LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120921\
Data File : BP008323.D
Acq On : 09 Dec 2021 21:41
Operator : CG/JU
Sample : M4967-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-7D

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: BP008323.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	16	rVB	255850	290370	5.82%	1.130%
2	3.969	162	167	173	rVB2	36112	55446	1.11%	0.216%
3	4.522	257	261	268	rVB	40344	54953	1.10%	0.214%
4	4.899	320	325	332	rBV	44555	68174	1.37%	0.265%
5	5.363	397	404	410	rBV	1709702	2514861	50.44%	9.790%
6	5.410	410	412	424	rVB	87037	170295	3.42%	0.663%
7	5.781	469	475	483	rVB	37777	57396	1.15%	0.223%
8	6.957	668	675	686	rBV	1535271	2629904	52.75%	10.237%
9	7.763	805	812	822	rVB	291533	471060	9.45%	1.834%
10	8.928	1003	1010	1026	rVB	953722	1666564	33.43%	6.487%
11	10.369	1247	1255	1273	rBV	103507	264648	5.31%	1.030%
12	10.563	1281	1288	1299	rBV	349010	607014	12.18%	2.363%
13	13.039	1700	1709	1726	rBV	2171811	3315105	66.49%	12.905%
14	14.422	1937	1944	1957	rVB	502620	812118	16.29%	3.161%
15	15.845	2181	2186	2192	rBV	123821	164992	3.31%	0.642%
16	15.922	2192	2199	2218	rVV	1655328	2632825	52.81%	10.249%
17	17.186	2407	2414	2422	rBV	617886	984371	19.74%	3.832%
18	17.310	2430	2435	2441	rVB4	69442	99109	1.99%	0.386%
19	17.845	2522	2526	2527	rBV	45572	51224	1.03%	0.199%
20	18.086	2562	2567	2575	rBV	162643	245092	4.92%	0.954%
21	18.998	2720	2722	2729	rVB2	65771	72018	1.44%	0.280%
22	19.321	2774	2777	2785	rBV4	38542	61462	1.23%	0.239%
23	19.757	2845	2851	2862	rVB	4146982	4985724	100.00%	19.408%
24	20.504	2975	2978	2981	rBV	85812	87918	1.76%	0.342%
25	21.004	3059	3063	3071	rBV	352116	523841	10.51%	2.039%
26	21.198	3093	3096	3102	rVB	183040	211074	4.23%	0.822%
27	21.292	3107	3112	3121	rVV	894391	1202482	24.12%	4.681%
28	22.174	3259	3262	3268	rVB	115642	154185	3.09%	0.600%
29	23.674	3511	3517	3529	rVB2	598966	1234984	24.77%	4.807%

Sum of corrected areas: 25689209

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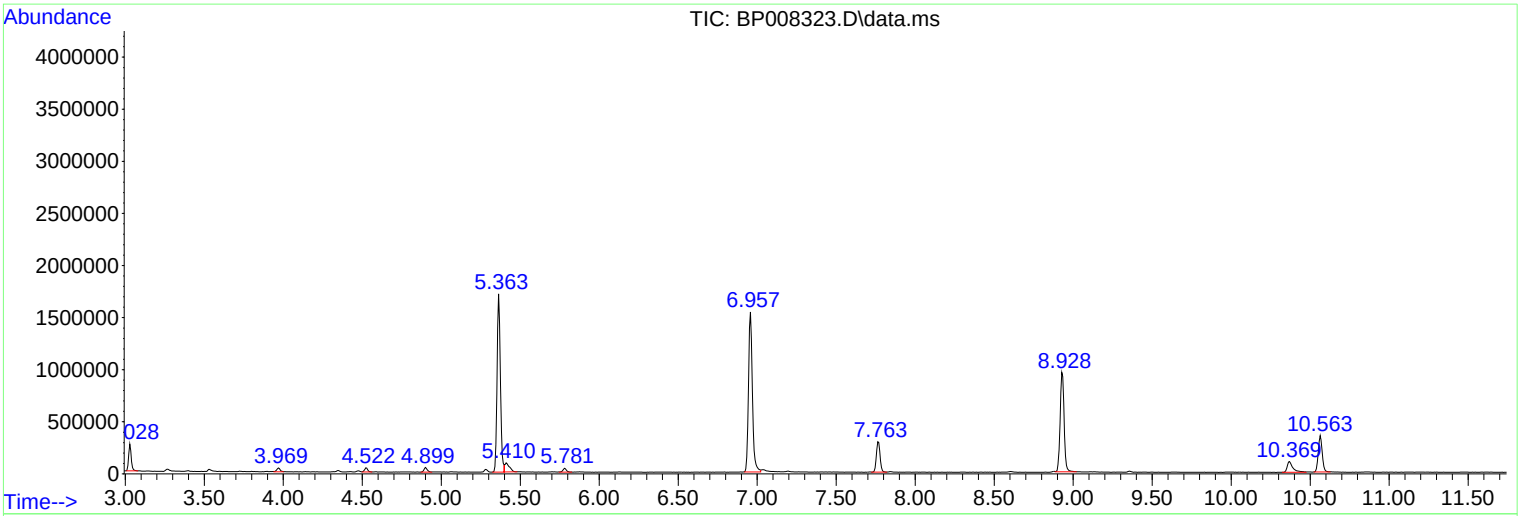
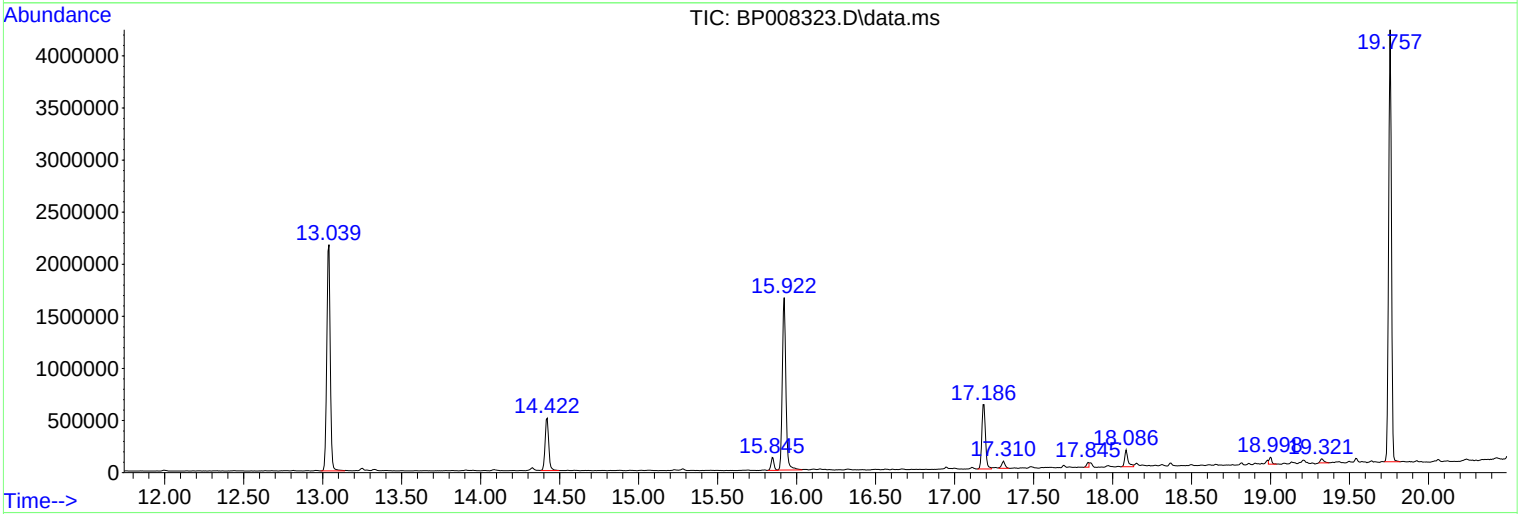
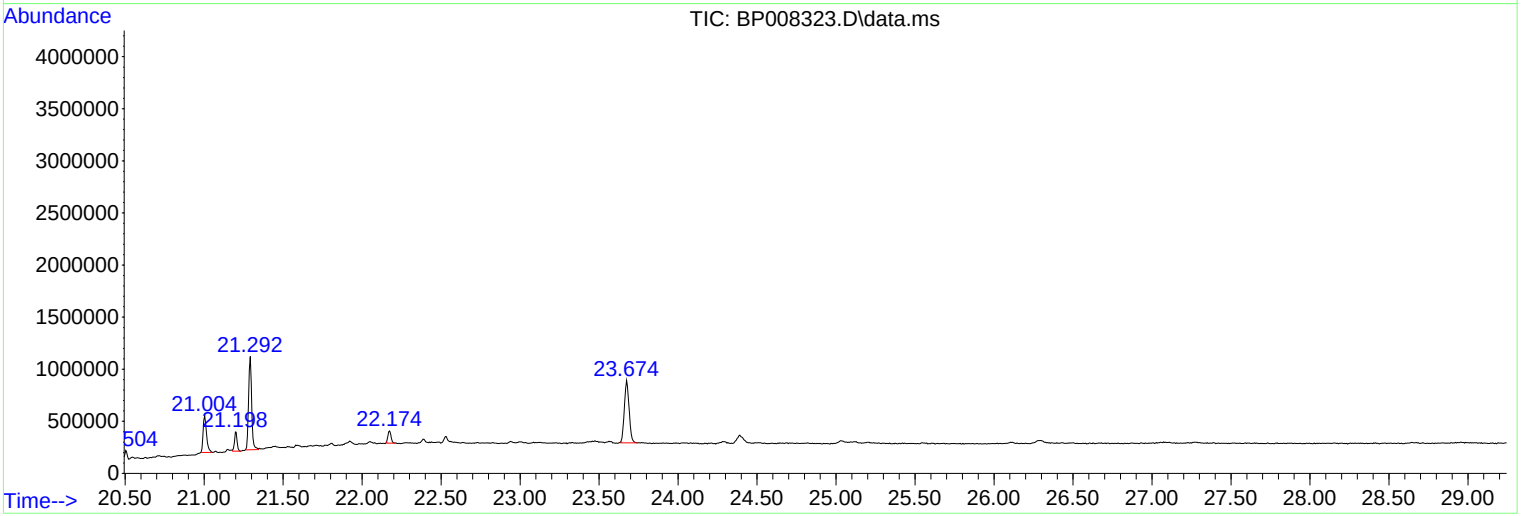
Instrument :
BNA_P
ClientSampleId :
TP-7D

