LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110122\
Data File : BF130898.D
Acq On : 01 Nov 2022 13:43
Operator : CG\JU
Sample : N5371-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-6-WC

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: BF130898.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	25	34	40	rVB	476109	617051	20.85%	3.173%
2	2.399	47	53	58	rBV	46991	62394	2.11%	0.321%
3	5.175	518	525	536	rVB	278899	367604	12.42%	1.890%
4	5.557	585	590	593	rBV	2394031	2271891	76.75%	11.683%
5	6.557	754	760	777	rVB	2018919	2446728	82.66%	12.582%
6	6.934	820	824	827	rBV	679634	549147	18.55%	2.824%
7	7.498	914	920	923	rBV	1519200	1573023	53.14%	8.089%
8	8.116	1021	1025	1037	rBV	54233	116547	3.94%	0.599%
9	8.216	1037	1042	1046	rVV	799157	736544	24.88%	3.788%
10	9.298	1220	1226	1229	rBV	3253398	2959982	100.00%	15.222%
11	9.981	1337	1342	1345	rBV	1064879	902542	30.49%	4.641%
12	10.775	1472	1477	1480	rBV	2002966	1885304	63.69%	9.695%
13	11.475	1592	1596	1599	rBV	1053890	906317	30.62%	4.661%
14	11.539	1604	1607	1610	rVB2	38768	33904	1.15%	0.174%
15	11.986	1679	1683	1688	rBV2	37857	34850	1.18%	0.179%
16	12.569	1776	1782	1786	rBV2	41029	40162	1.36%	0.207%
17	13.063	1862	1866	1869	rBV	2682639	2491487	84.17%	12.812%
18	13.627	1953	1962	1965	rBV2	38691	44898	1.52%	0.231%
19	13.957	2015	2018	2023	rBV	35276	36917	1.25%	0.190%
20	14.033	2023	2031	2037	rBV5	34451	116756	3.94%	0.600%
21	14.121	2042	2046	2049	rVV	569699	499554	16.88%	2.569%
22	14.216	2057	2062	2067	rBV	55090	69155	2.34%	0.356%
23	14.280	2069	2073	2076	rVB	30709	32755	1.11%	0.168%
24	14.580	2121	2124	2127	rBV	38938	37827	1.28%	0.195%
25	14.886	2173	2176	2178	rBV2	36226	40679	1.37%	0.209%
26	15.263	2236	2240	2244	rVB	40446	47675	1.61%	0.245%
27	15.633	2298	2303	2314	rVB	334751	459478	15.52%	2.363%
28	16.127	2383	2387	2392	rVB	44788	64784	2.19%	0.333%

