LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120921\
Data File : BP008327.D
Acq On : 09 Dec 2021 23:56
Operator : CG/JU
Sample : M4966-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : P1-COMP

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_P\Methods\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008327.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.022	3	6	14	rVB	172134	198687	6.01%	1.103%
2	3.393	65	69	74	rBV	37412	42210	1.28%	0.234%
3	3.969	162	167	175	rVB2	27349	41907	1.27%	0.233%
4	4.893	319	324	337	rBV	412744	566729	17.13%	3.148%
5	5.364	396	404	410	rBV	1049802	1620761	48.99%	9.002%
6	5.411	410	412	421	rVB	65011	114464	3.46%	0.636%
7	5.781	467	475	485	rVB	25070	42142	1.27%	0.234%
8	6.958	667	675	695	rBV	898488	1694641	51.23%	9.412%
9	7.763	805	812	822	rVB	255104	398172	12.04%	2.211%
10	8.928	1003	1010	1027	rBV	588684	1034457	31.27%	5.745%
11	10.563	1279	1288	1301	rBV	273683	501140	15.15%	2.783%
12	13.034	1701	1708	1722	rBV	1307718	2052503	62.04%	11.399%
13	13.245	1738	1744	1748	rBV	22099	33277	1.01%	0.185%
14	14.328	1919	1928	1934	rBV3	23310	44269	1.34%	0.246%
15	14.422	1937	1944	1960	rVB	395878	660873	19.98%	3.670%
16	15.845	2181	2186	2192	rBV	76157	102401	3.10%	0.569%
17	15.922	2192	2199	2217	rBV	993062	1671080	50.51%	9.281%
18	17.181	2407	2413	2422	rBV	500464	807085	24.40%	4.482%
19	17.845	2523	2526	2534	rVB8	14876	33222	1.00%	0.185%
20	18.086	2563	2567	2571	rBV2	46199	63553	1.92%	0.353%
21	18.980	2715	2719	2726	rVB3	25322	42504	1.28%	0.236%
22	19.757	2845	2851	2861	rVB	2755127	3308121	100.00%	18.373%
23	20.504	2975	2978	2982	rBV	60248	58375	1.76%	0.324%
24	21.004	3059	3063	3073	rVB	228191	355495	10.75%	1.974%
25	21.198	3093	3096	3103	rVB	128645	149452	4.52%	0.830%
26	21.292	3107	3112	3120	rBV	770047	1089895	32.95%	6.053%
27	22.174	3259	3262	3267	rVB2	88718	115038	3.48%	0.639%
28	23.674	3511	3517	3530	rVB2	544819	1162796	35.15%	6.458%