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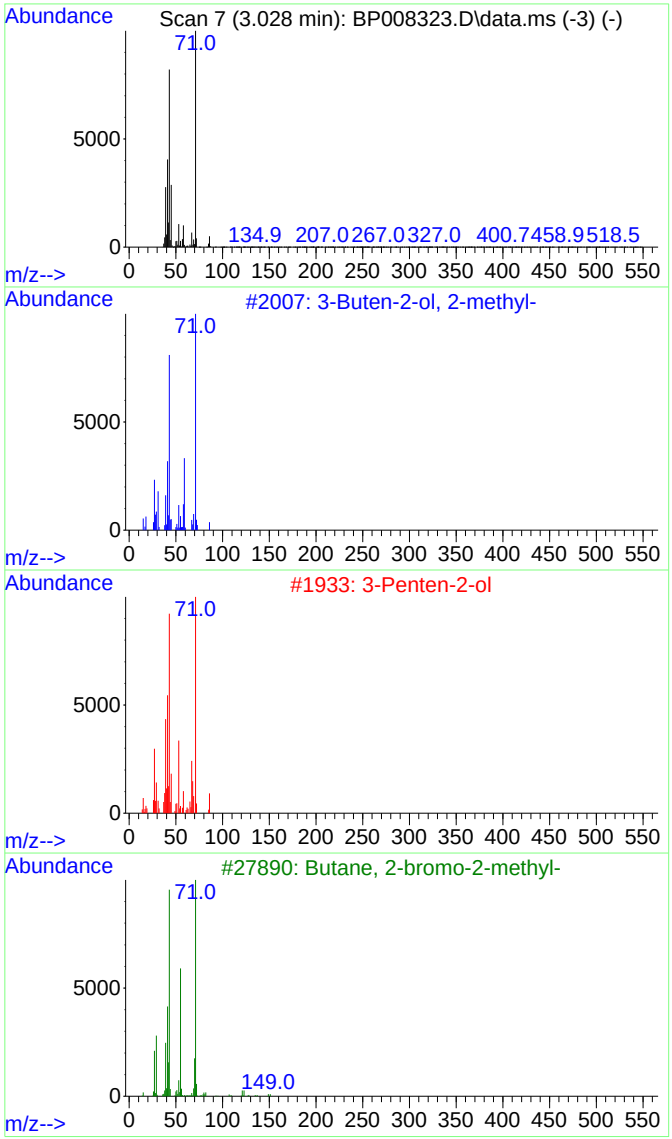
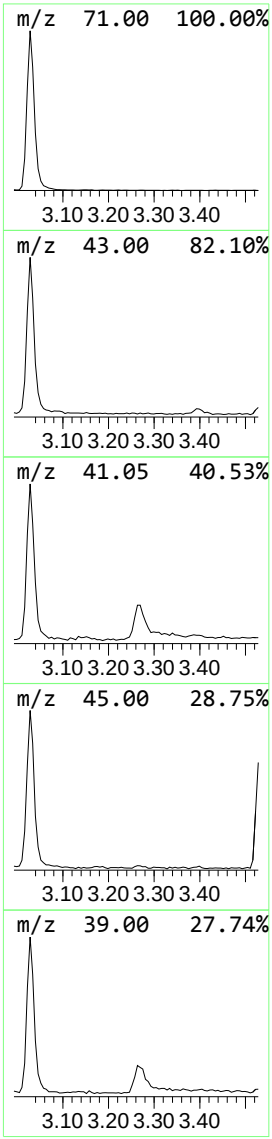
****