Sum of corrected areas: 19445955

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Misc :
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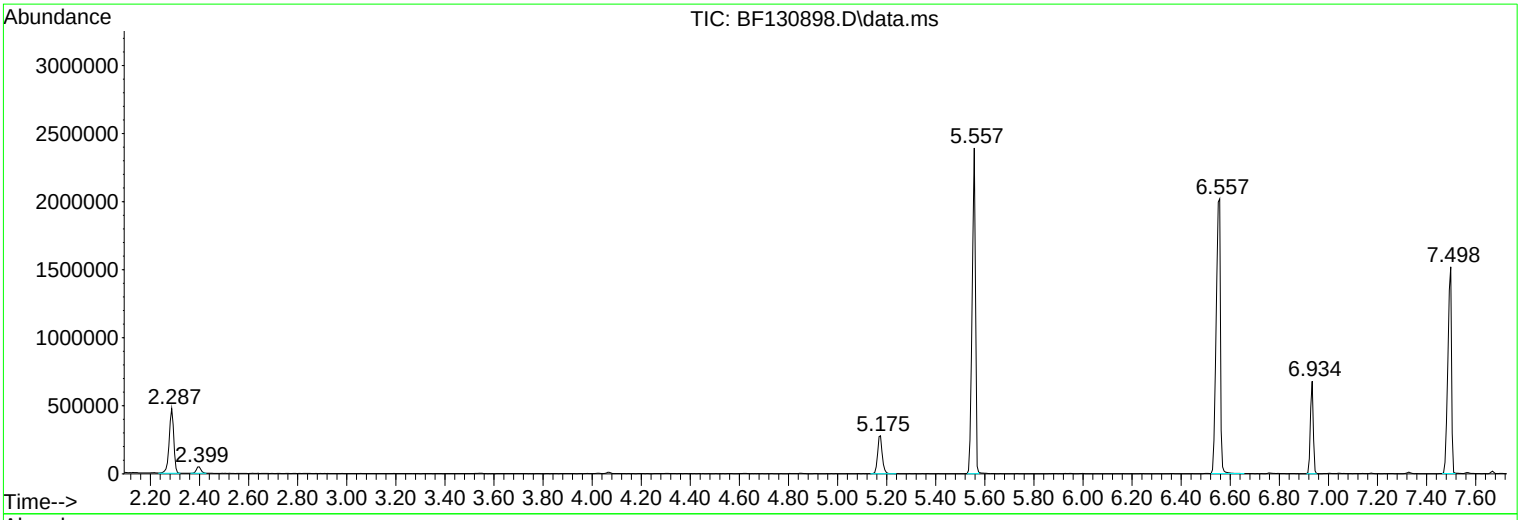
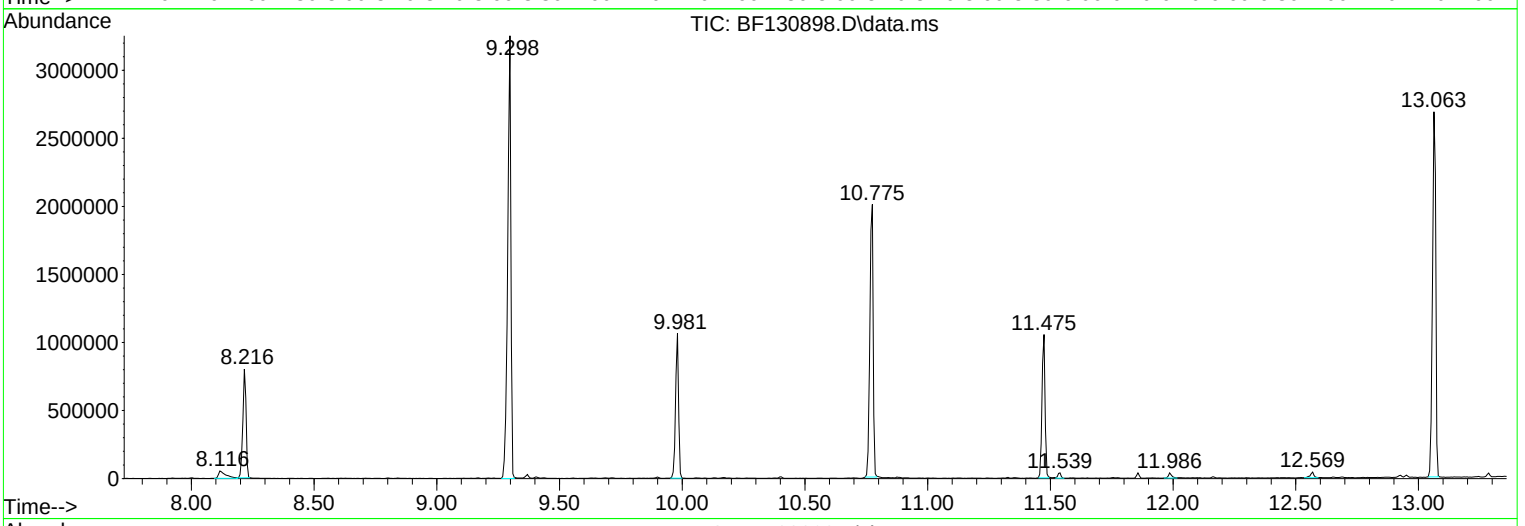
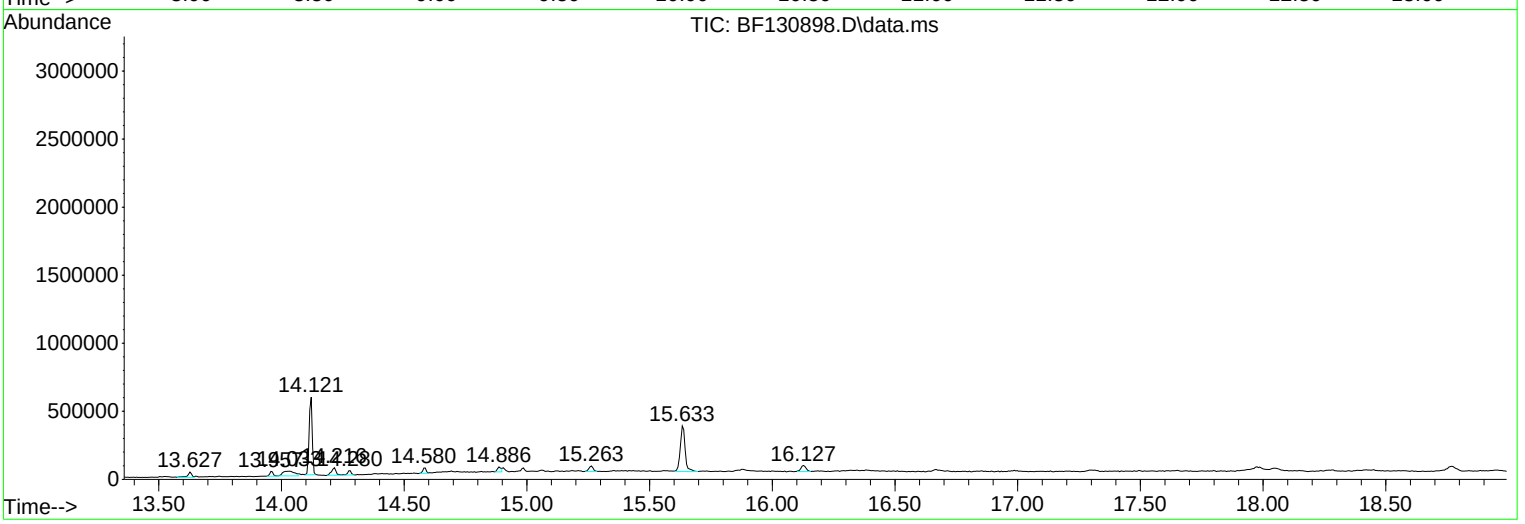
Instrument :
BNA_F
ClientSampleId :
MH-6-WC

