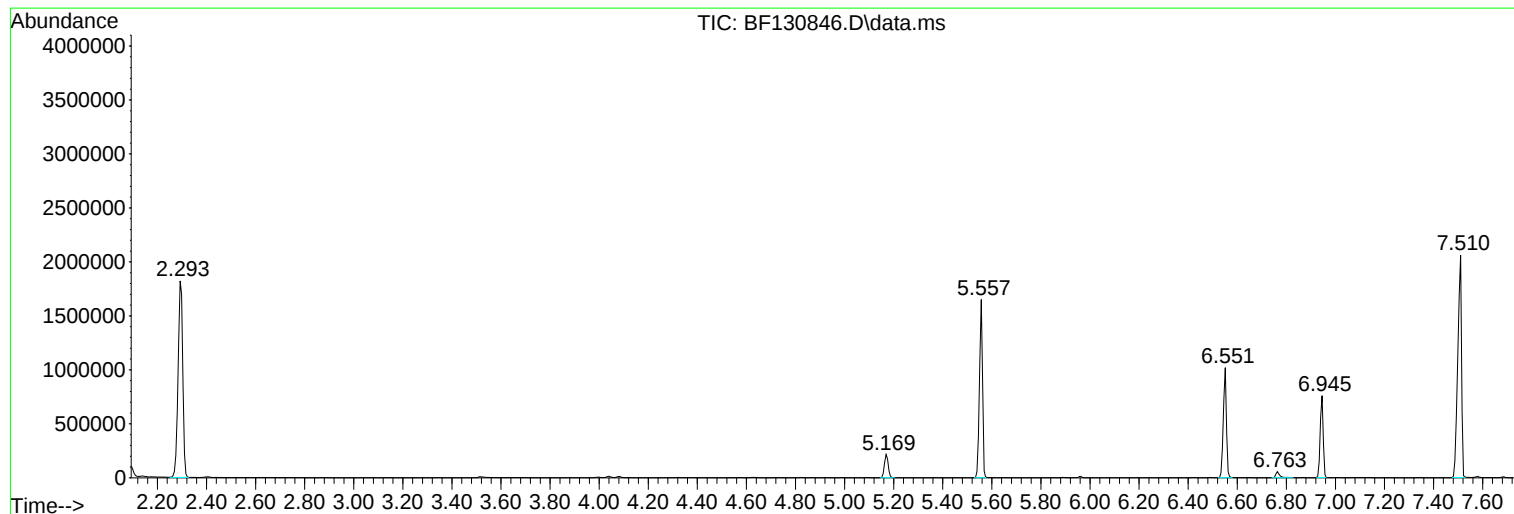
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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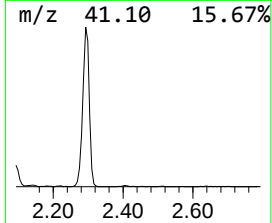
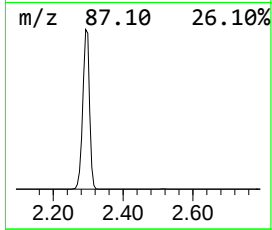
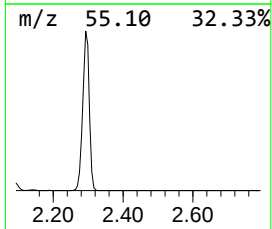
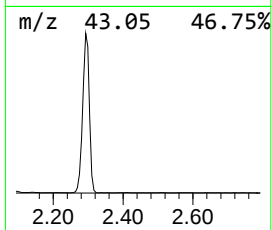
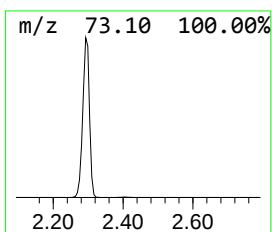
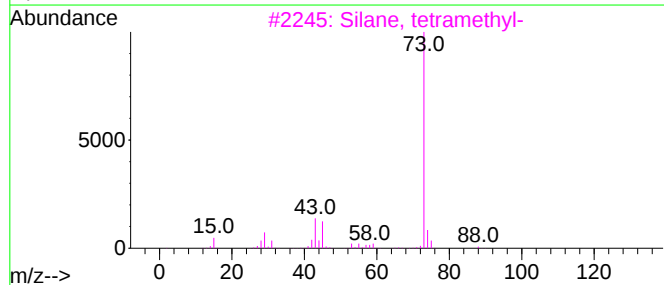
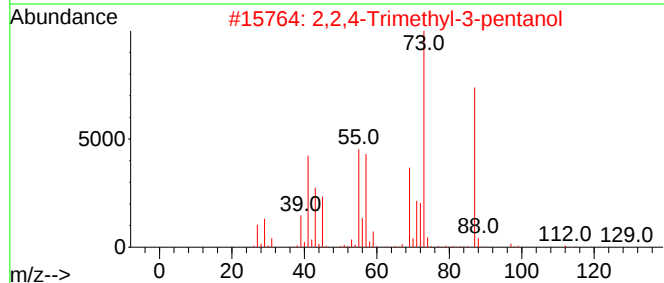
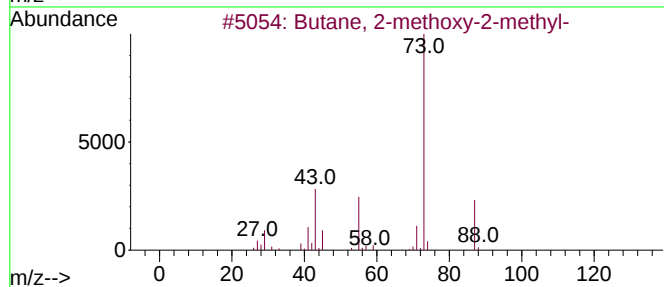
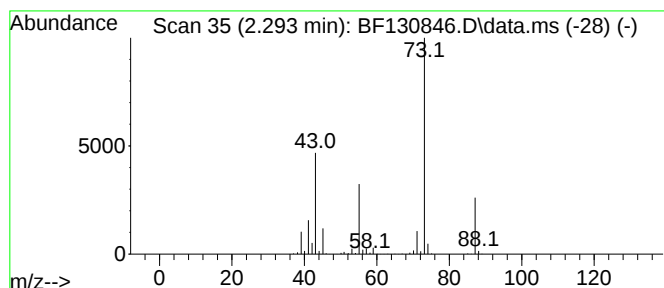
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.293	75.12 ng	2395740	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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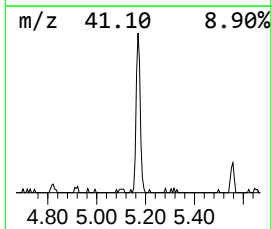