Peak Number 1 3-Buten-2-ol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	12.33 ng	290370	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
2	3-Penten-2-ol	86	C5H10O	001569-50-2	72
3	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	59
4	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	56
5	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	53





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Misc :
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Instrument :
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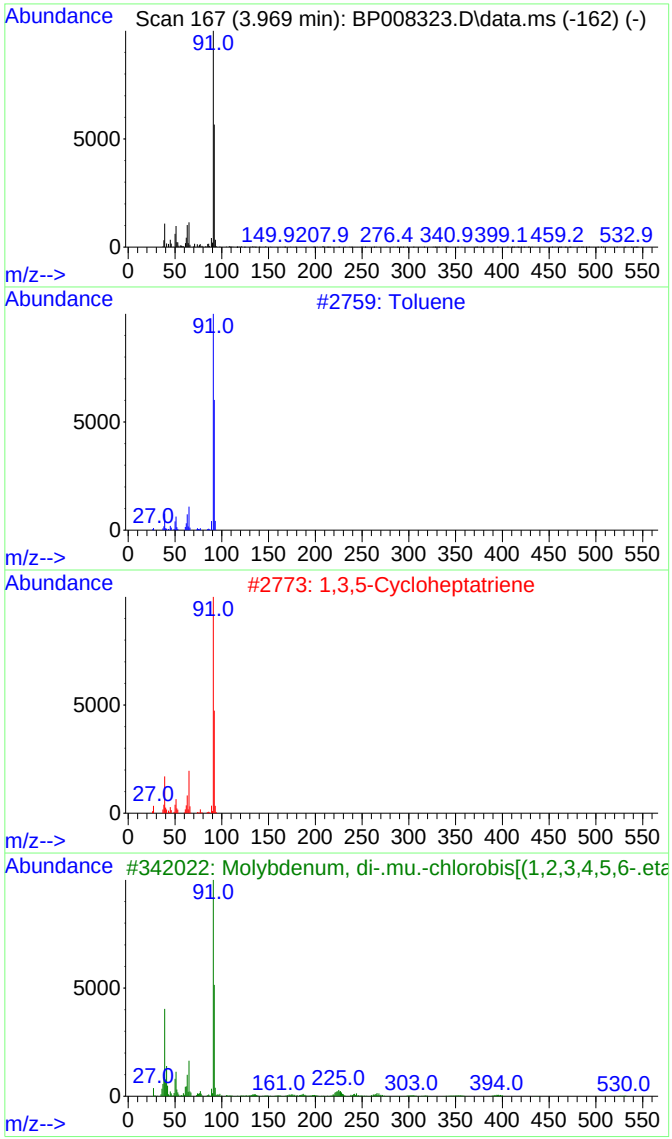
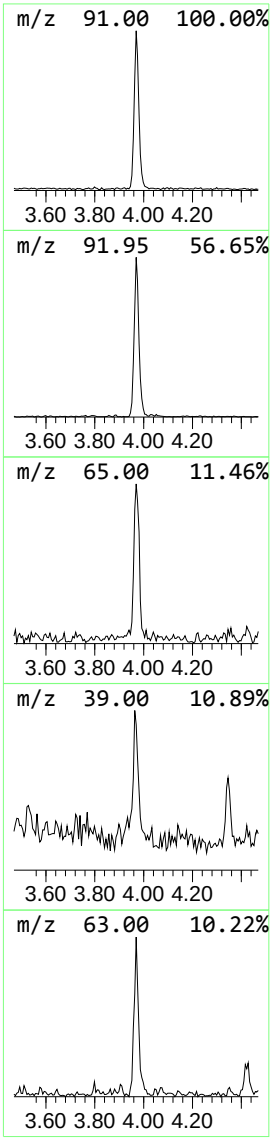
Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.969	2.35 ng	55446	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	91
2	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	91
3	Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	78
4	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	72
5	Acetaldehyde dibenzyl acetal	242	C16H18O2	1000431-44-3	64





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Sample : M4967-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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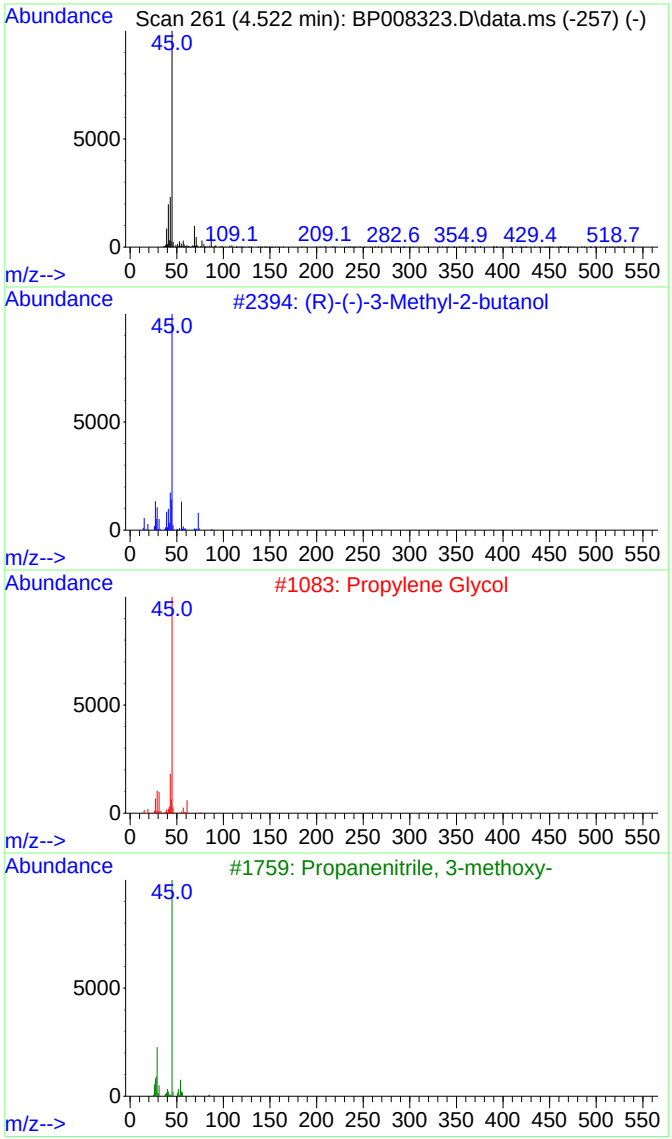
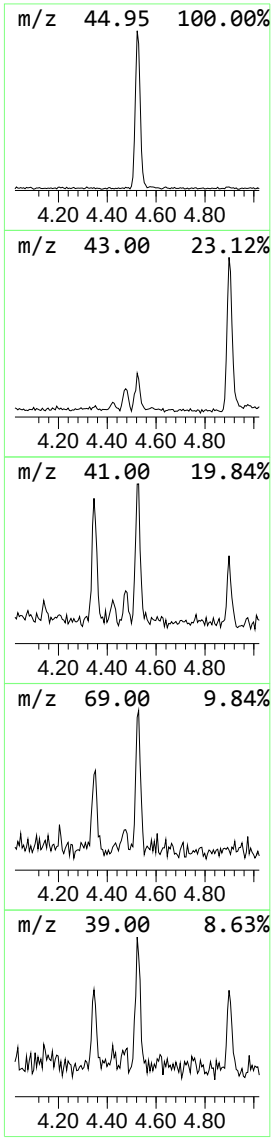
****