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

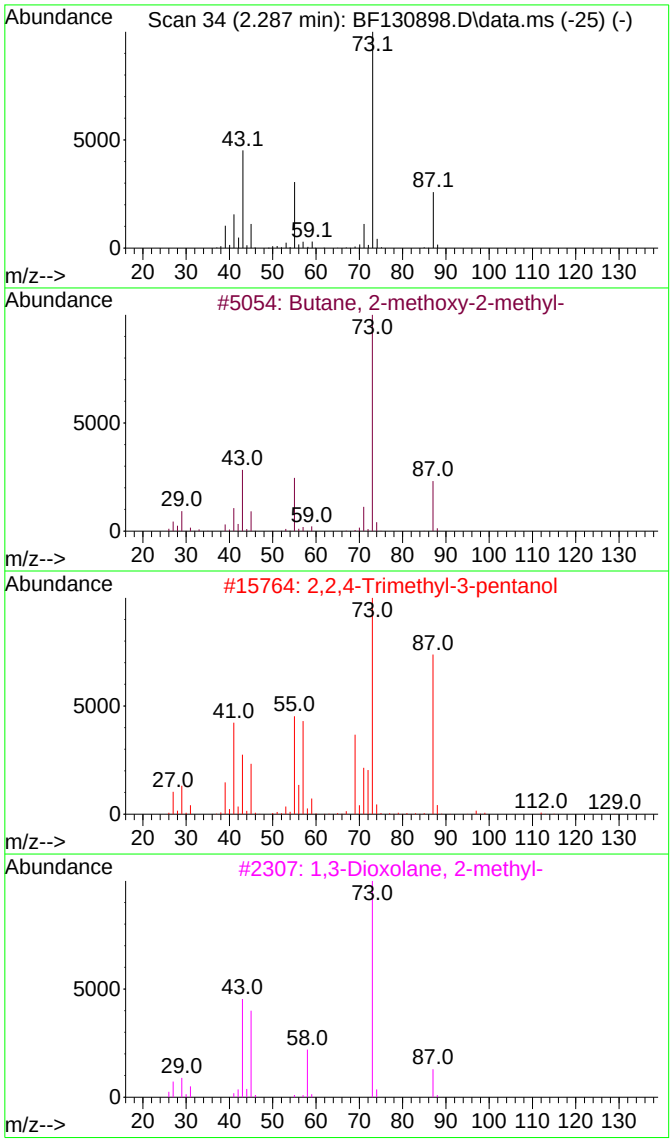
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

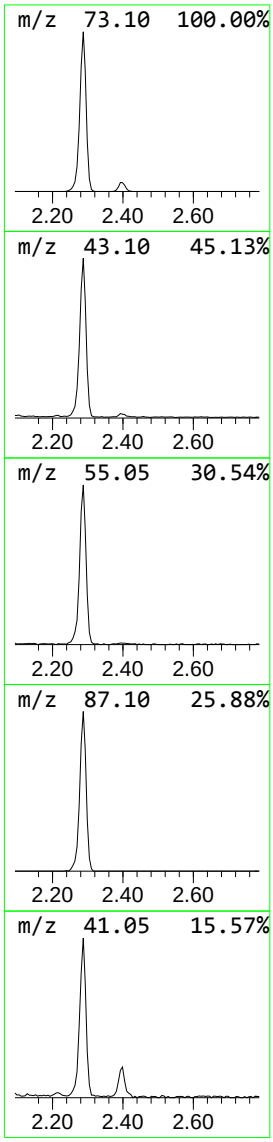
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	22.47 ng	617051	1,4-Dichlorobenzene-d4	6.934