Sum of corrected areas: 18005249

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Misc :
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Instrument :
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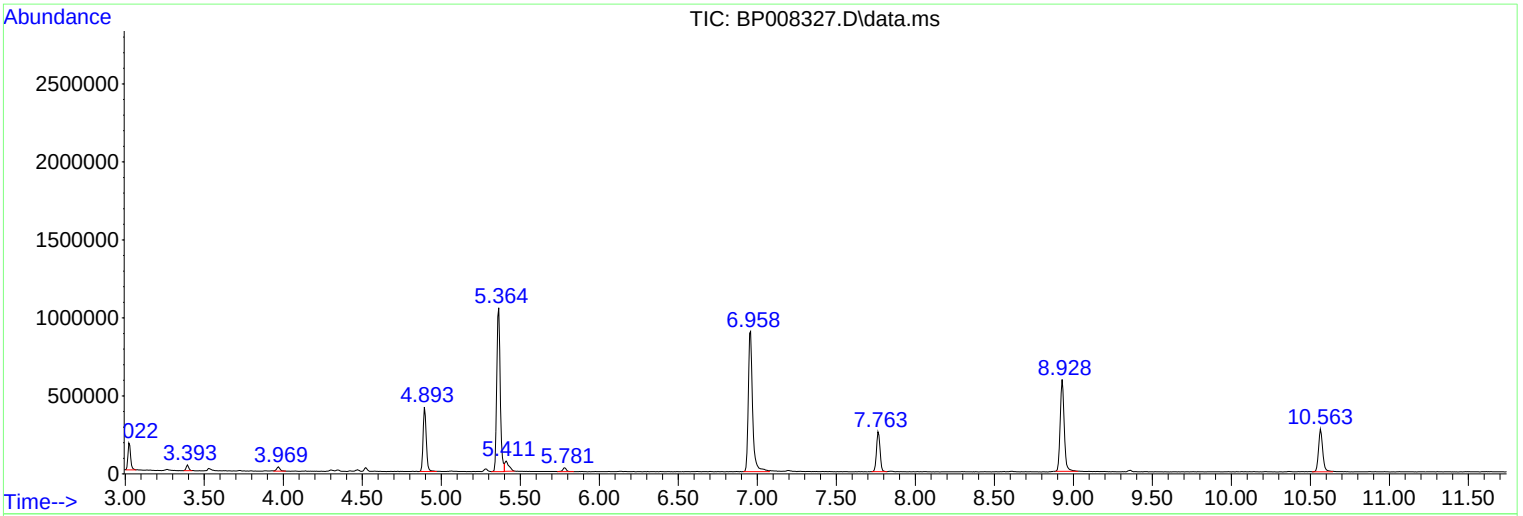
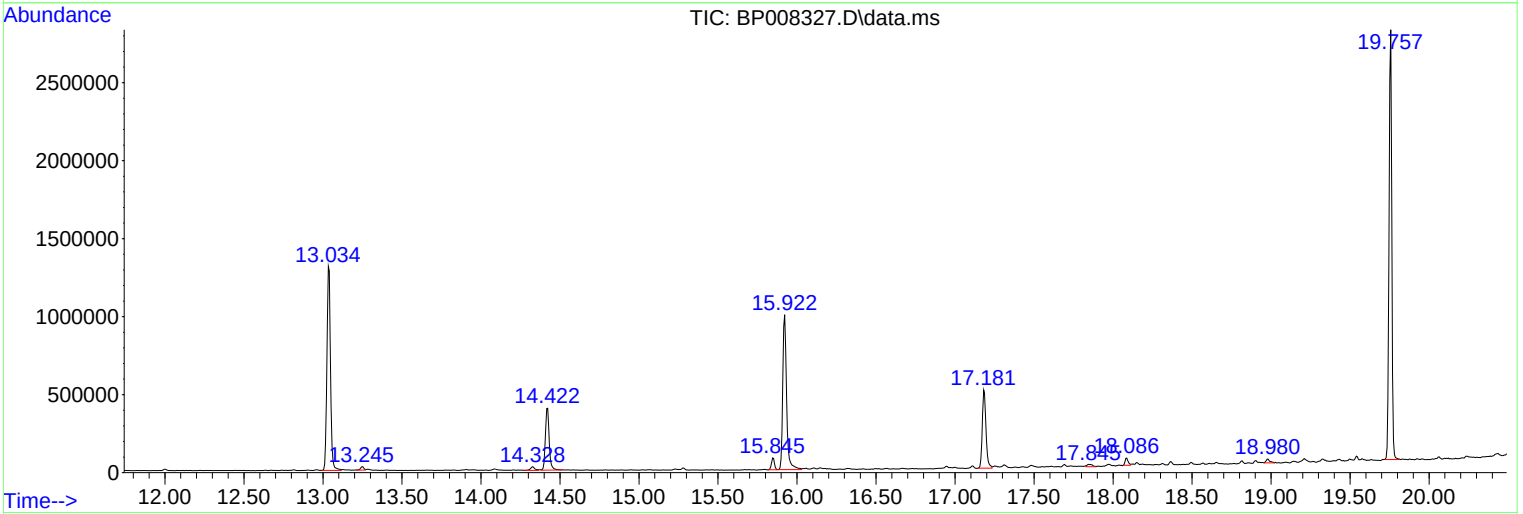
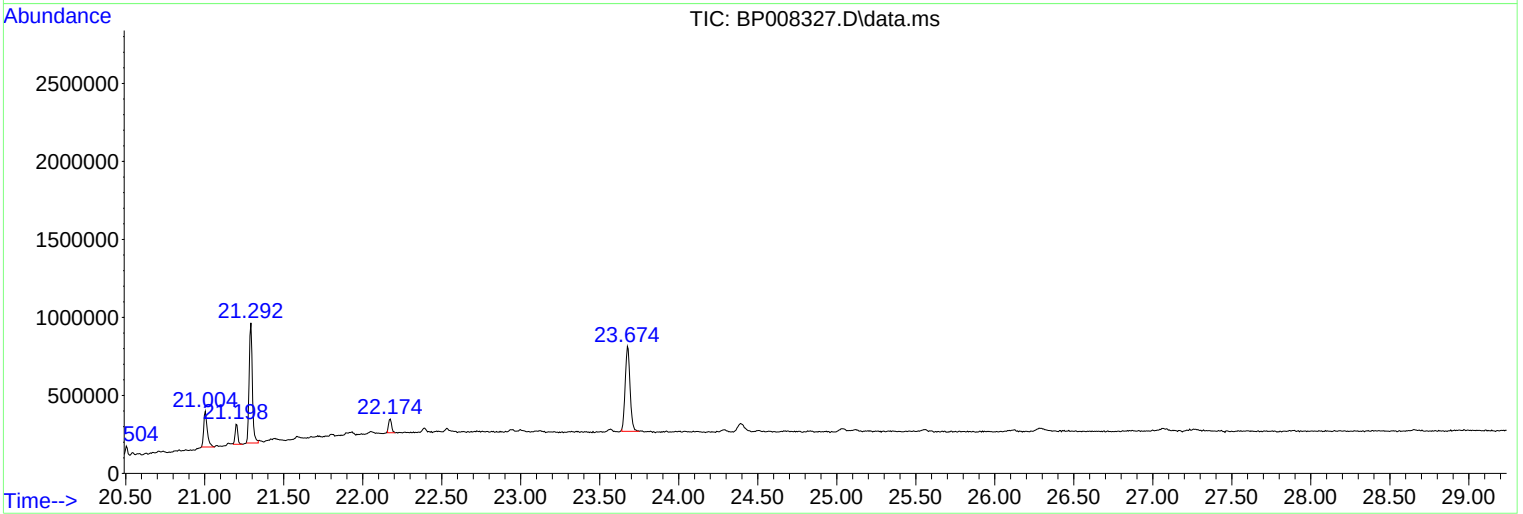
ClientSampleId :
P1-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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

