LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
Data File : BP011676.D
Acq On : 09 Sep 2022 22:34
Operator : CG/JU
Sample : N4549-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-62

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-BP090222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011676.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.011	3	4	13	rVB	1213454	1433152	3.72%	0.927%
2	3.093	13	18	45	rVB	12151086	15228115	39.49%	9.854%
3	3.634	105	110	121	rBV	1057823	1466198	3.80%	0.949%
4	5.517	423	430	441	rBV	3856019	5801499	15.05%	3.754%
5	7.111	694	701	714	rVB	2335751	3770560	9.78%	2.440%
6	7.958	838	845	852	rBV	1325390	2056555	5.33%	1.331%
7	8.334	903	909	923	rVB	935654	1526573	3.96%	0.988%
8	9.075	1028	1035	1037	rBV2	255158	403540	1.05%	0.261%
9	9.128	1037	1044	1058	rVB	4437691	8233375	21.35%	5.328%
10	9.593	1118	1123	1132	rVB	384443	618553	1.60%	0.400%
11	10.169	1212	1221	1230	rBV	471777	836440	2.17%	0.541%
12	10.769	1312	1323	1329	rBV	1710406	3068507	7.96%	1.986%
13	13.228	1733	1741	1753	rVB	11233017	16957333	43.98%	10.973%
14	14.322	1921	1927	1934	rBV	379471	595634	1.54%	0.385%
15	14.598	1967	1974	1980	rBV	2602363	3827108	9.92%	2.476%
16	15.775	2169	2174	2178	rBV	346915	535159	1.39%	0.346%
17	16.087	2220	2227	2236	rBV	8620593	12543410	32.53%	8.117%
18	17.351	2436	2442	2448	rBV	3201047	4210826	10.92%	2.725%
19	18.234	2588	2592	2614	rBV2	901281	1709858	4.43%	1.106%
20	19.463	2797	2801	2812	rBV	631141	989299	2.57%	0.640%
21	19.904	2870	2876	2881	rBV	16848207	20616553	53.47%	13.341%
22	21.428	3130	3135	3141	rBV	3575643	4686420	12.15%	3.033%
23	21.563	3151	3158	3182	rBV	23912923	38560705	100.00%	24.952%
24	23.898	3548	3555	3565	rVB	2376295	4864144	12.61%	3.148%