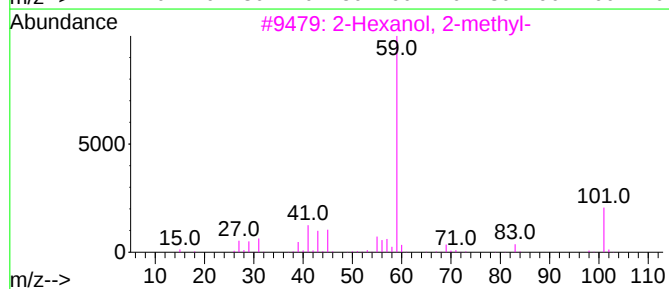
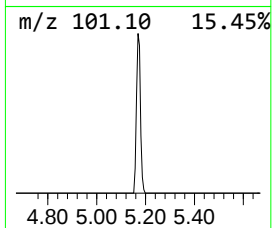
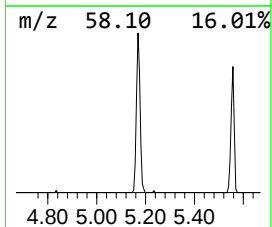
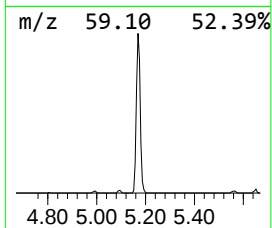
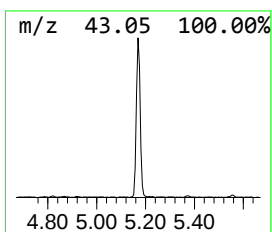
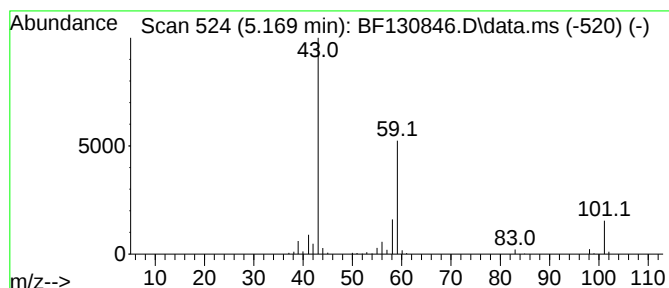
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	7.24 ng	230782	1,4-Dichlorobenzene-d4	6.945

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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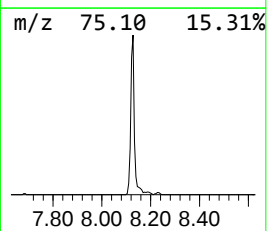
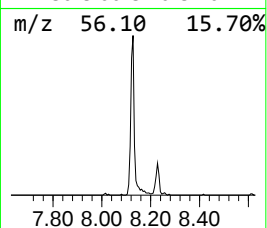
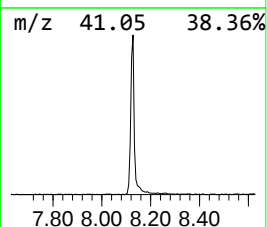
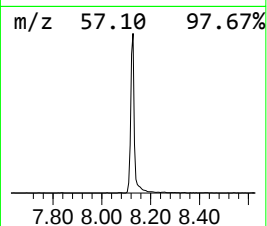
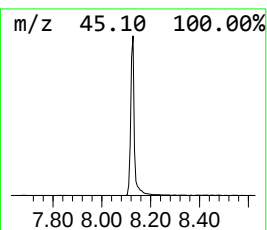
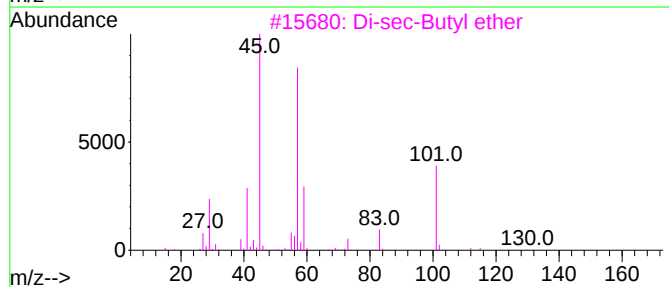
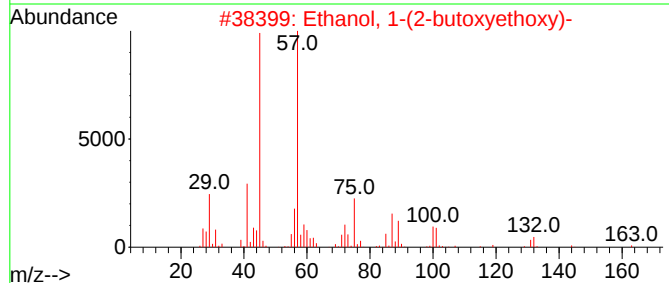
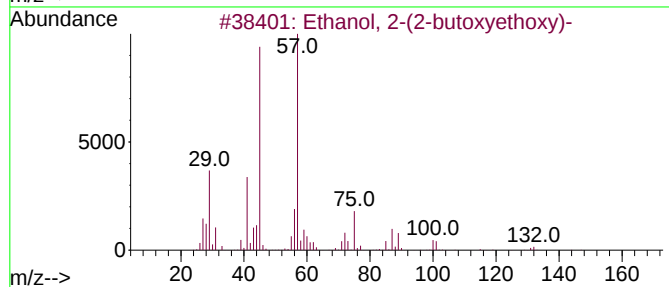
