LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
Data File : BP007933.D
Acq On : 10 Nov 2021 22:47
Operator : CG/JU
Sample : M4572-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
2

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-BP110221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007933.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.440	359	366	377	rVB	952456	1353747	17.60%	4.832%
2	7.028	628	636	648	rBV	499747	791378	10.29%	2.825%
3	7.852	768	776	784	rBV	394400	623080	8.10%	2.224%
4	9.010	966	973	984	rBV	1199558	1953764	25.40%	6.973%
5	10.651	1242	1252	1263	rBV	473119	786043	10.22%	2.806%
6	11.304	1352	1363	1370	rBV	98197	185320	2.41%	0.661%
7	12.857	1622	1627	1641	rBV	67308	108699	1.41%	0.388%
8	13.116	1663	1671	1687	rBV	2948633	4393572	57.12%	15.682%
9	13.245	1687	1693	1704	rVB	85310	162519	2.11%	0.580%
10	14.492	1896	1905	1916	rBV	654896	993040	12.91%	3.544%
11	14.710	1937	1942	1948	rBV	54545	78136	1.02%	0.279%
12	15.987	2151	2159	2176	rBV	2411159	3736428	48.58%	13.336%
13	17.245	2367	2373	2382	rBV	864635	1261123	16.40%	4.501%
14	17.922	2483	2488	2494	rVB2	102579	129536	1.68%	0.462%
15	19.810	2803	2809	2817	rBV	6282847	7691531	100.00%	27.453%
16	21.051	3017	3020	3027	rBV5	85256	120942	1.57%	0.432%
17	21.339	3064	3069	3074	rBV	1277512	1712789	22.27%	6.113%
18	23.745	3472	3478	3488	rVB2	922344	1935876	25.17%	6.910%