Sum of corrected areas: 154539516

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Instrument :
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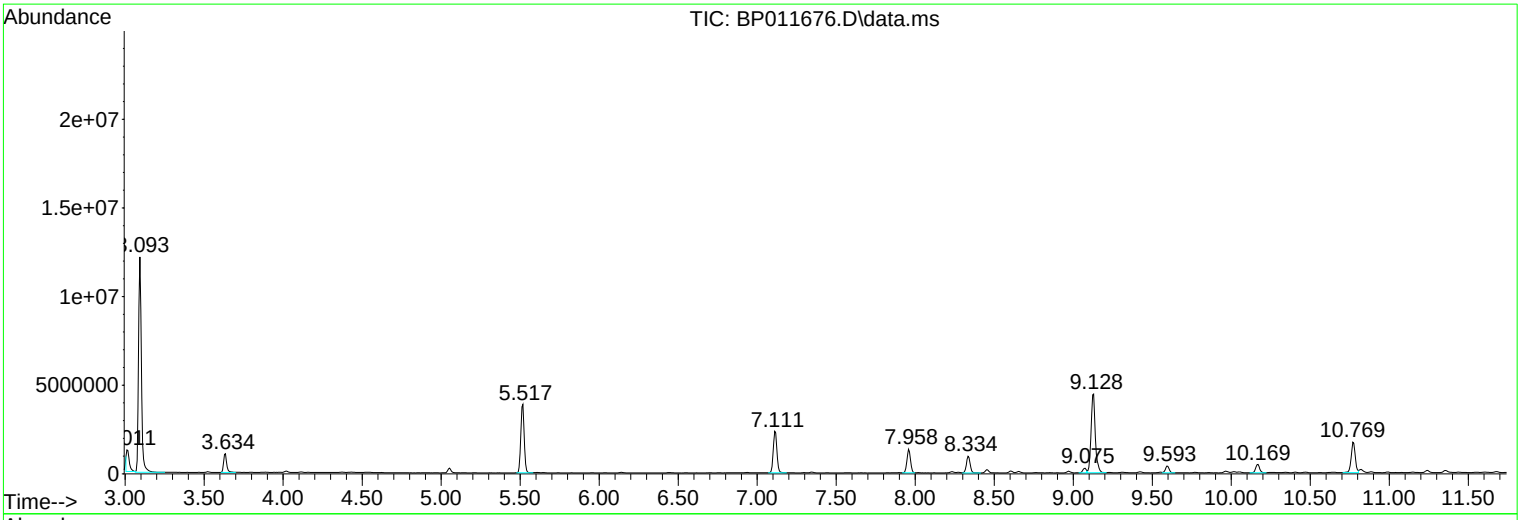
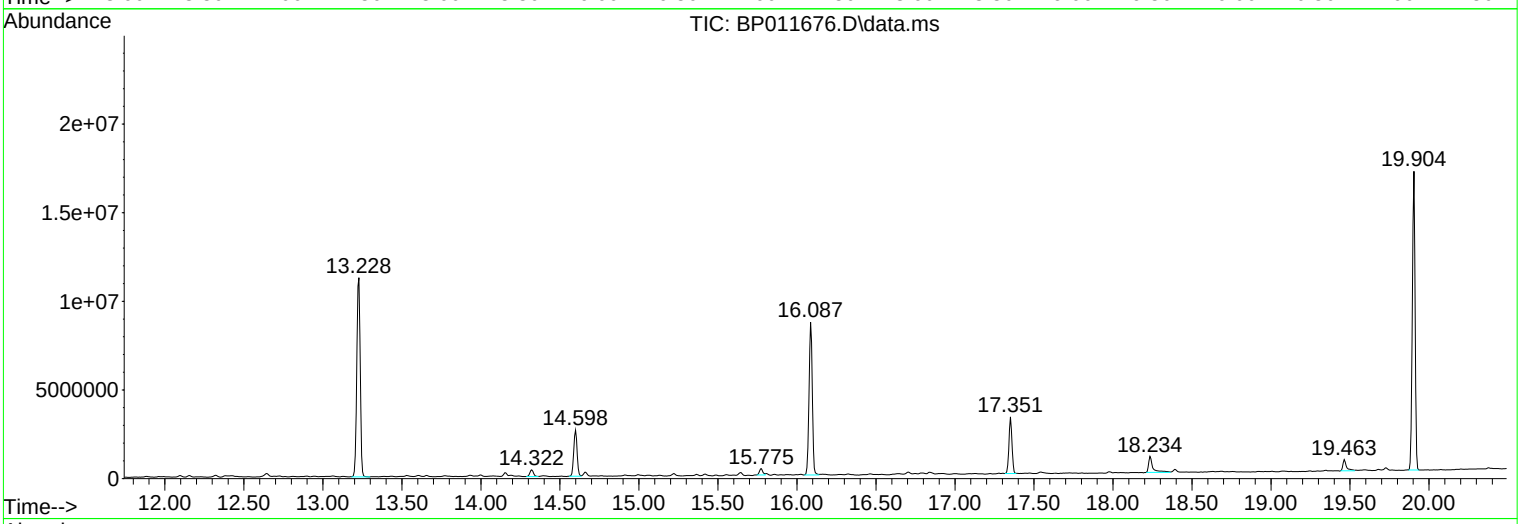
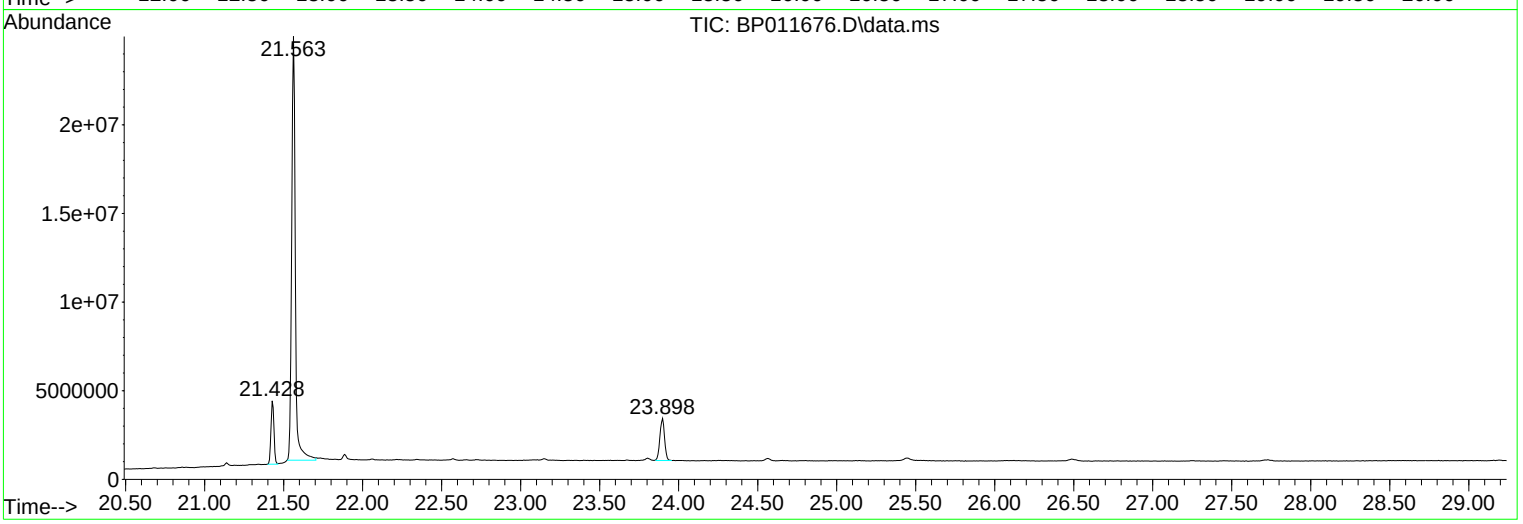
ClientSampleId :
MW-62