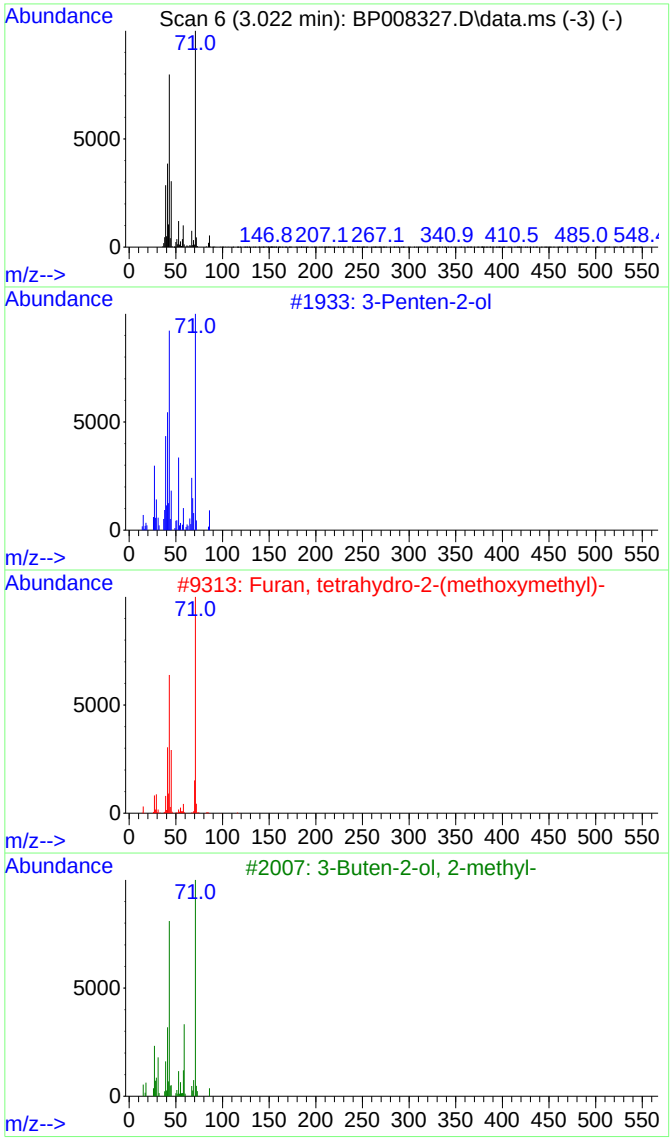
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

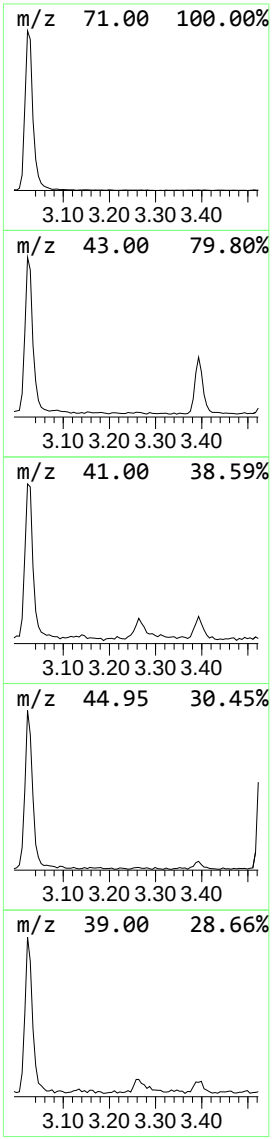
****

Peak Number 1 3-Penten-2-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.022	9.98 ng	198687	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	72
2	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	72
3	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
4	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	53
5	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	45