Peak Number 3 (R)-(-)-3-Methyl-2-butanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.522	2.33 ng	54953	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	53
2	Propylene Glycol	76	C3H8O2	000057-55-6	53
3	Propanenitrile, 3-methoxy-	85	C4H7NO	000110-67-8	42
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	42
5	2-Hexanol	102	C6H14O	000626-93-7	40





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ClientSampleId :
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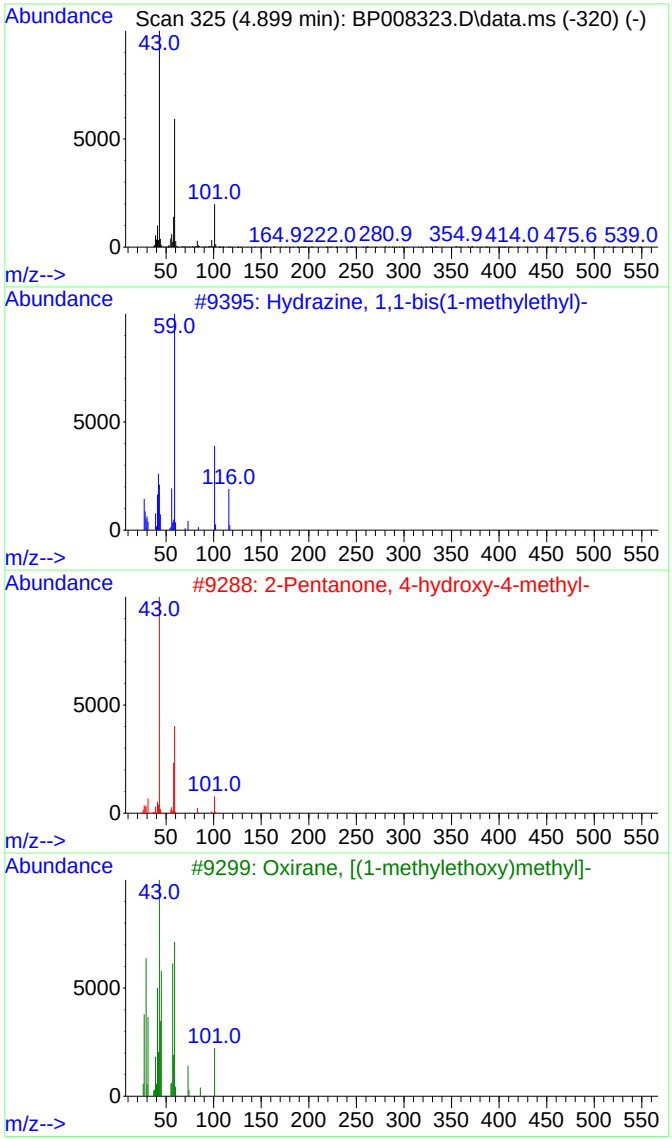
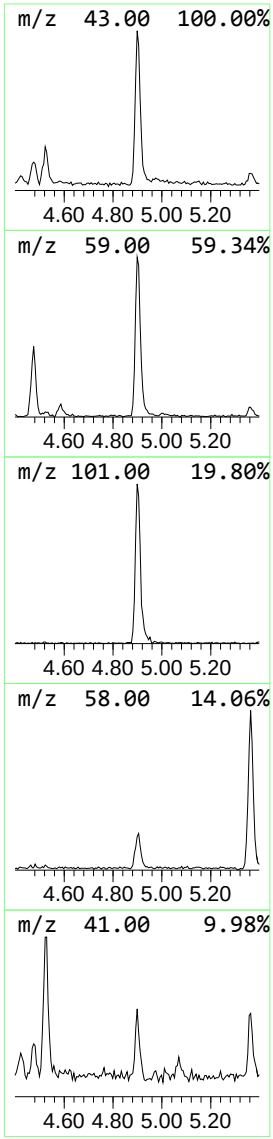
****
Peak Number 4 Hydrazine, 1,1-bis(1-methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.899	2.89 ng	68174	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	38
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
5	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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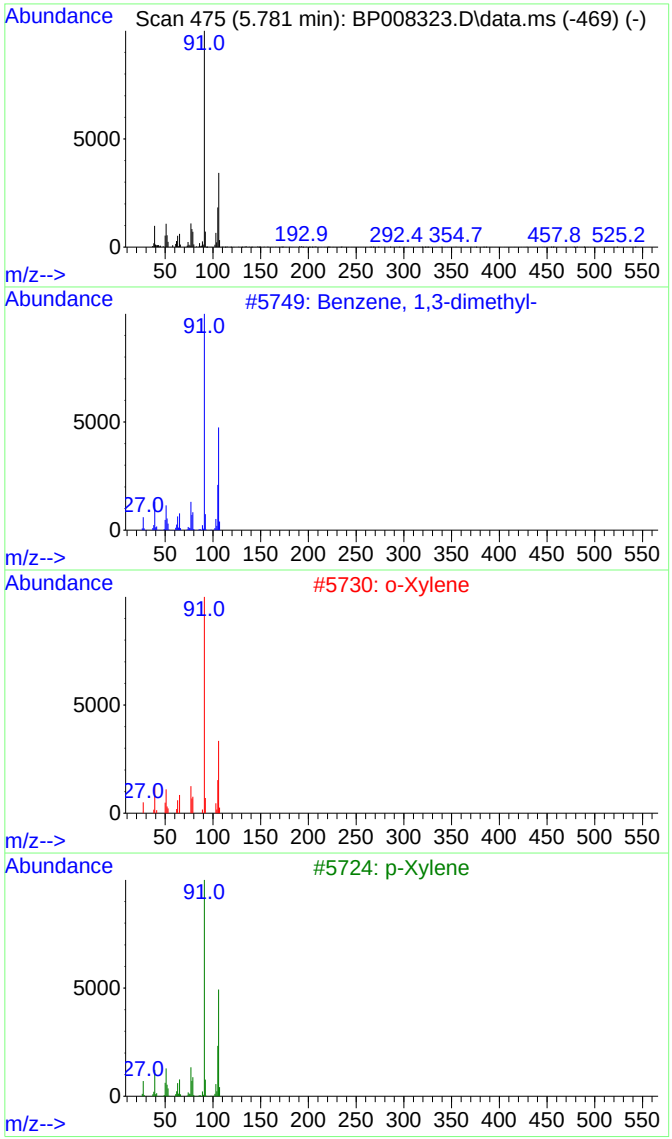
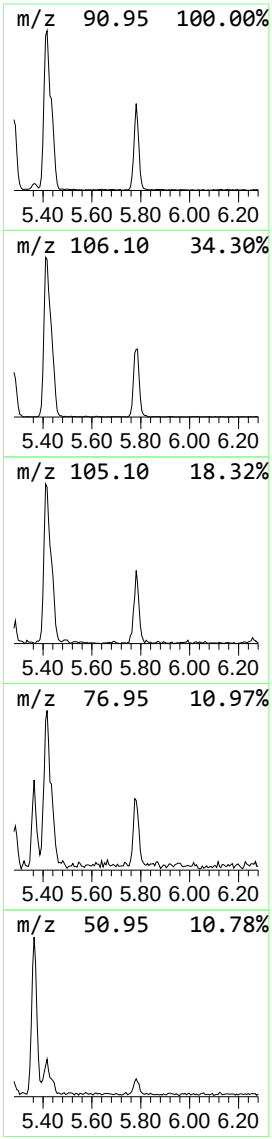
****