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.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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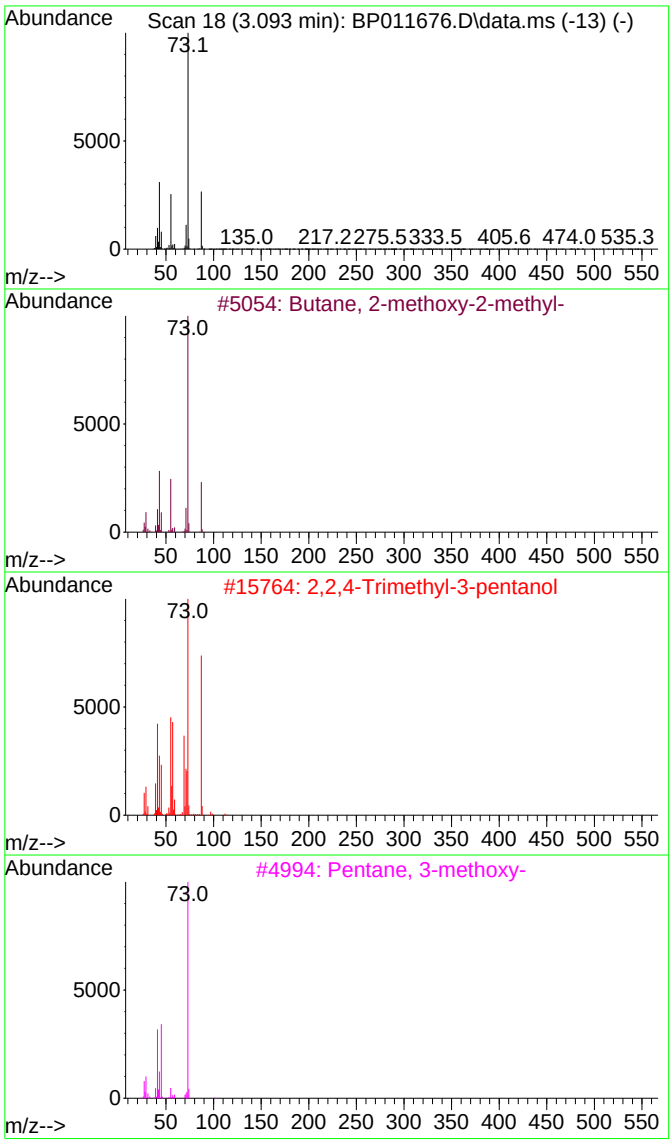
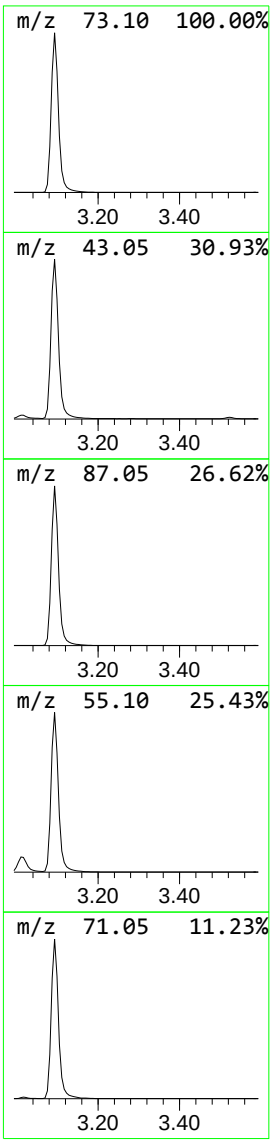
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.093	148.09 ng	15228100	1,4-Dichlorobenzene-d4	7.958