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Acq On : 09 Dec 2021 23:56
Operator : CG/JU
Sample : M4966-05
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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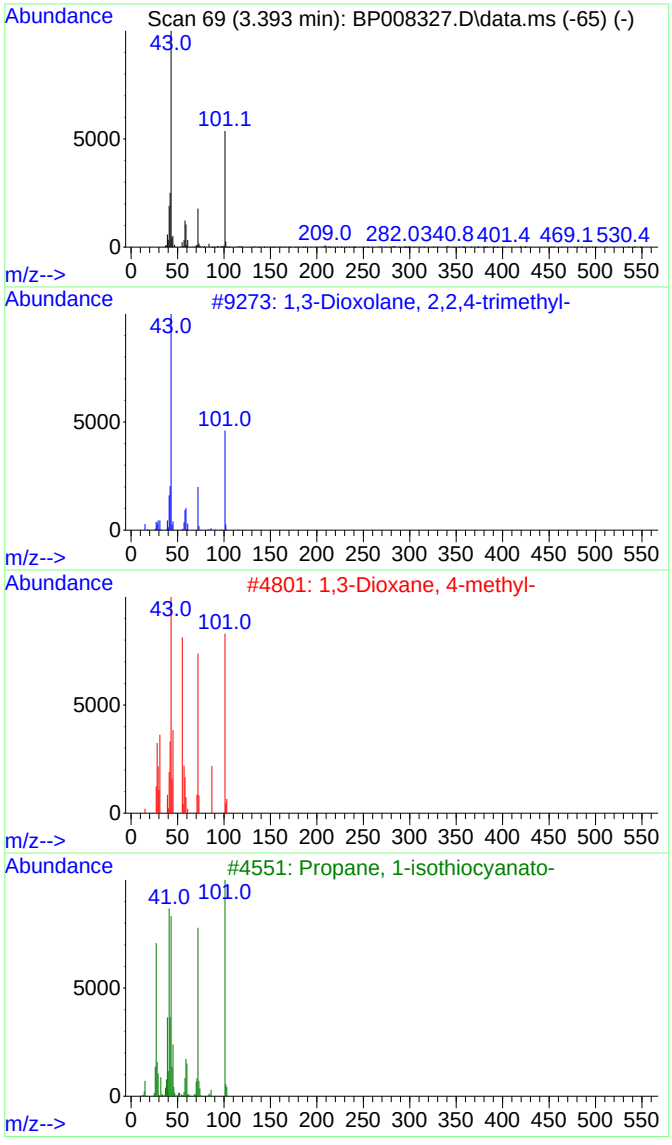
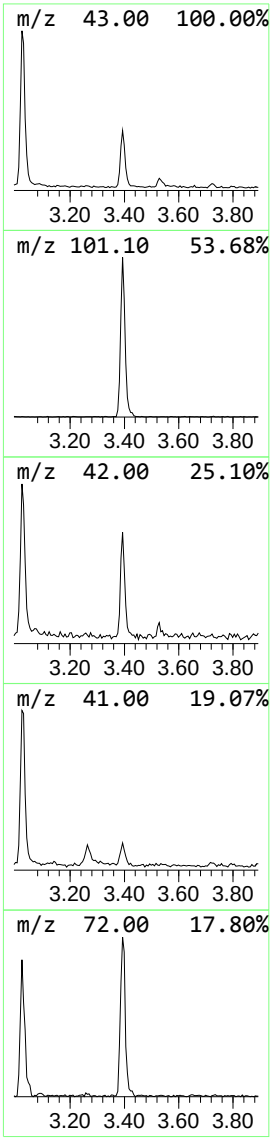
****
Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	2.12 ng	42210	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	86
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	53
3	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	50
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	45
5	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	43





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
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TIC Library : C:\Database\NIST20.L
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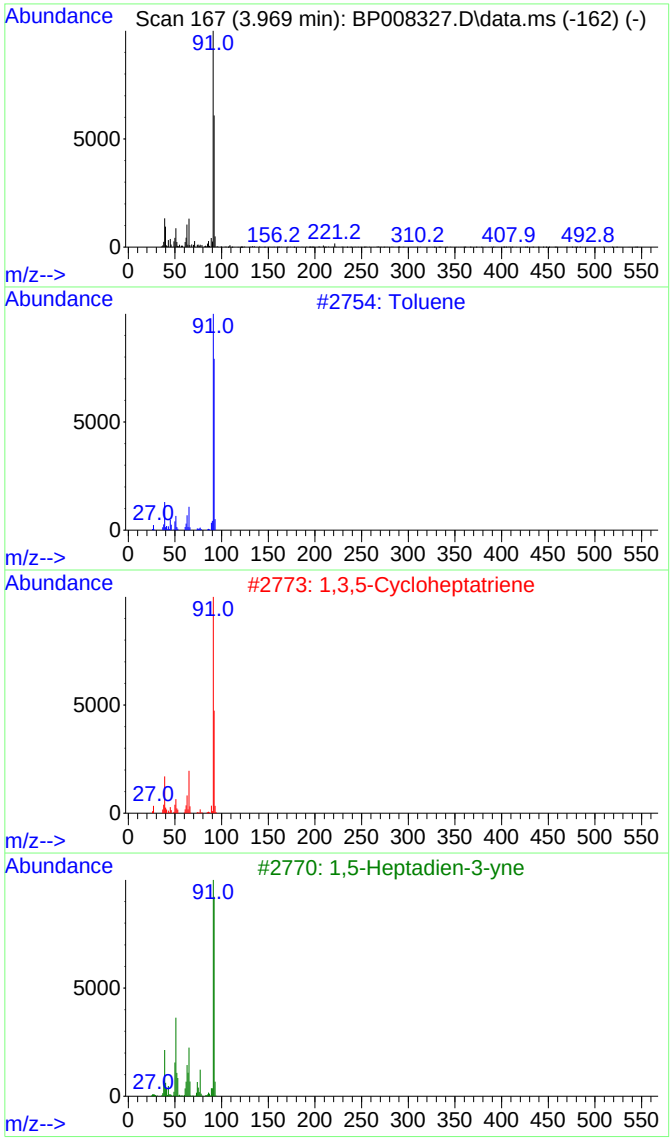
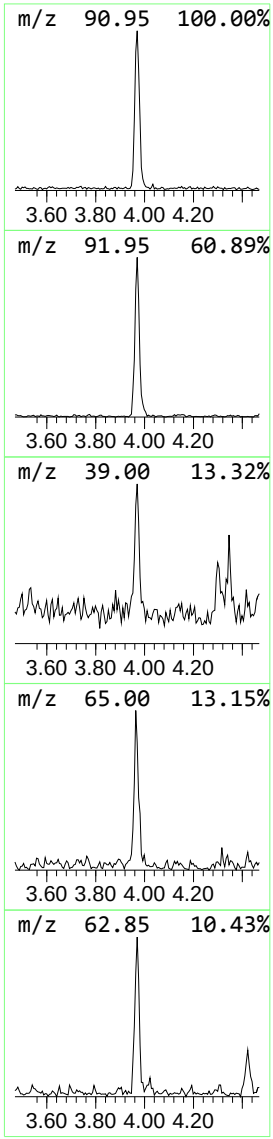
****