Sum of corrected areas: 28017523

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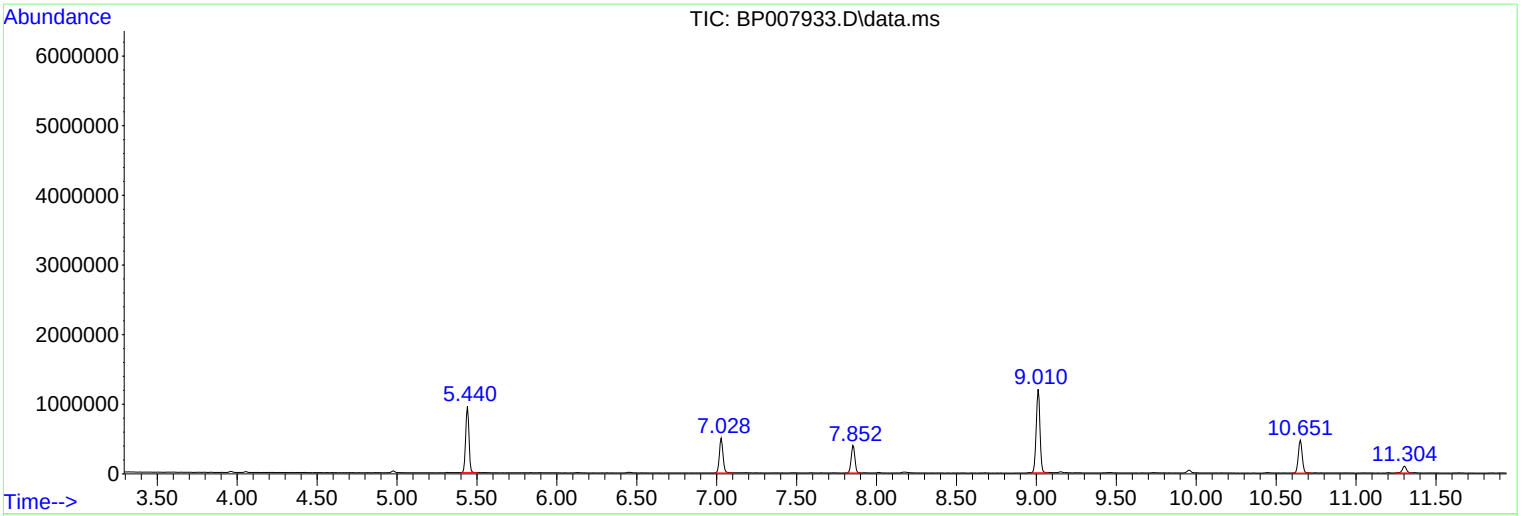
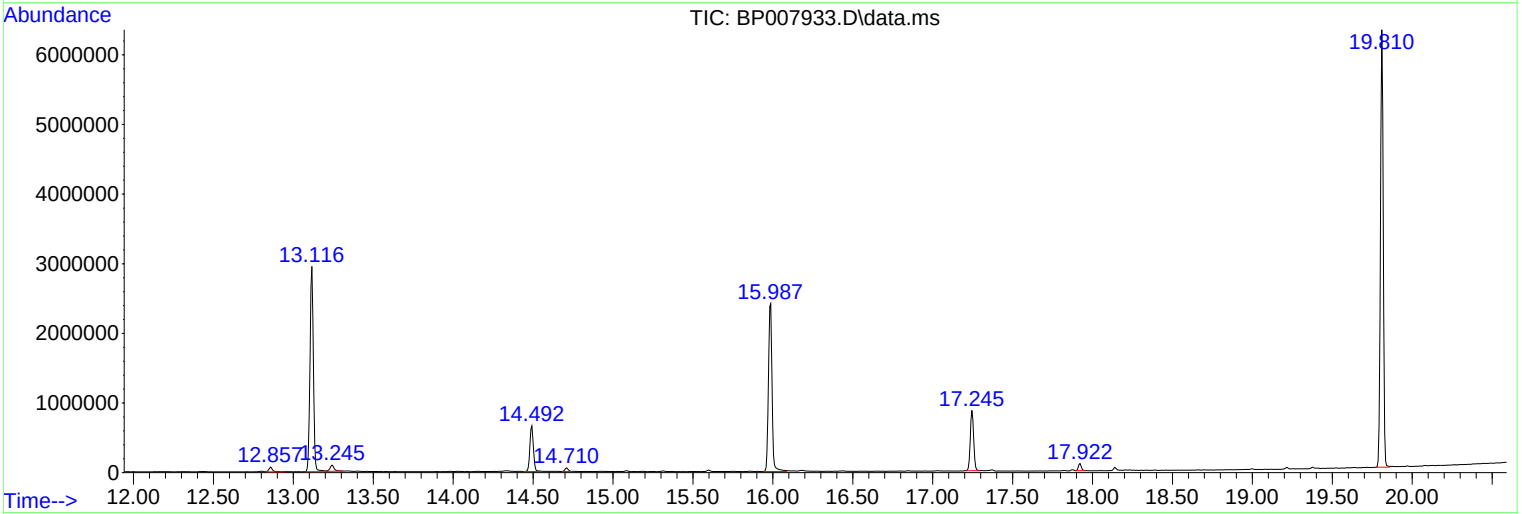
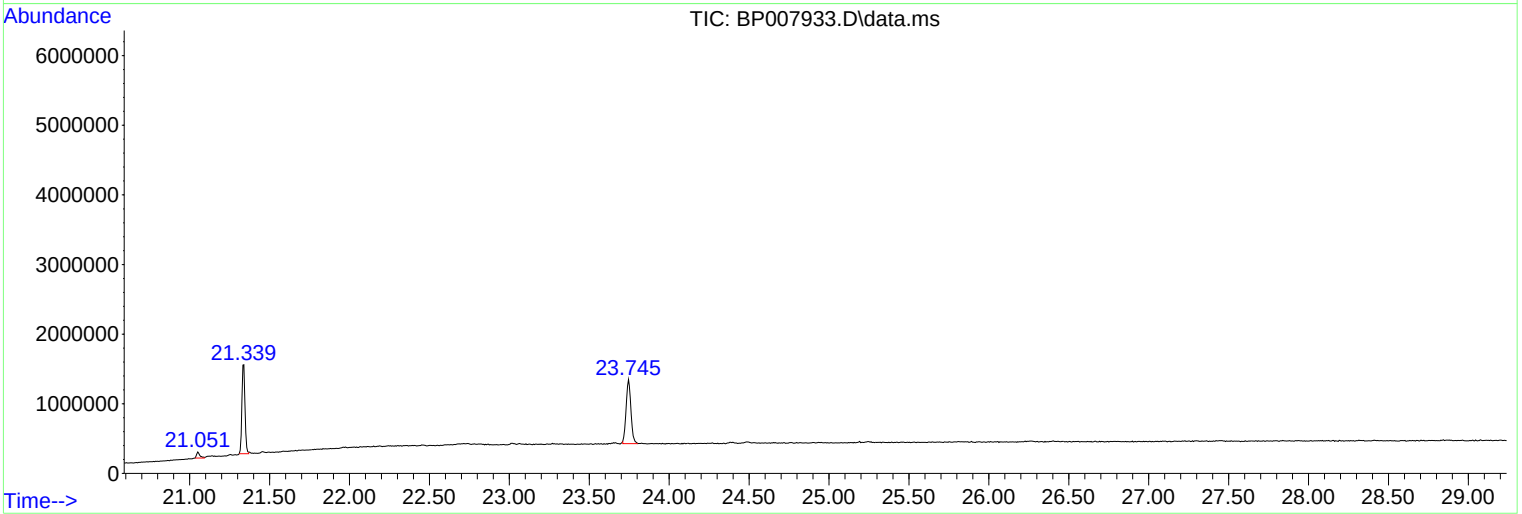
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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