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	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BP011676.D
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Operator : CG/JU
Sample : N4549-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-62

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.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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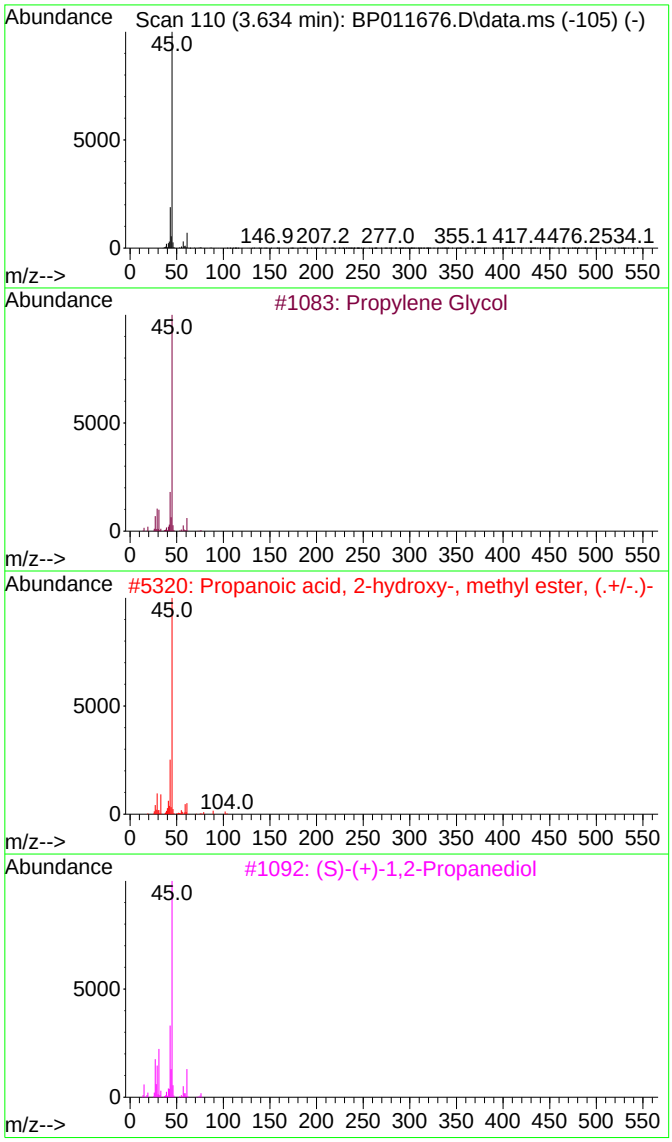
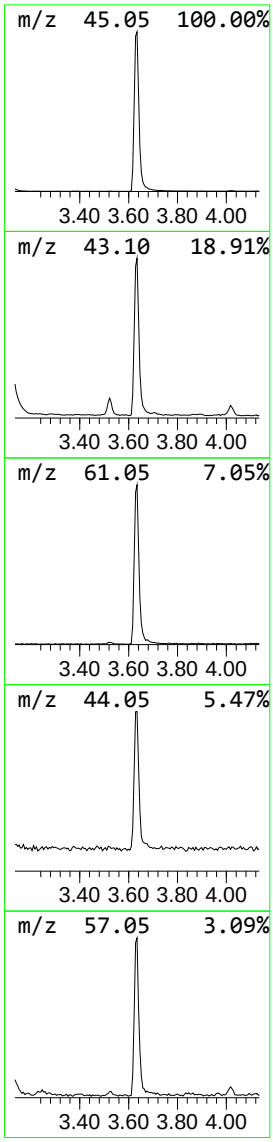
Peak Number 3 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.634	14.26 ng	1466200	1,4-Dichlorobenzene-d4	7.958