Peak Number 3 Toluene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.969	2.10 ng	41907	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	90
2	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	86
3	1,5-Heptadien-3-yne	92	C7H8	003511-27-1	72
4	Benzene, (ethoxymethyl)-	136	C9H12O	000539-30-0	59
5	Benzene, (butoxymethyl)-	164	C11H16O	000588-67-0	59





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Instrument :
BNA_P
ClientSampleId :
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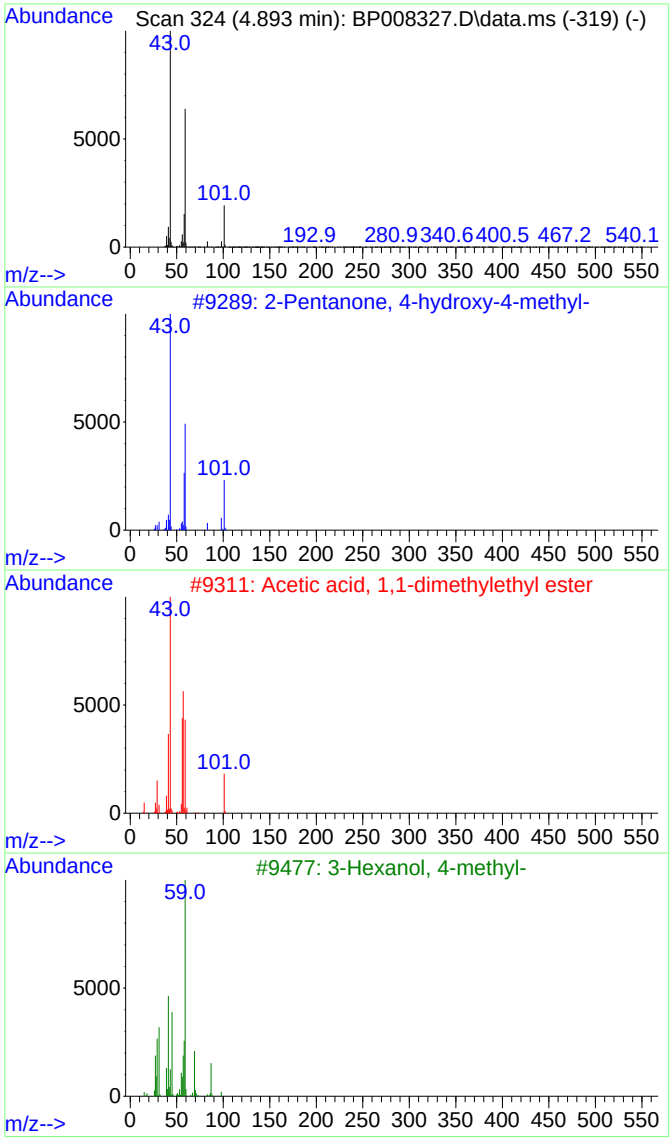
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