Peak Number 5 Benzene, 1,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.781	2.44 ng	57396	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	95
2	o-Xylene	106	C8H10	000095-47-6	94
3	p-Xylene	106	C8H10	000106-42-3	93
4	Ethylbenzene	106	C8H10	000100-41-4	87
5	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	72





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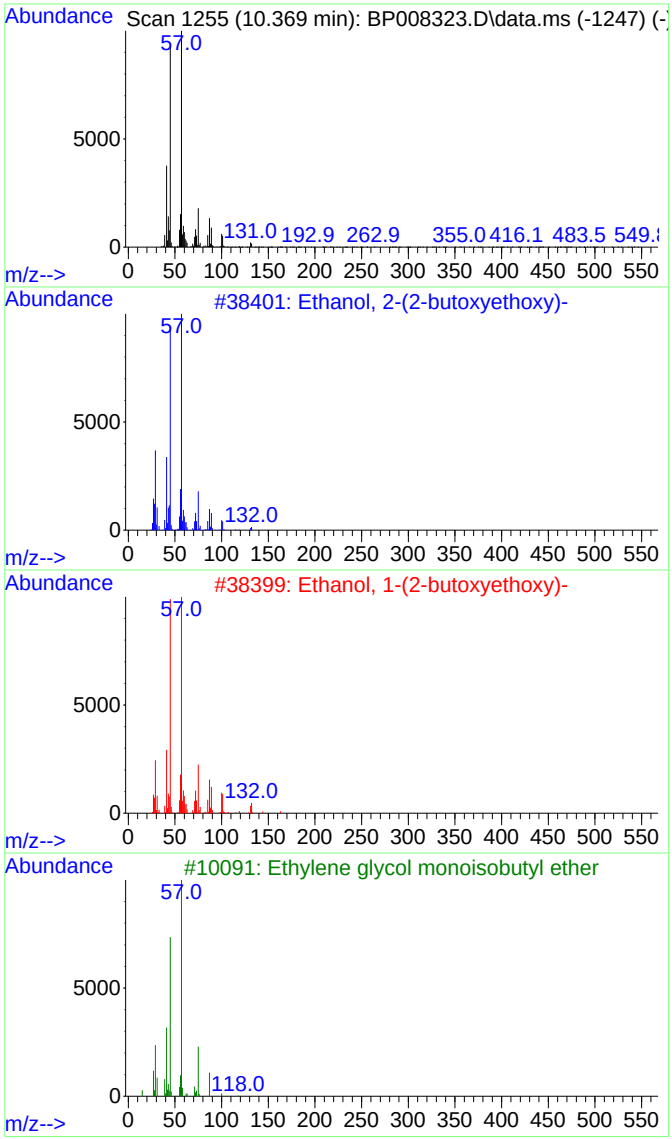
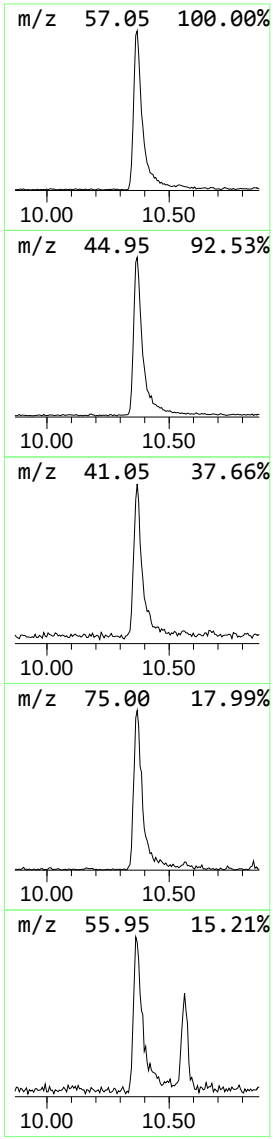
****
Peak Number 6 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.369	8.72 ng	264648	Naphthalene-d8	10.563

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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53