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	83
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	25
4	2-Pentanol	88	C5H12O	006032-29-7	9
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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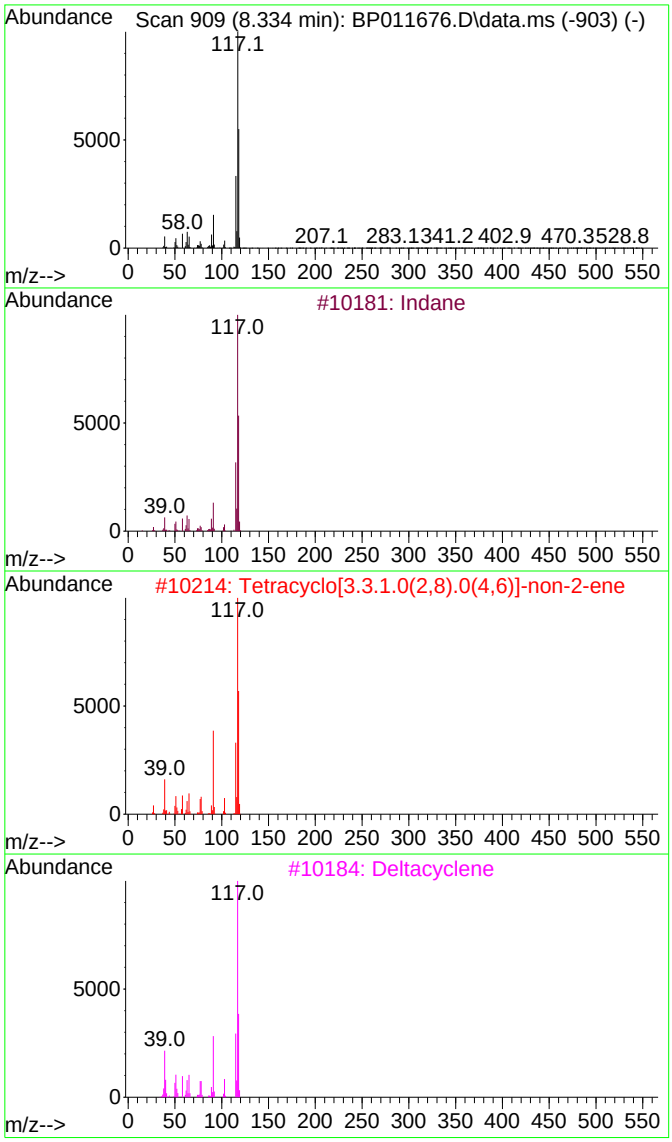
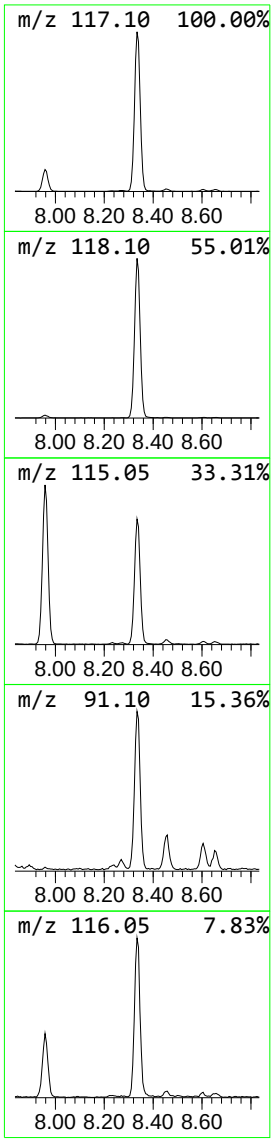
Peak Number 4 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.334	14.85 ng	1526570	1,4-Dichlorobenzene-d4	7.958