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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Data File : BF130898.D
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Sample : N5371-01
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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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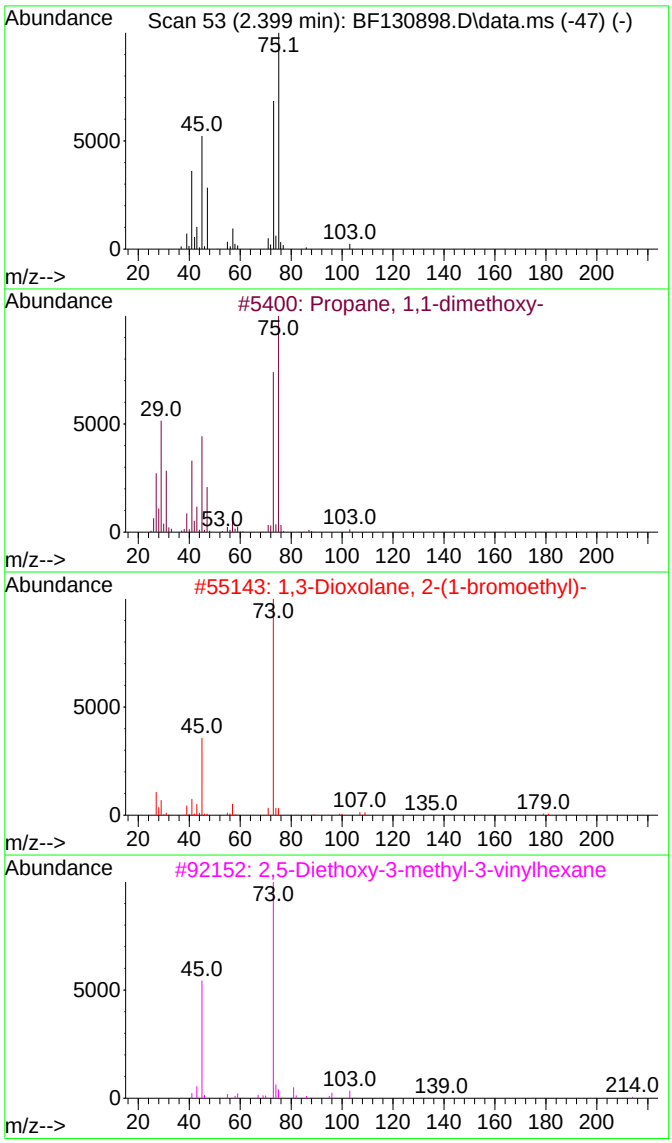
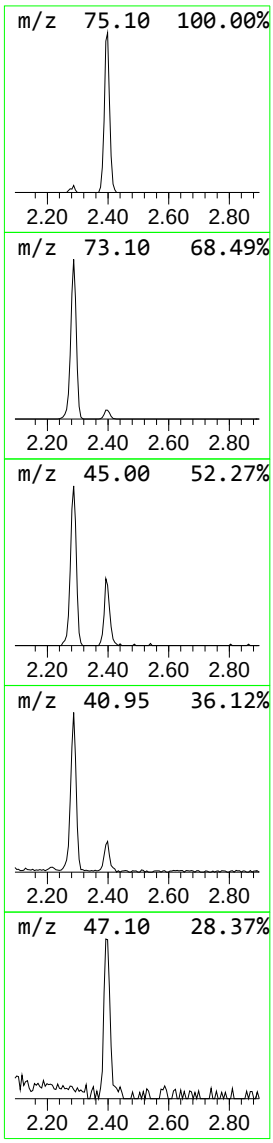
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	2.27 ng	62394	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	22
3	2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	12
4	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	10
5	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	9





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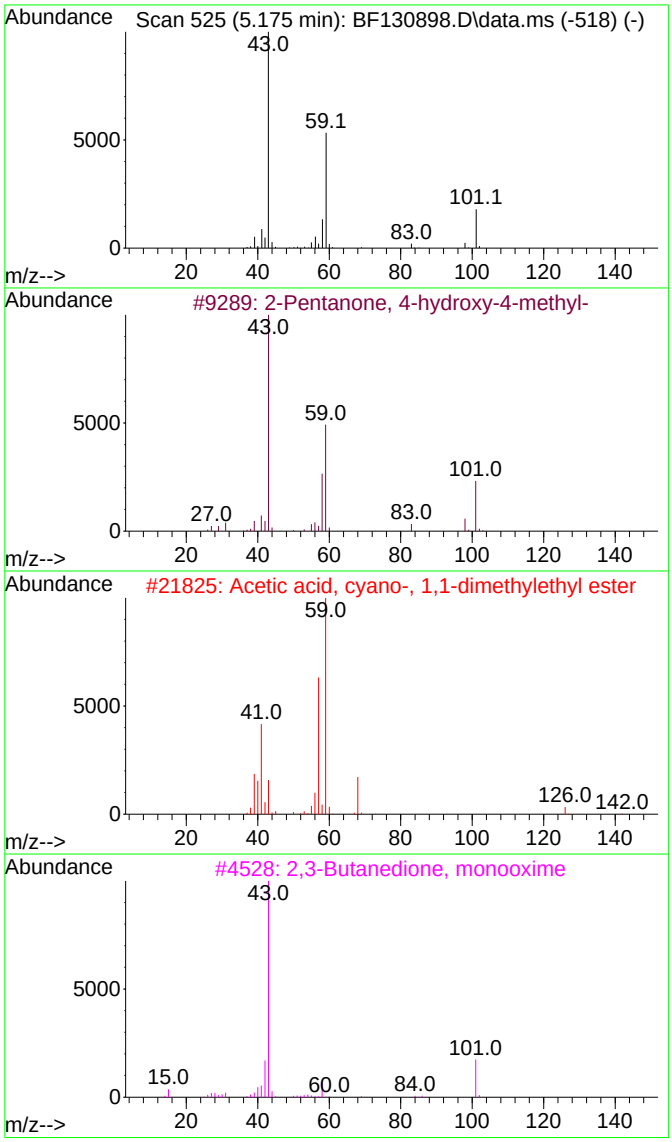
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