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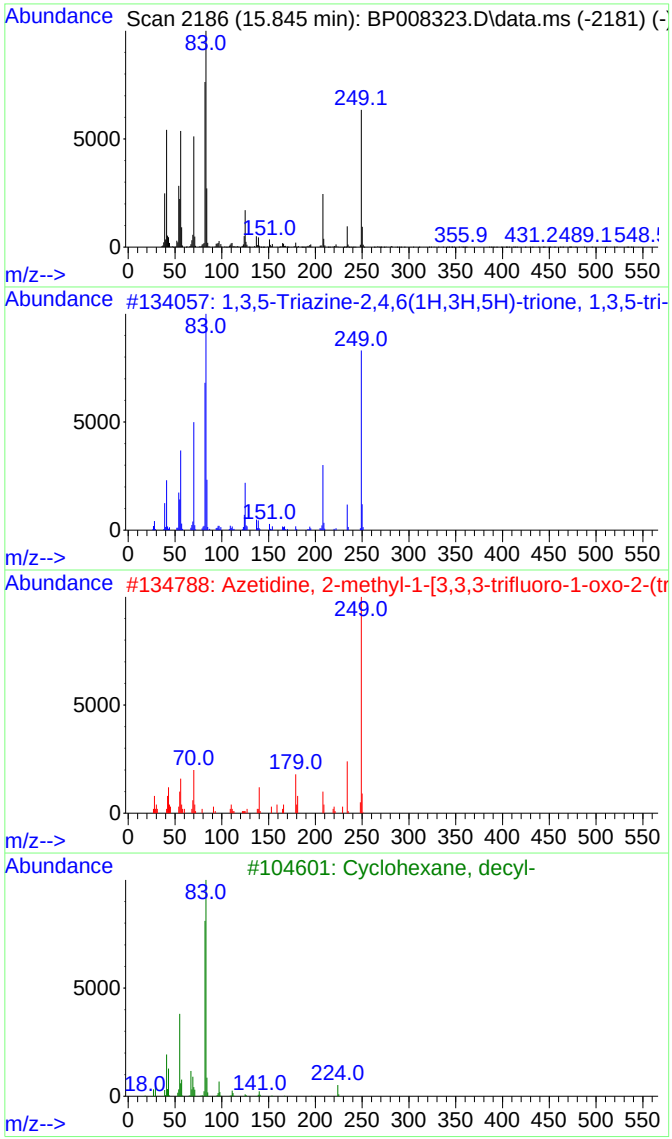
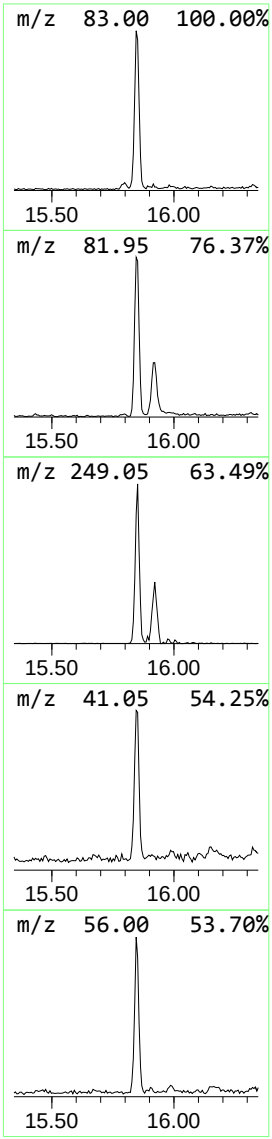
****
Peak Number 7 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.845	3.35 ng	164992	Phenanthrene-d10	17.186

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	Azetidine, 2-methyl-1-[3,3,3-tri...	249	C8H9F6NO	050837-79-1	27
3	Cyclohexane, decyl-	224	C16H32	001795-16-0	25
4	n-Nonylcyclohexane	210	C15H30	002883-02-5	22
5	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	12





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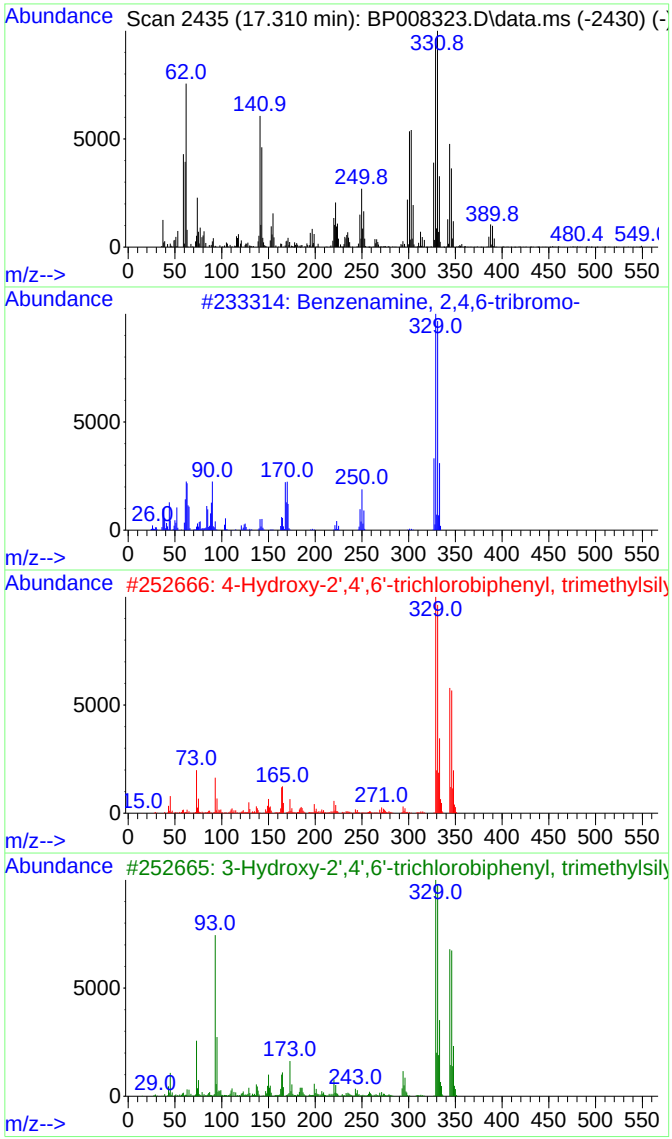
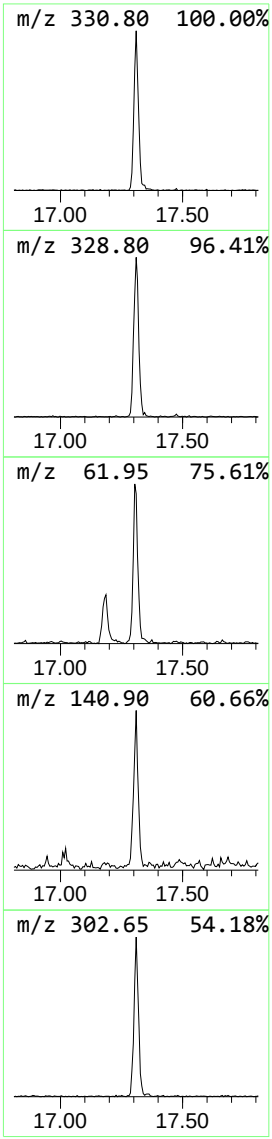
****