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
3	Deltacyclene	118	C9H10	007785-10-6	72
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64





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BNA_P
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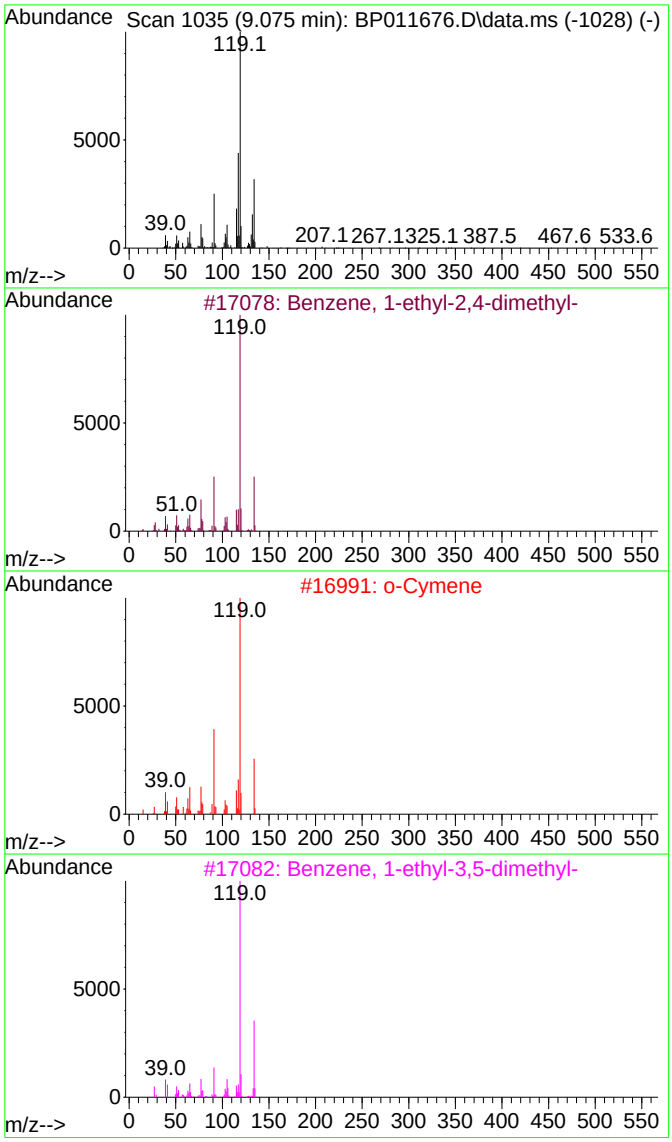
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