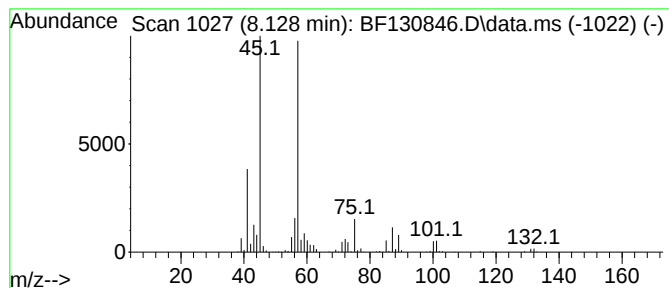
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.128	20.54 ng	838517	Naphthalene-d8	8.228

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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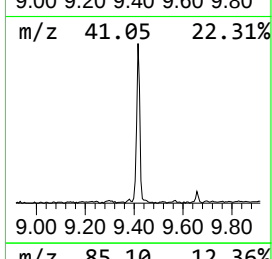
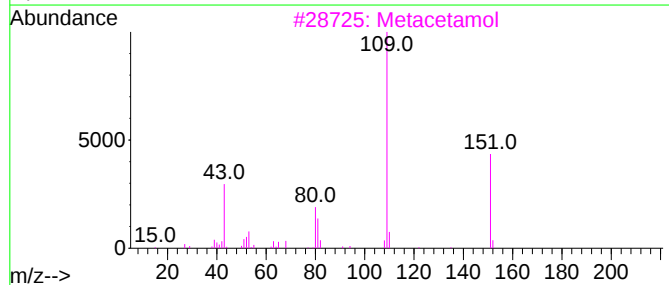
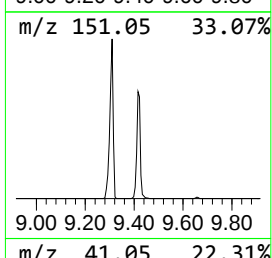
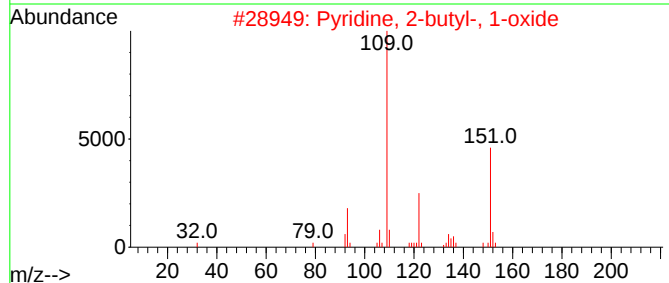
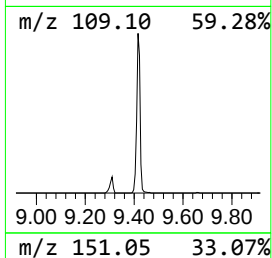
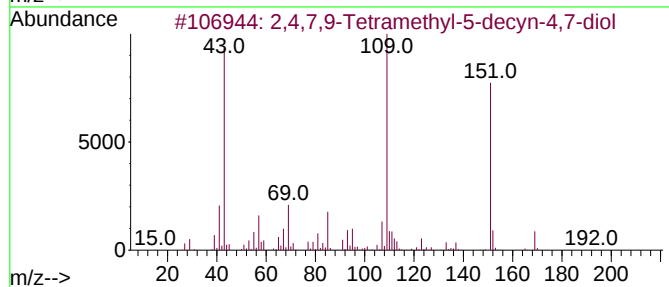
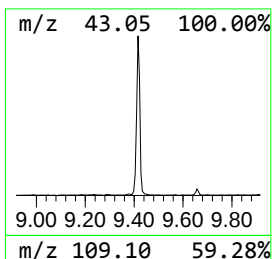
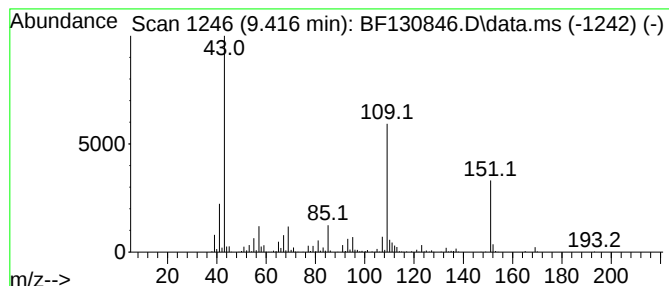
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.416	12.05 ng	553790	Acenaphthene-d10			9.992

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	53