Peak Number 8 Benzenamine, 2,4,6-tribromo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.310	2.01 ng	99109	Phenanthrene-d10	17.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	59
2	4-Hydroxy-2',4',6'-trichlorobiph...	344	C15H15Cl3OSi	1000447-71-9	22
3	3-Hydroxy-2',4',6'-trichlorobiph...	344	C15H15Cl3OSi	1000447-69-8	12
4	Methyl 3,5-diamino-6-chloropyraz...	346	C12H23ClN4O2Si2	1000293-06-3	10
5	1,3,4-Oxadiazol-2-amine, 5-(2-br...	329	C11H12BrN3O4	1000350-74-8	10





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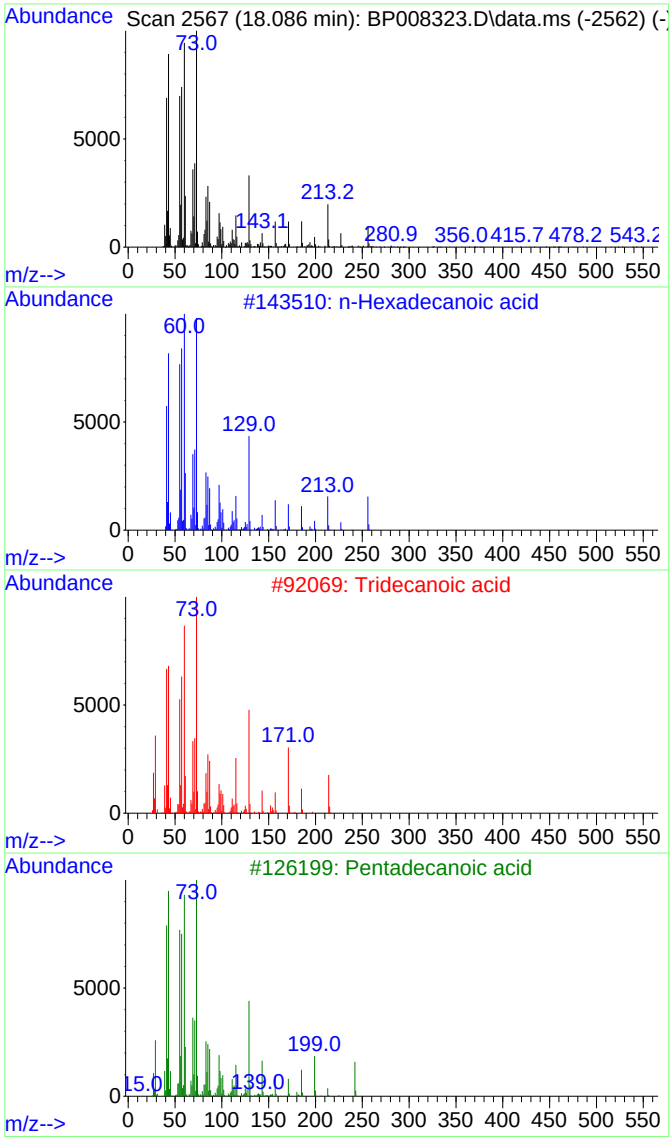
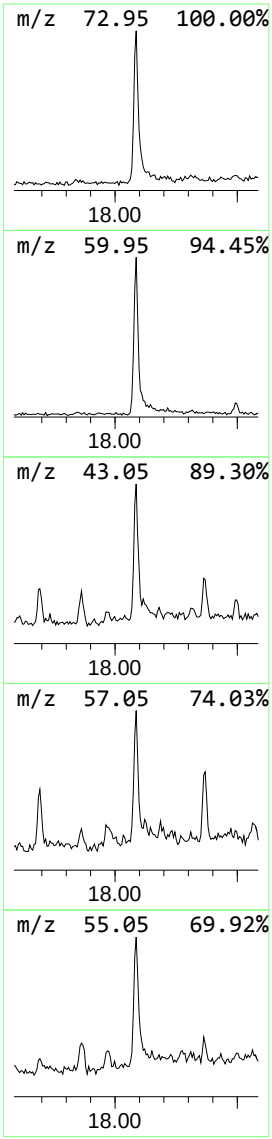
Peak Number 9 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.086	4.98 ng	245092	Phenanthrene-d10	17.186

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Dodecanoic acid	200	C12H24O2	000143-07-7	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Data File : BP008323.D
Acq On : 09 Dec 2021 21:41
Operator : CG/JU
Sample : M4967-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-7D

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

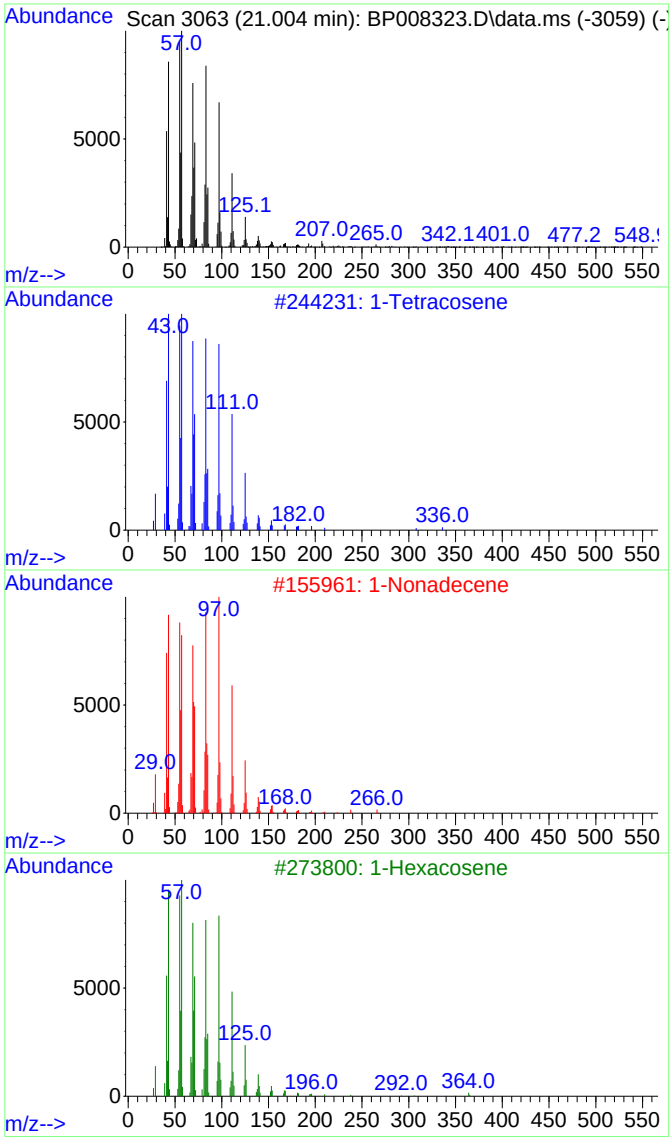
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