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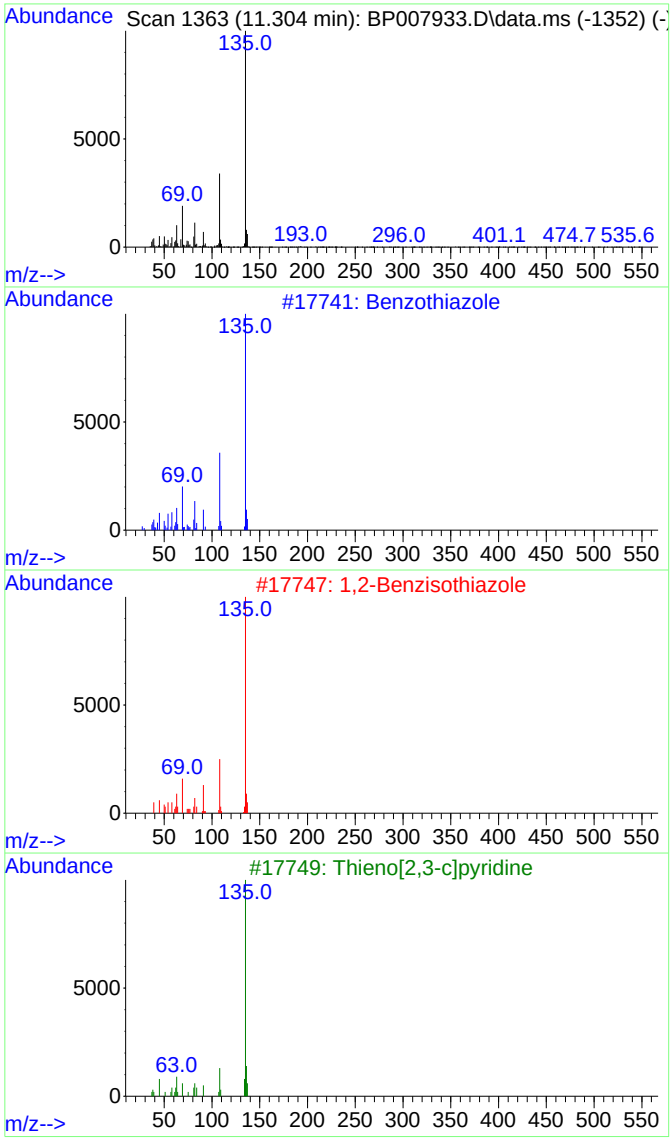
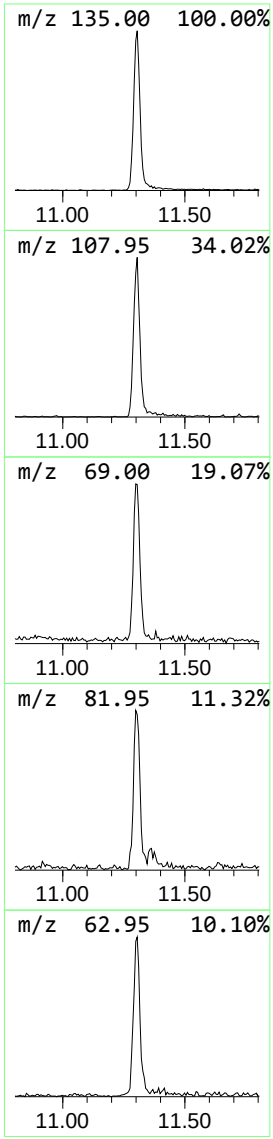
Peak Number 1 Benzothiazole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.304	4.72 ng	185320	Naphthalene-d8	10.652