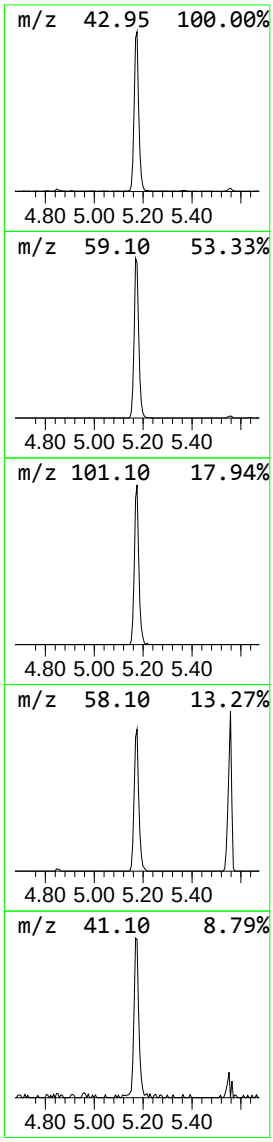
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	13.39 ng	367604	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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ClientSampleId :
MH-6-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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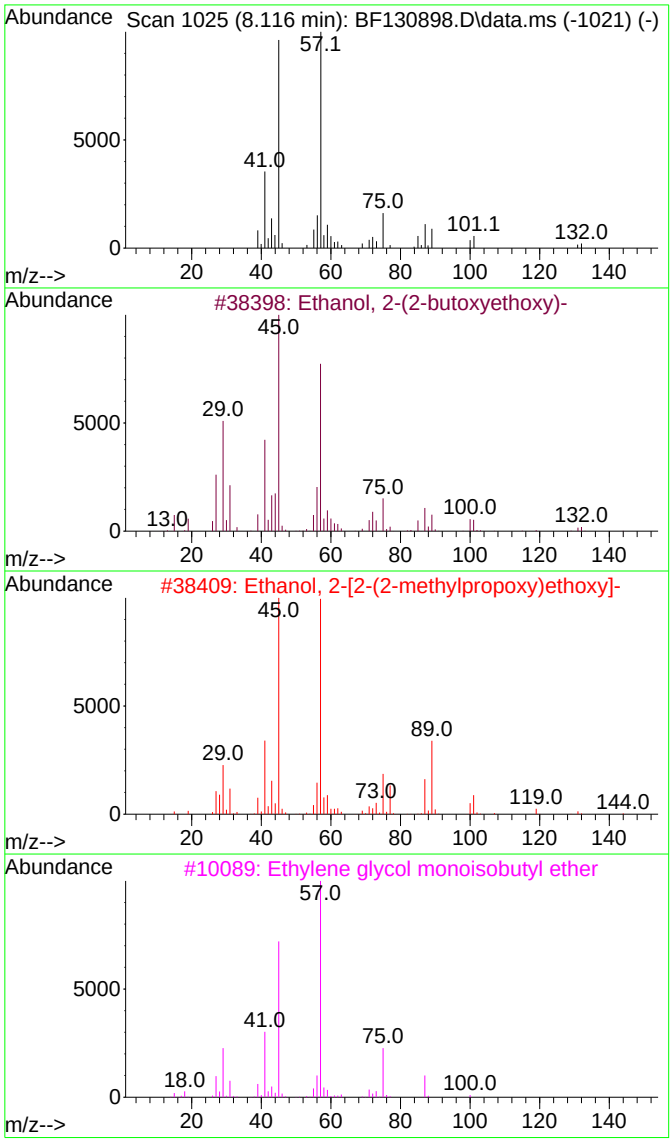
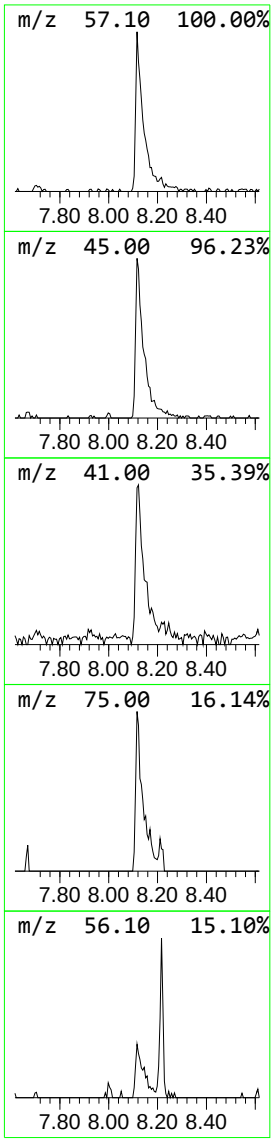
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.116	3.16 ng	116547	Naphthalene-d8	8.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	56
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





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Sample : N5371-01
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Instrument :
BNA_F
ClientSampleId :
MH-6-WC