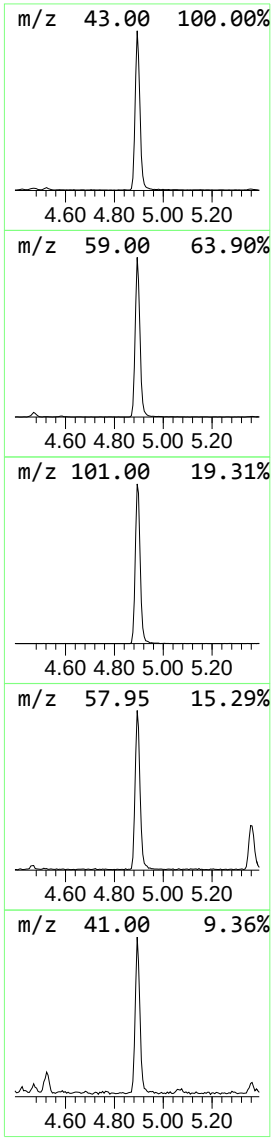
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	28.47 ng	566729	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
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TIC Library : C:\Database\NIST20.L
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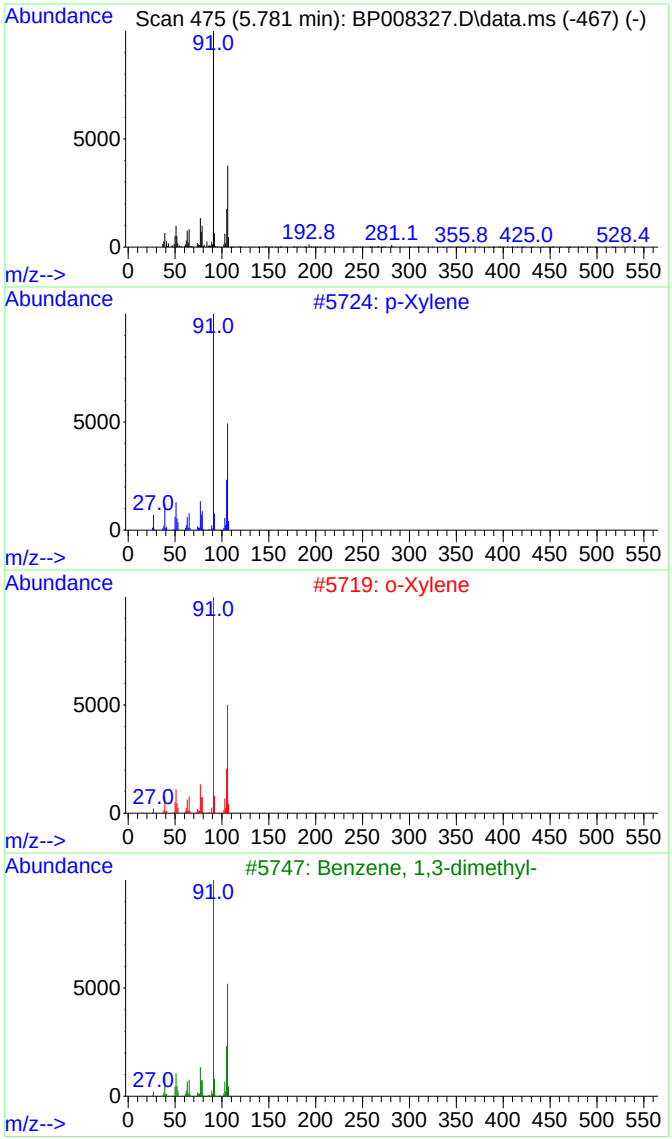
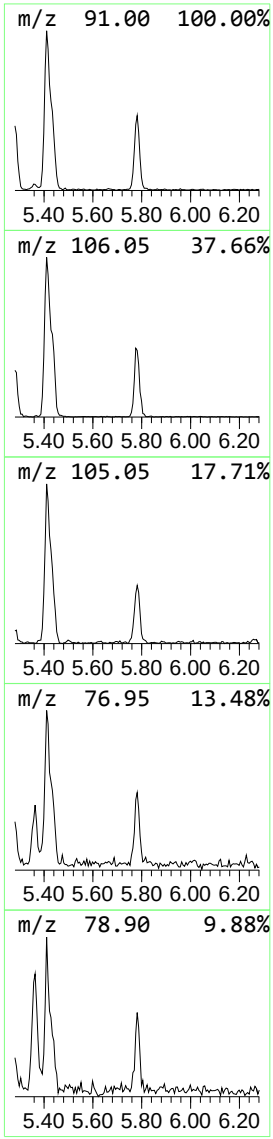
****

Peak Number 5 p-Xylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.781	2.12 ng	42142	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Xylene	106	C8H10	000106-42-3	97
2	o-Xylene	106	C8H10	000095-47-6	97
3	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
4	Ethylbenzene	106	C8H10	000100-41-4	83
5	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	72