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	95
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	83
3	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	72
4	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
5	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	59





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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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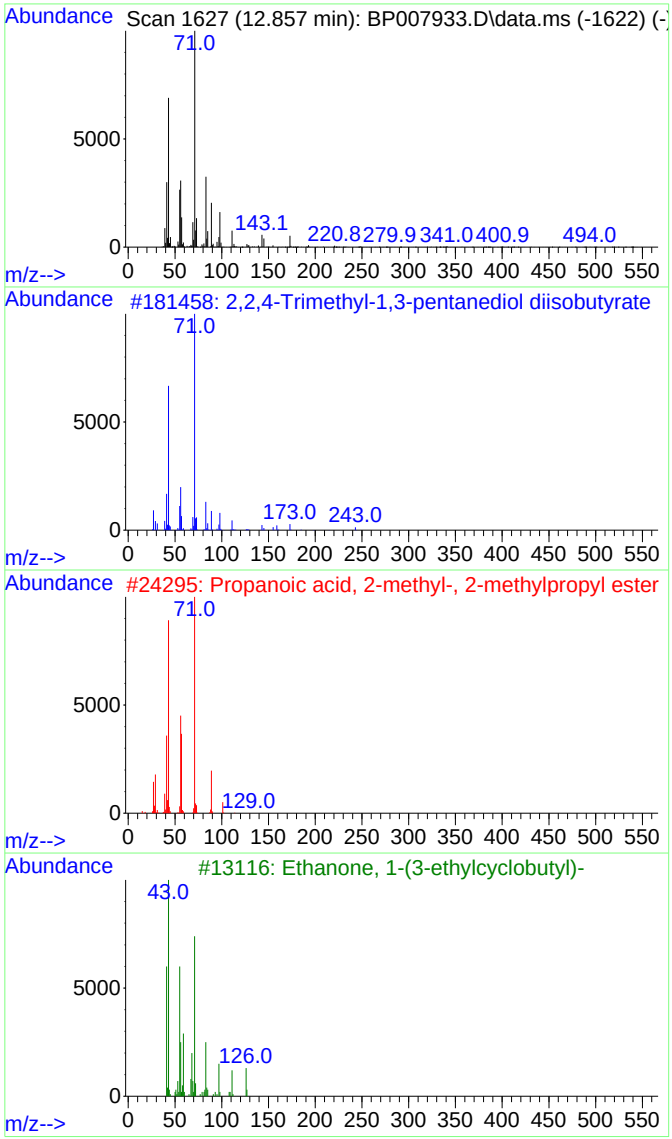
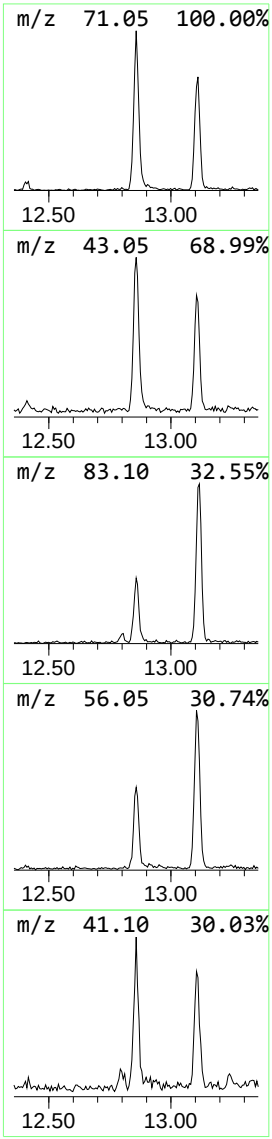
Peak Number 2 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.857	2.19 ng	108699	Acenaphthene-d10	14.493

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	59
2	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	53
3	Ethanone, 1-(3-ethylcyclobutyl)-	126	C8H14O	056335-71-8	50
4	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	42
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42