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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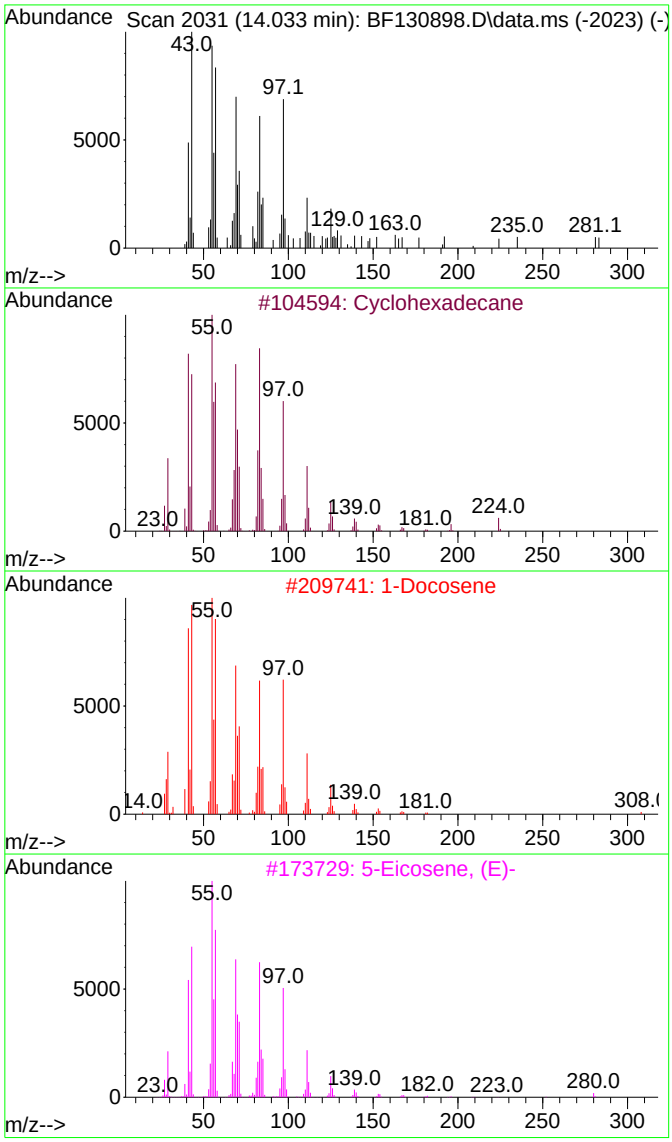
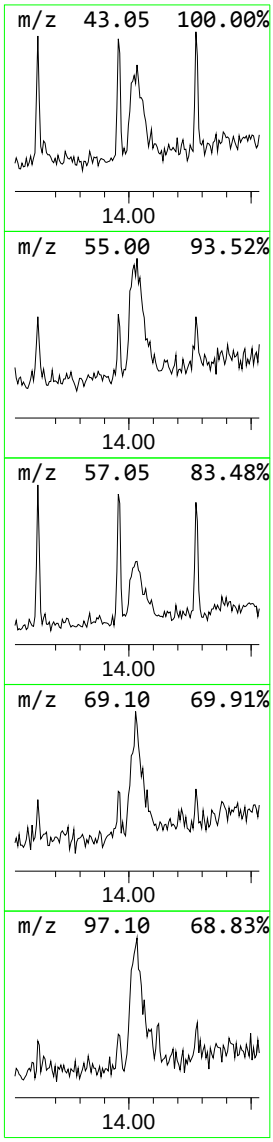
Peak Number 5 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	4.67 ng	116756	Chrysene-d12	14.121

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	1-Docosene	308	C22H44	001599-67-3	90
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
5	5-Fluoro-3-trifluoromethylbenzoi...	474	C27H42F4O2	1000338-91-1	87





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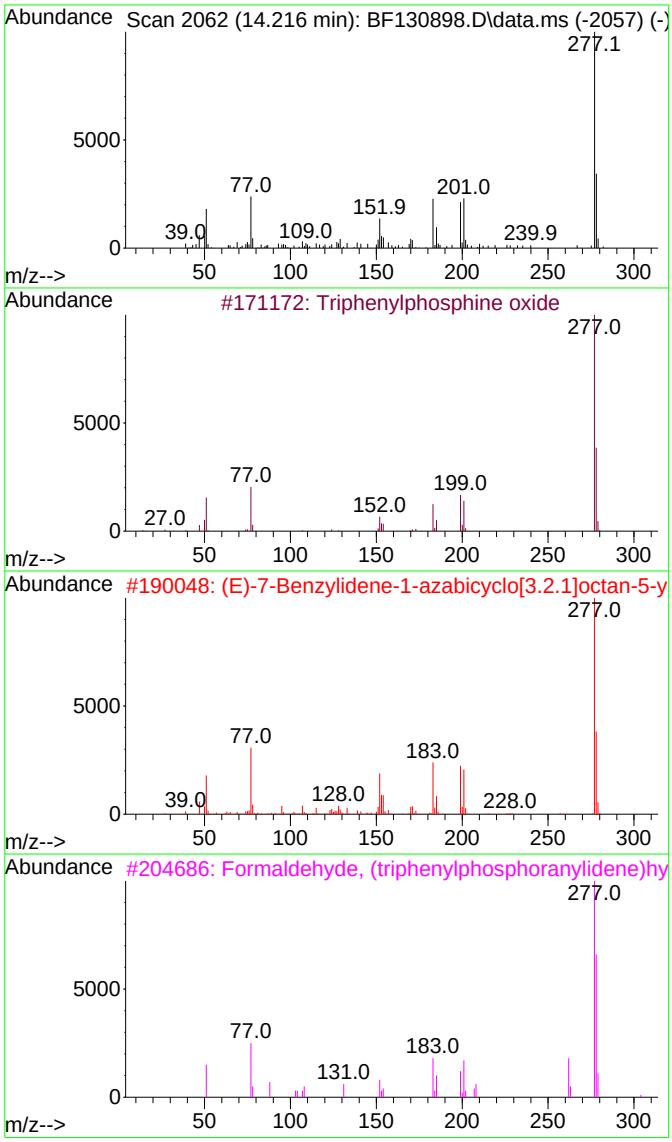
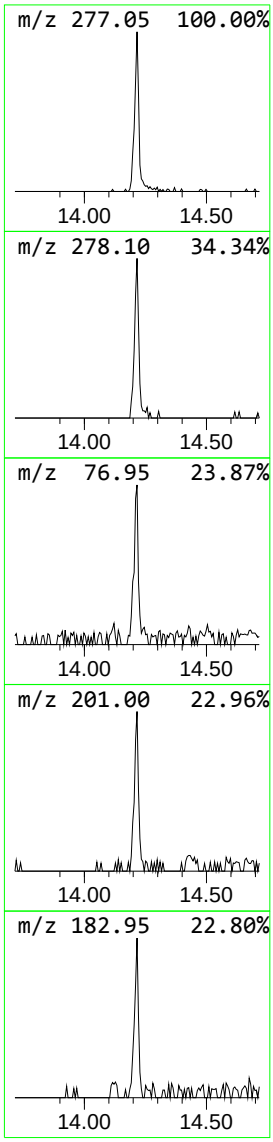
Peak Number 6 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.216	2.77 ng	69155	Chrysene-d12	14.121