3	Metacetamol	151	C8H9NO2		000621-42-1	47
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2		001006-96-8	47
5	2-Thiophenecarbonitrile	109	C5H3NS		001003-31-2	47



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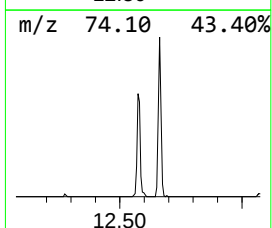
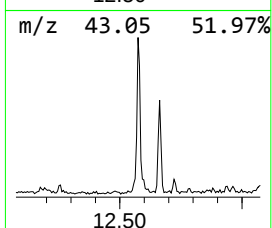
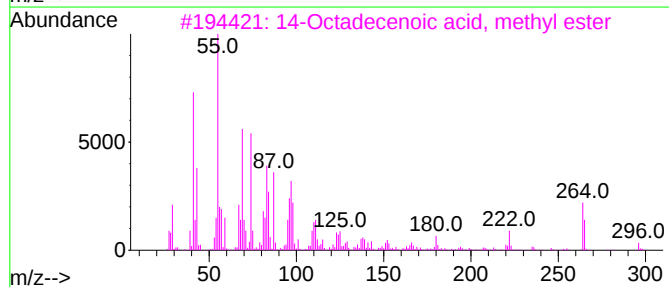
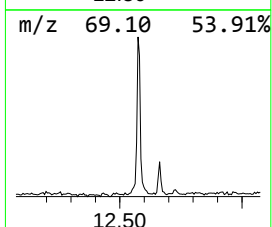
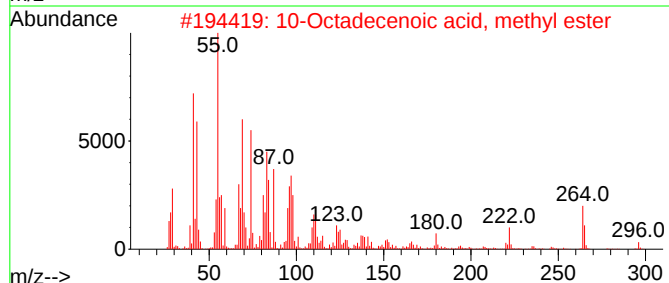
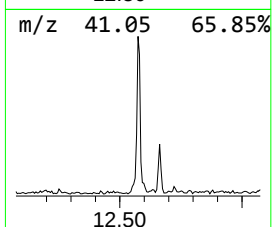
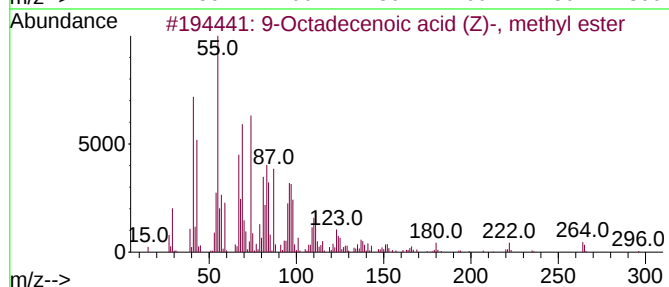
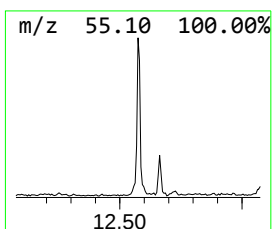
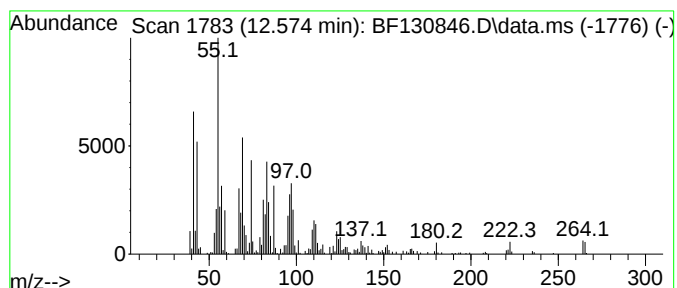
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TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.575	7.93 ng	371991	Phenanthrene-d10	11.480	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