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Data File : BP007933.D
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Operator : CG/JU
Sample : M4572-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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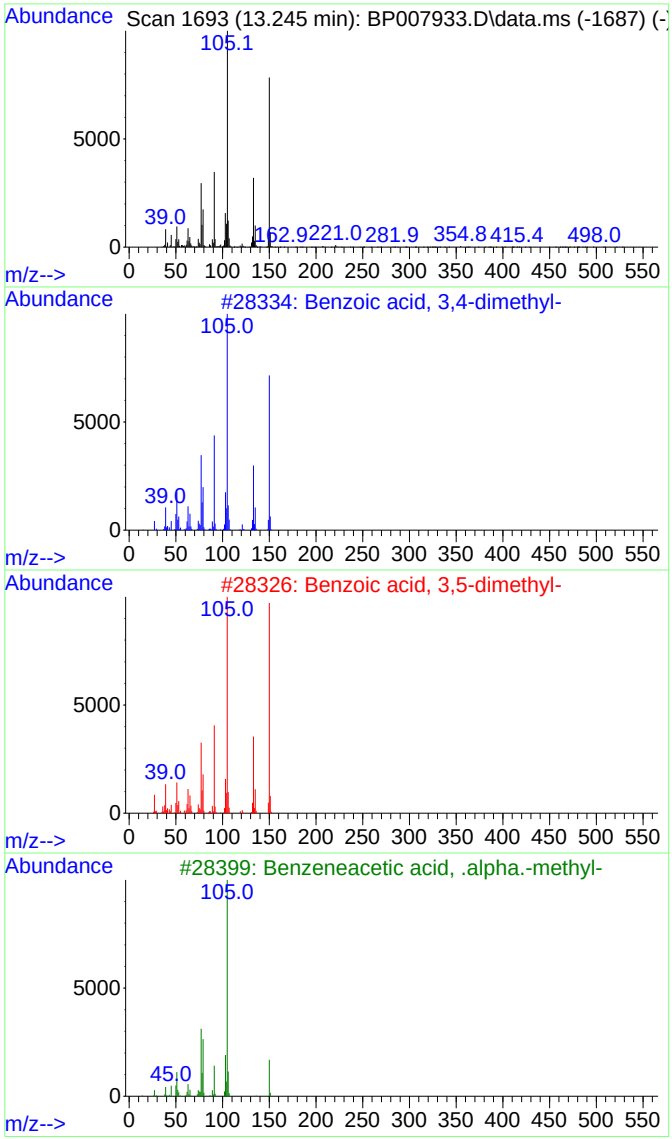
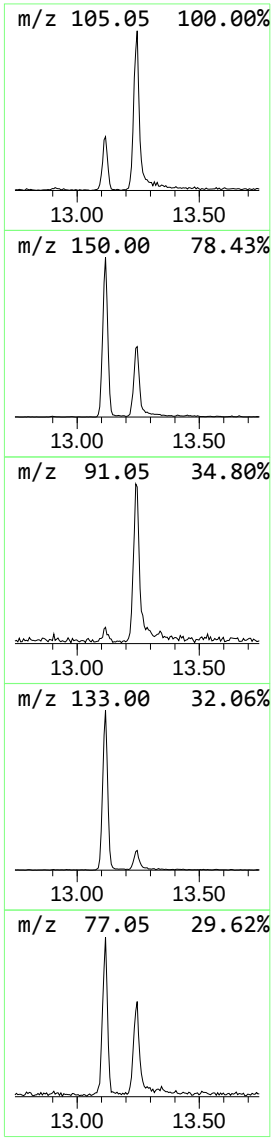
Peak Number 3 Benzoic acid, 3,4-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.246	3.27 ng	162519	Acenaphthene-d10	14.493

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 3,4-dimethyl-	150	C9H10O2	000619-04-5	97
2	Benzoic acid, 3,5-dimethyl-	150	C9H10O2	000499-06-9	95
3	Benzeneacetic acid, .alpha.-methyl-	150	C9H10O2	000492-37-5	81
4	p-Tolylacetic acid	150	C9H10O2	000622-47-9	81
5	m-Tolylacetic acid	150	C9H10O2	000621-36-3	81