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	74
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5	2-Indolinone, 2TMS derivative	277	C14H23NOSi2	010416-65-6	35





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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

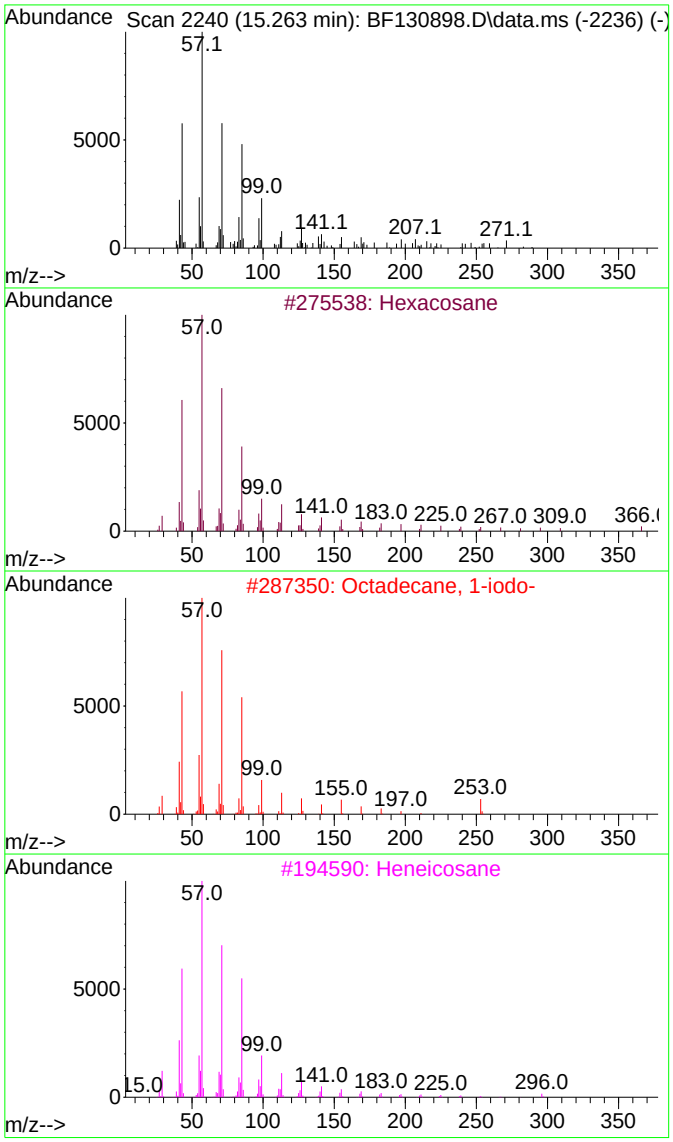
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

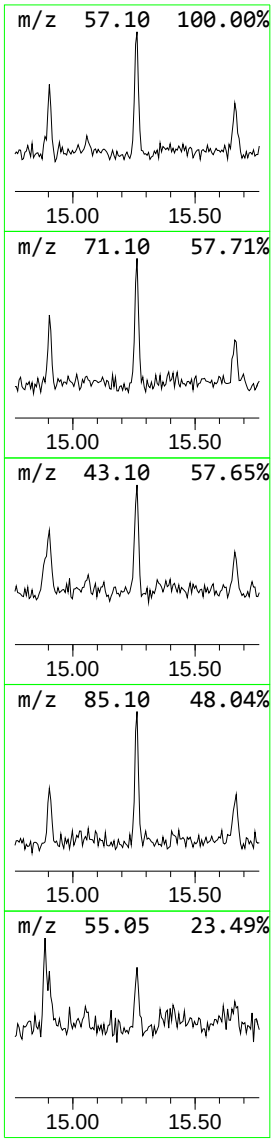
****

Peak Number 7 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.262	2.08 ng	47675	Perylene-d12	15.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	80
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
3	Heneicosane	296	C21H44	000629-94-7	72
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72
5	Octadecane	254	C18H38	000593-45-3	72