5	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	90



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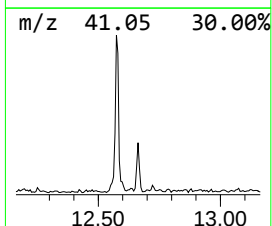
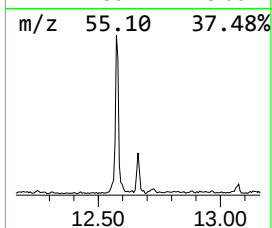
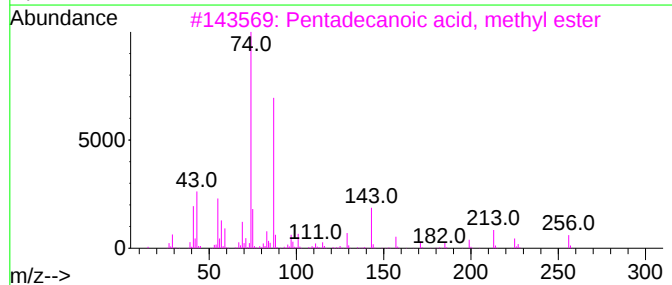
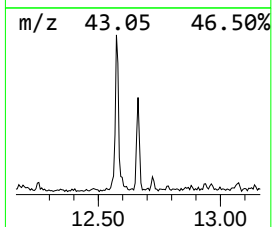
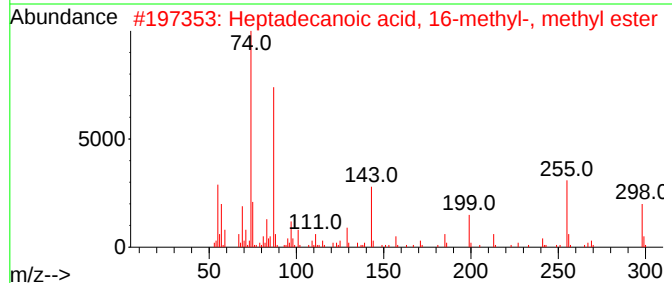
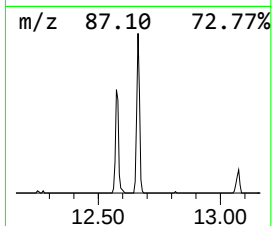
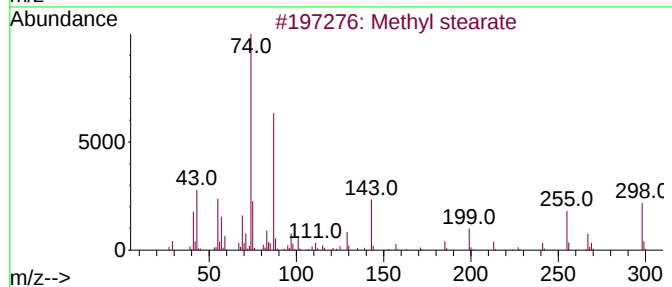
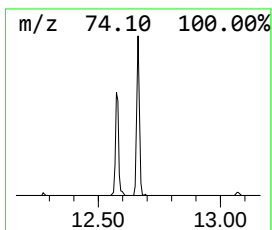
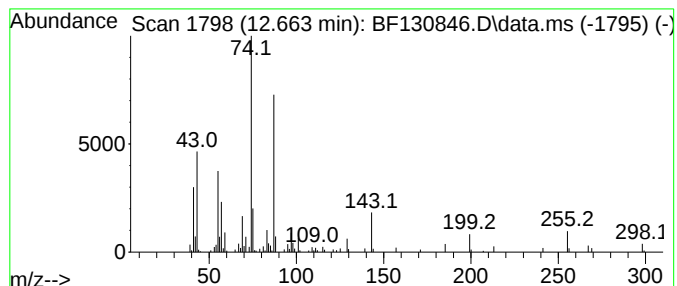
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	2.25 ng	105712	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102822\
Data File : BF130846.D
Acq On : 29 Oct 2022 02:58
Operator : CG\JU