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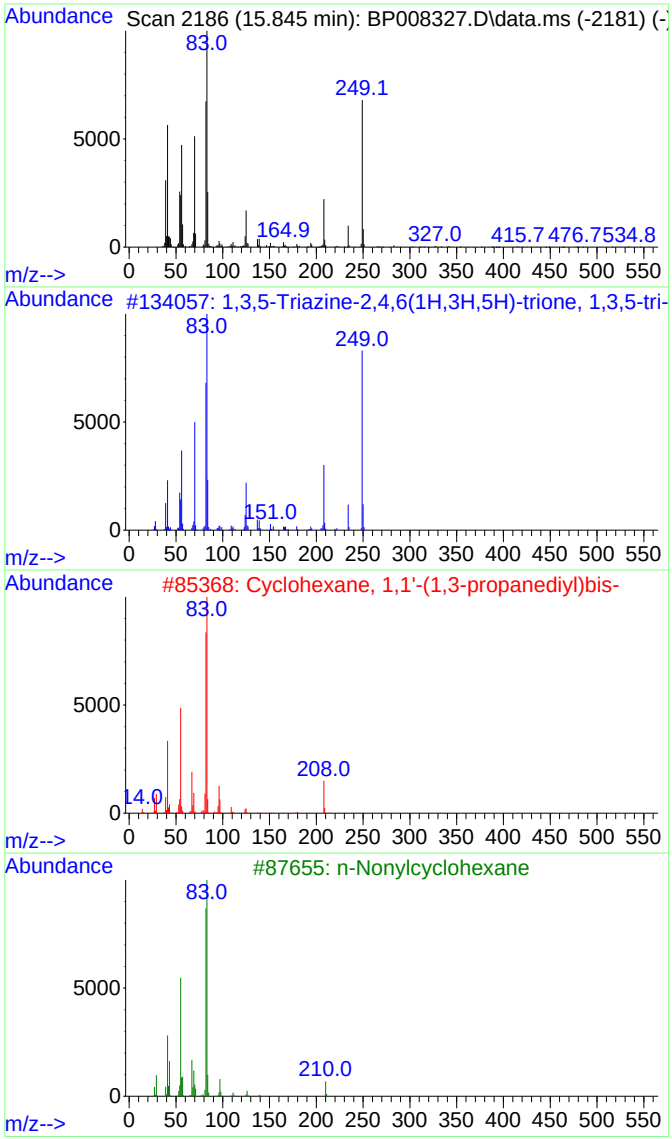
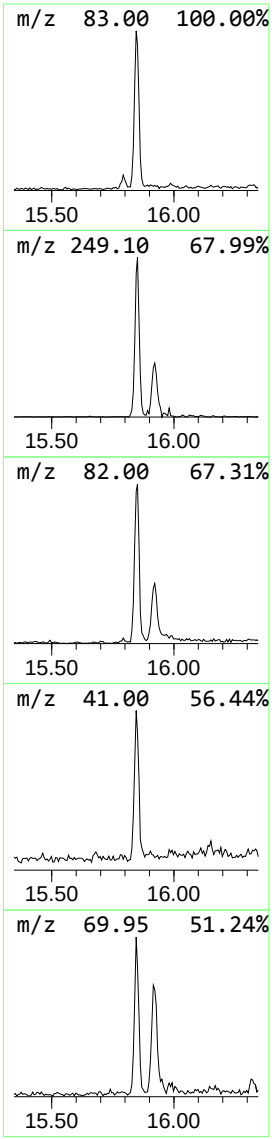
****
Peak Number 6 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.845	2.54 ng	102401	Phenanthrene-d10	17.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	98
2	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	35
3	n-Nonylcyclohexane	210	C15H30	002883-02-5	27
4	Cyclohexane, undecyl-	238	C17H34	054105-66-7	16
5	Succinic acid, 2-methylpent-3-yl...	284	C16H28O4	1000391-11-2	16





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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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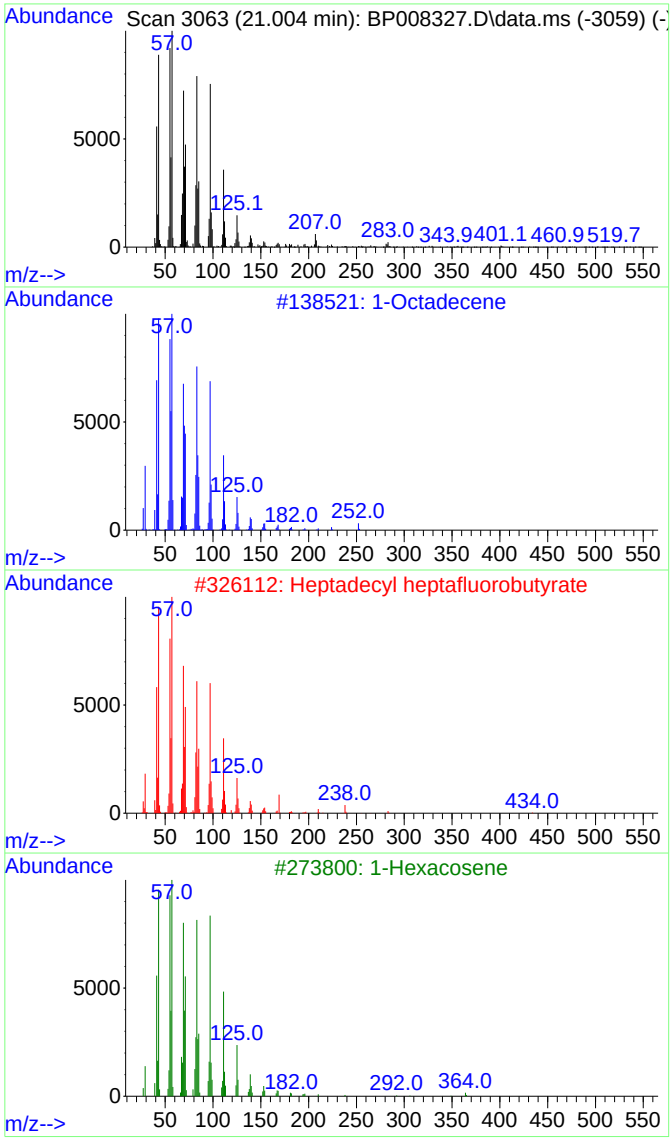
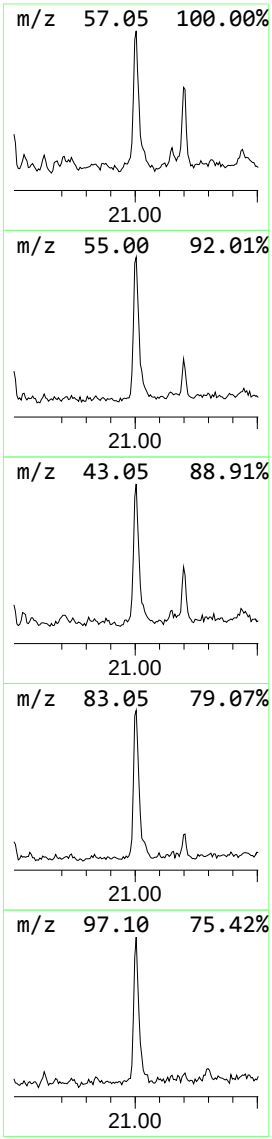
****