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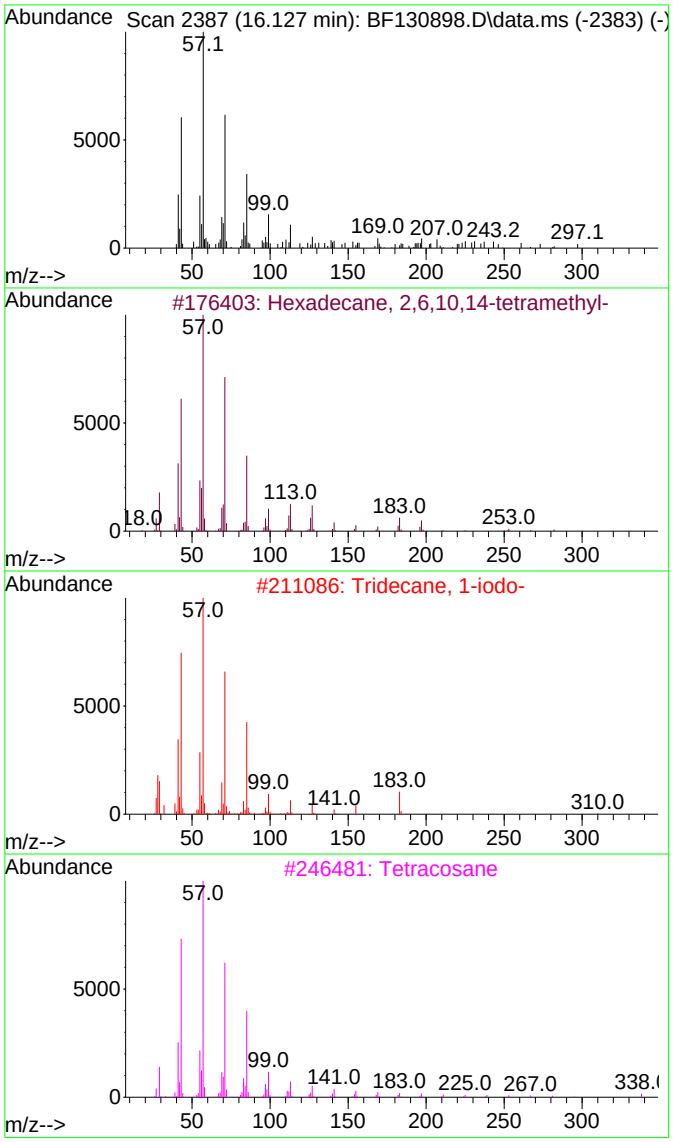
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

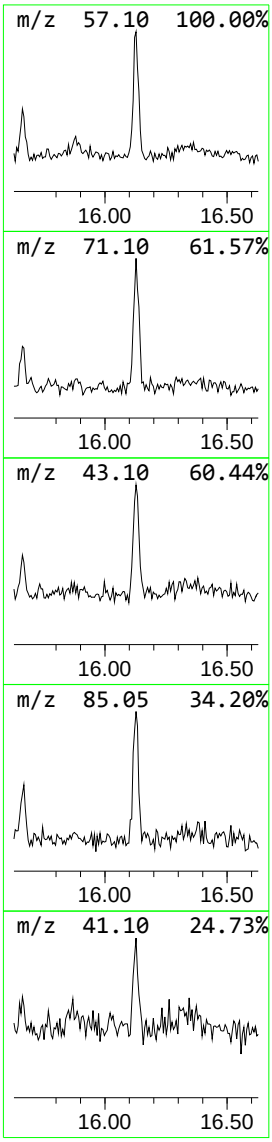
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexadecane, 2,6,10,14-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.127	2.82 ng	64784	Perylene-d12	15.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
3	Tetracosane	338	C24H50	000646-31-1	83
4	Heptacosane	380	C27H56	000593-49-7	83
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	83





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.287	22.5	ng	617051	1	6.934	549147	20.0
Propane, 1,1-di...	2.399	2.3	ng	62394	1	6.934	549147	20.0
2-Pentanone, 4-...	5.175	13.4	ng	367604	1	6.934	549147	20.0
Ethanol, 2-(2-b...	8.116	3.2	ng	116547	2	8.216	736544	20.0
Cyclohexadecane	14.033	4.7	ng	116756	5	14.121	499554	20.0
Triphenylphosph...	14.216	2.8	ng	69155	5	14.121	499554	20.0
Hexacosane	15.262	2.1	ng	47675	6	15.633	459478	20.0
Hexadecane, 2,6...	16.127	2.8	ng	64784	6	15.633	459478	20.0