Sample : N5292-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
251032-3

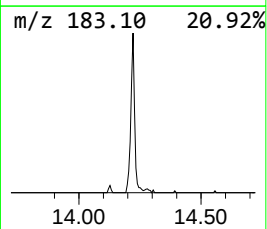
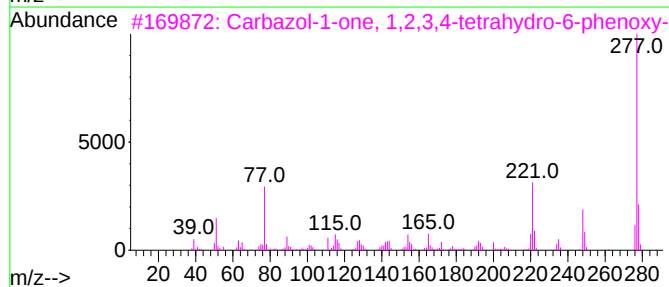
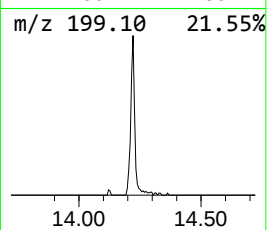
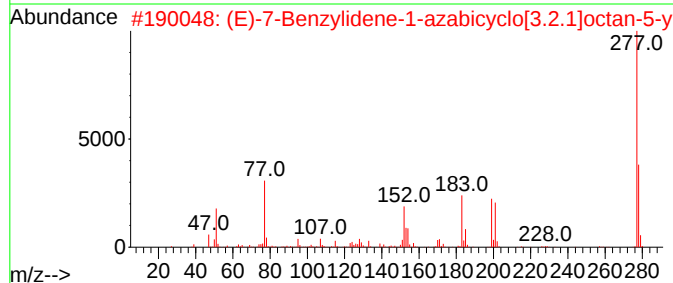
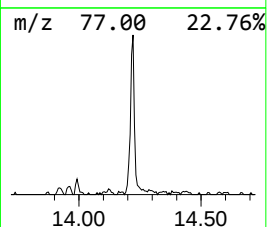
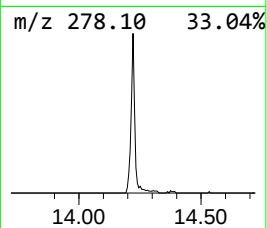
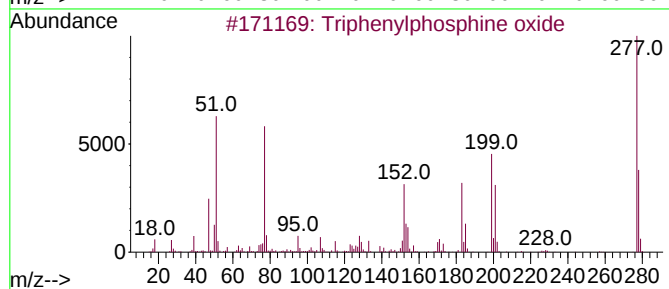
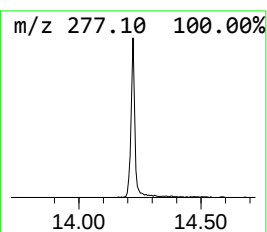
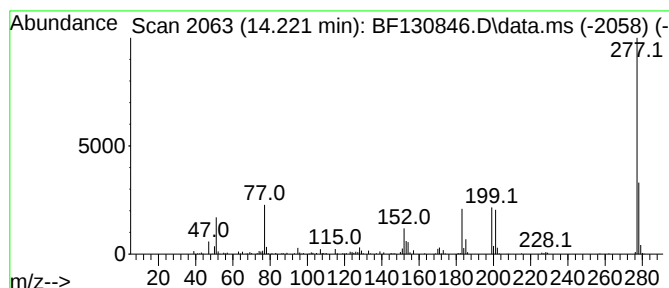
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	7.16 ng	252808	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	53
3			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	37
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	32
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102822\
Data File : BF130846.D