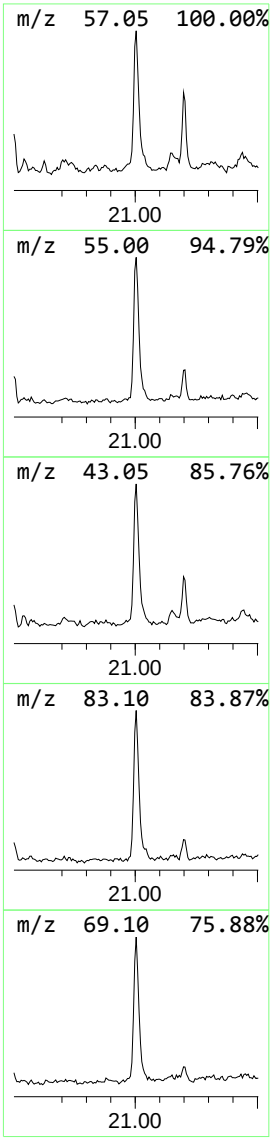
****

Peak Number 10 1-Tetracosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.004	8.71 ng	523841	Chrysene-d12	21.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	1-Hexacosene	364	C26H52	018835-33-1	91
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120921\
Data File : BP008323.D
Acq On : 09 Dec 2021 21:41
Operator : CG/JU
Sample : M4967-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-7D

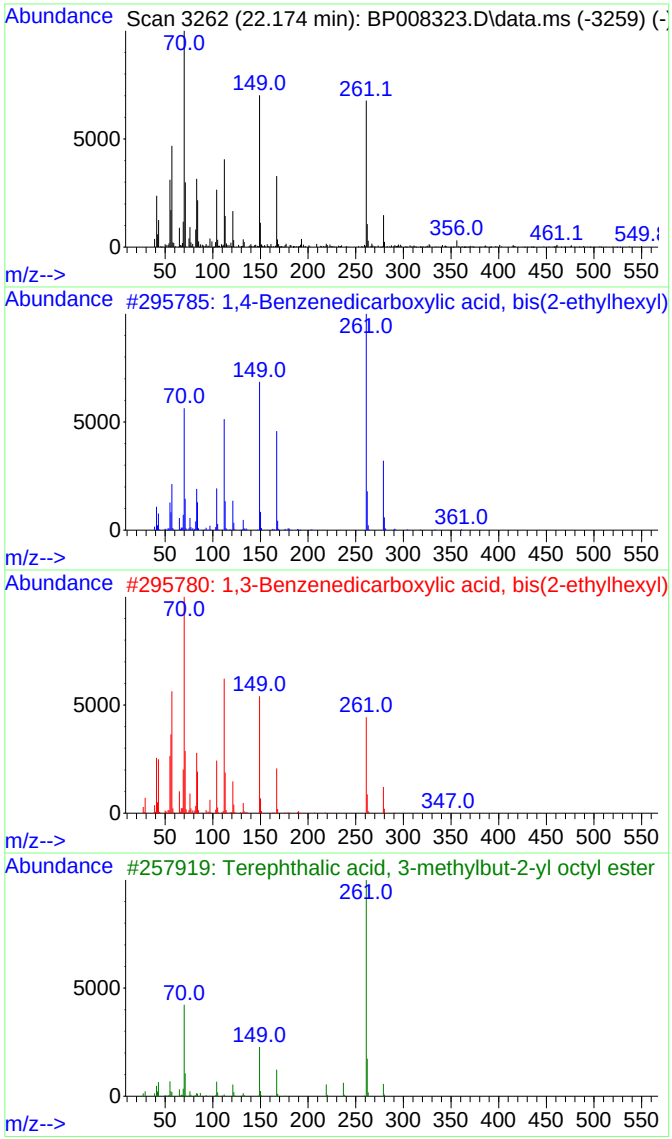
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

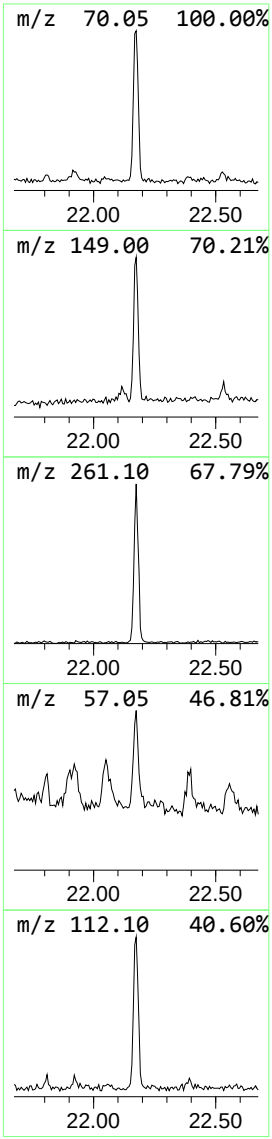
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1,4-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.174	2.56 ng	154185	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	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	43
4	Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	27
5	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120921\
Data File : BP008323.D
Acq On : 09 Dec 2021 21:41
Operator : CG/JU
Sample : M4967-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-7D

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Buten-2-ol, 2...	3.028	12.3	ng	290370	1	7.769	471060	20.0
1,3,5-Cyclohept...	3.969	2.4	ng	55446	1	7.769	471060	20.0
(R)-(-)-3-Methy...	4.522	2.3	ng	54953	1	7.769	471060	20.0
Hydrazine, 1,1-...	4.899	2.9	ng	68174	1	7.769	471060	20.0
Benzene, 1,3-di...	5.781	2.4	ng	57396	1	7.769	471060	20.0
Ethanol, 2-(2-b...	10.369	8.7	ng	264648	2	10.563	607014	20.0
1,3,5-Triazine-...	15.845	3.4	ng	164992	4	17.186	984371	20.0
Benzenamine, 2,...	17.310	2.0	ng	99109	4	17.186	984371	20.0
n-Hexadecanoic ...	18.086	5.0	ng	245092	4	17.186	984371	20.0
1-Tetracosene	21.004	8.7	ng	523841	5	21.292	1202480	20.0
1,4-Benzenedica...	22.174	2.6	ng	154185	5	21.292	1202480	20.0