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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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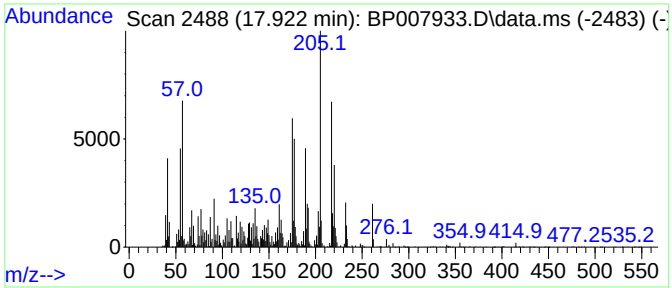
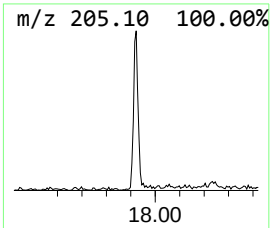
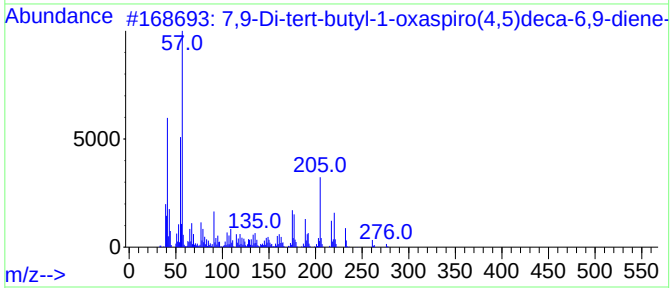
Peak Number 4 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 4

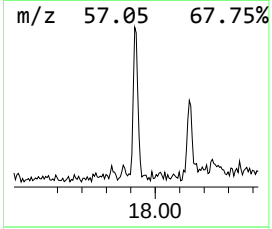
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.922	2.05 ng	129536	Phenanthrene-d10	17.245

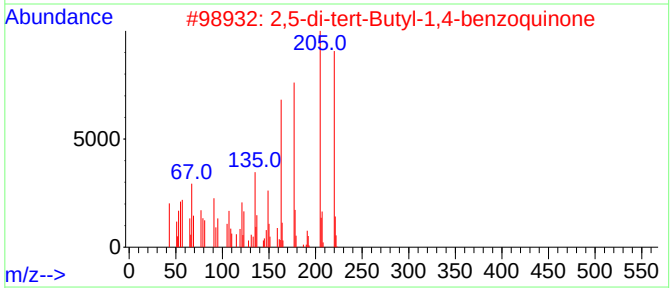
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	46
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	46
4	3-Acetylphenanthrene	220	C16H12O	002039-76-1	45
5	2-Hydroxy-4-methoxy-5-(2-methylb...	220	C13H16O3	2108511-28-8	45

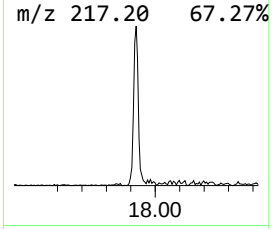


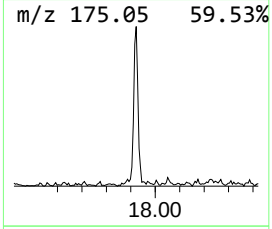


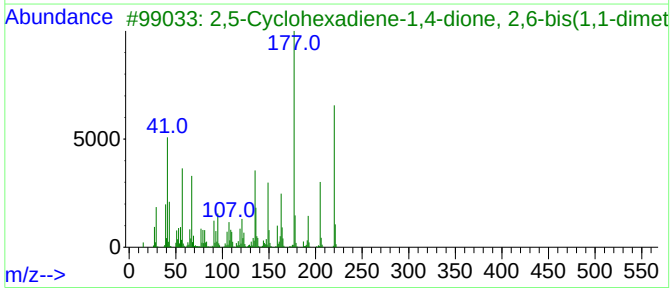


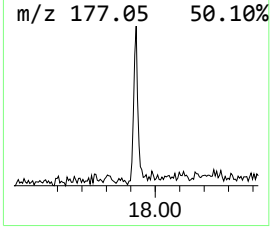












Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzothiazole	11.304	4.7	ng	185320	2	10.652	786043	20.0
2,2,4-Trimethyl...	12.857	2.2	ng	108699	3	14.493	993040	20.0
Benzoic acid, 3...	13.246	3.3	ng	162519	3	14.493	993040	20.0
7,9-Di-tert-but...	17.922	2.0	ng	129536	4	17.245	1261120	20.0