Acq On : 29 Oct 2022 02:58
Operator : CG\JU
Sample : N5292-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
251032-3

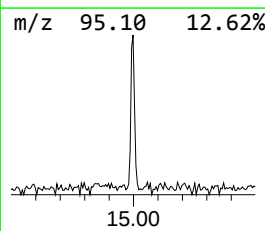
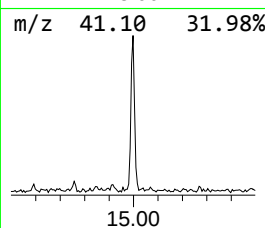
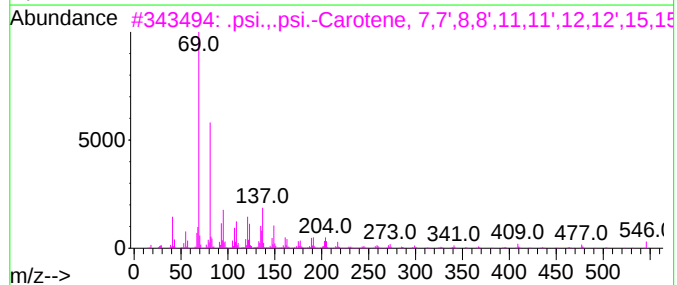
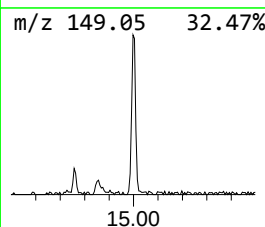
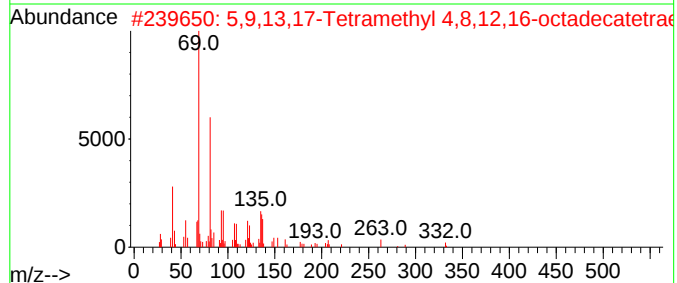
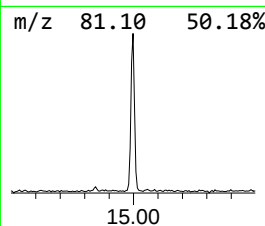
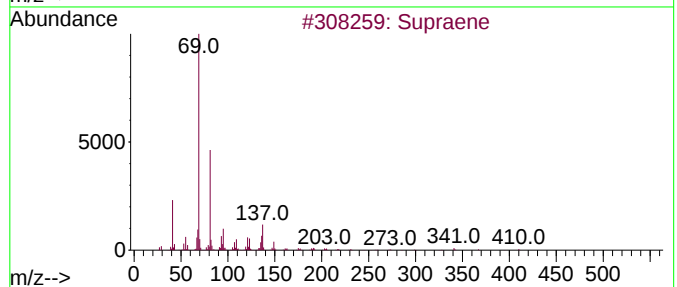
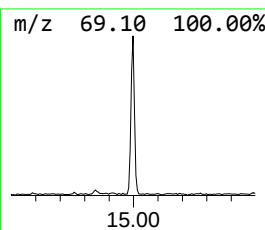
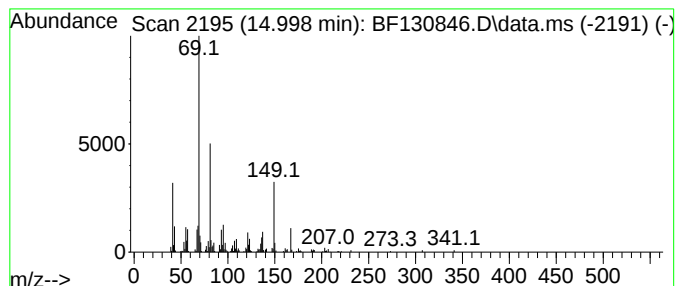
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	8.68 ng	224098	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	74
2			5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	59
3			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	59
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	53
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102822\
Data File : BF130846.D
Acq On : 29 Oct 2022 02:58
Operator : CG\JU
Sample : N5292-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
251032-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.293	75.1	ng	2395740	1	6.945	637854	20.0
2-Pentanone, 4-...	5.169	7.2	ng	230782	1	6.945	637854	20.0
Ethanol, 2-(2-b...	8.128	20.5	ng	838517	2	8.228	816413	20.0
2,4,7,9-Tetrame...	9.416	12.1	ng	553790	3	9.992	919274	20.0
9-Octadecenoic ...	12.575	7.9	ng	371991	4	11.480	938180	20.0
Methyl stearate	12.663	2.3	ng	105712	4	11.480	938180	20.0
Triphenylphosph...	14.221	7.2	ng	252808	5	14.127	705732	20.0
Supraene	14.998	8.7	ng	224098	6	15.639	516403	20.0