Peak Number 7 1-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.004	6.52 ng	355495	Chrysene-d12	21.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Hexacosene	364	C26H52	018835-33-1	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94





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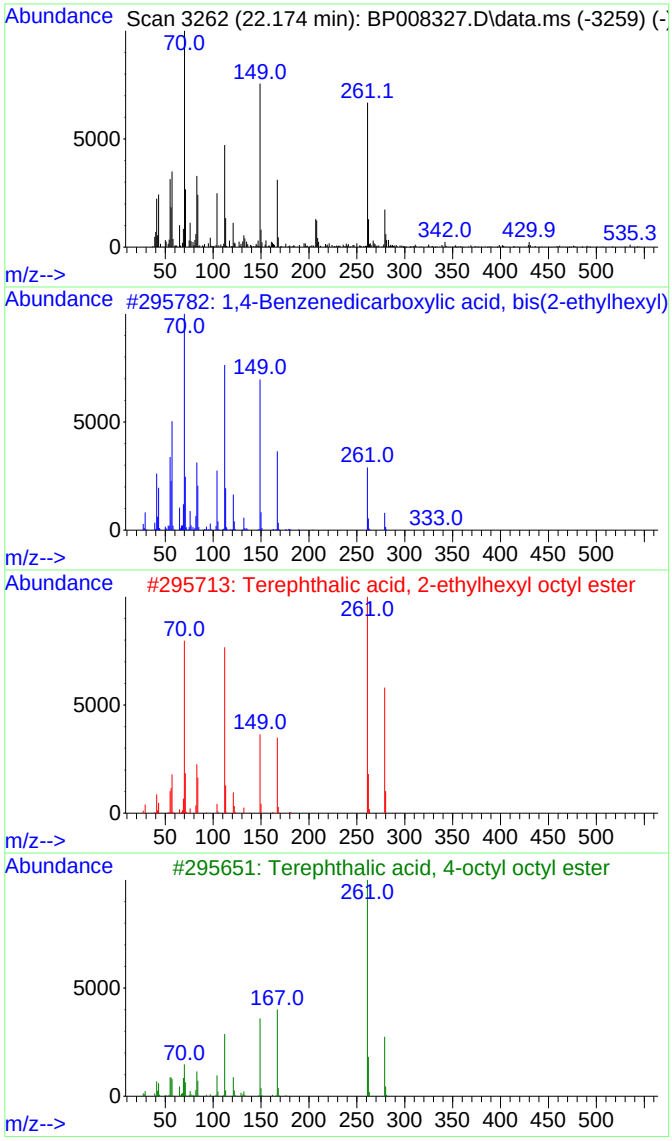
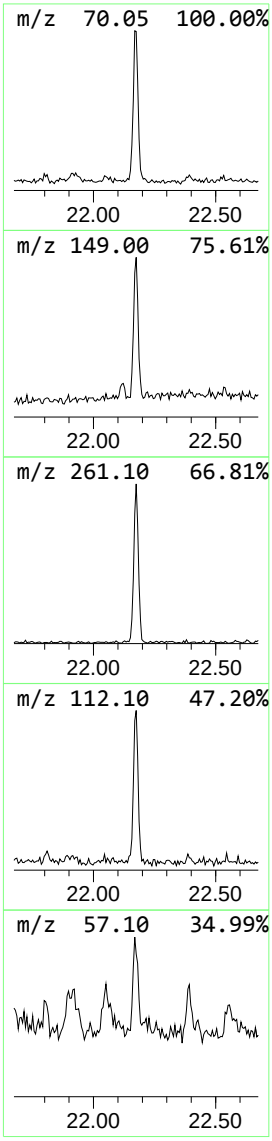
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,4-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.174	2.11 ng	115038	Chrysene-d12	21.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
2	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	35
3	Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	30
4	4-Nitrobenzoic acid, cyclobutyl ...	221	C11H11NO4	070335-00-1	22
5	1,4-benzenedicarboxylic acid, mo...	208	C11H12O4	1000400-56-6	22





Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument :
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-ol	3.022	10.0	ng	198687	1	7.763	398172	20.0
1,3-Dioxolane, ...	3.393	2.1	ng	42210	1	7.763	398172	20.0
Toluene	3.969	2.1	ng	41907	1	7.763	398172	20.0
2-Pentanone, 4-...	4.893	28.5	ng	566729	1	7.763	398172	20.0
p-Xylene	5.781	2.1	ng	42142	1	7.763	398172	20.0
1,3,5-Triazine-...	15.845	2.5	ng	102401	4	17.181	807085	20.0
1-Octadecene	21.004	6.5	ng	355495	5	21.292	1089900	20.0
1,4-Benzenedica...	22.174	2.1	ng	115038	5	21.292	1089900	20.0