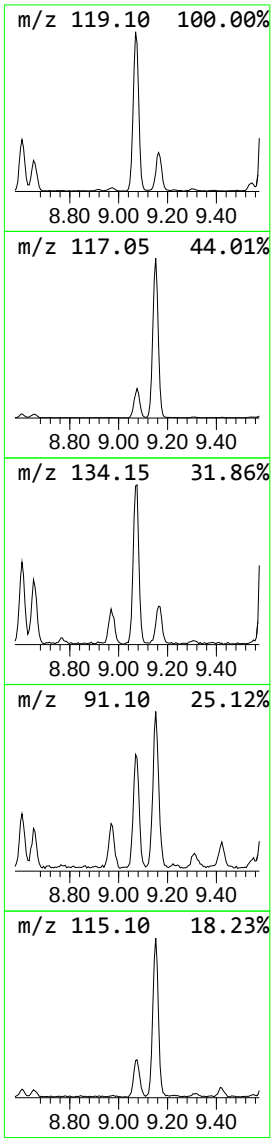
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.075	3.92 ng	403540	1,4-Dichlorobenzene-d4	7.958

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	70
2	o-Cymene	134	C10H14	000527-84-4	70
3	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	64
4	p-Cymene	134	C10H14	000099-87-6	64
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	64





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ALS Vial : 17 Sample Multiplier: 1

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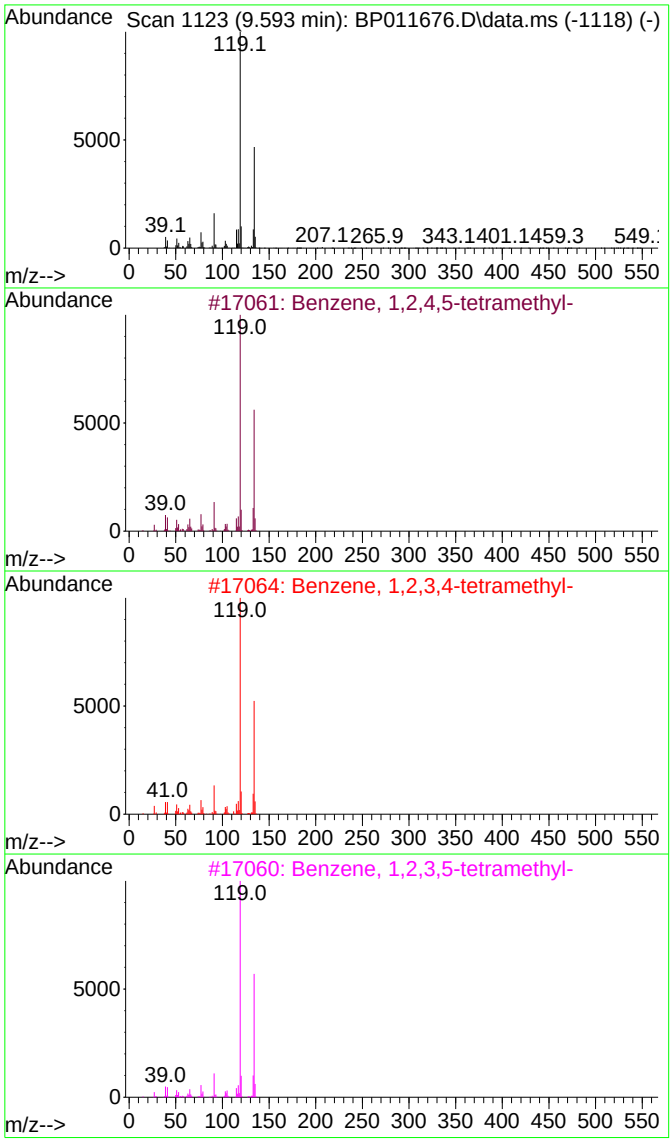
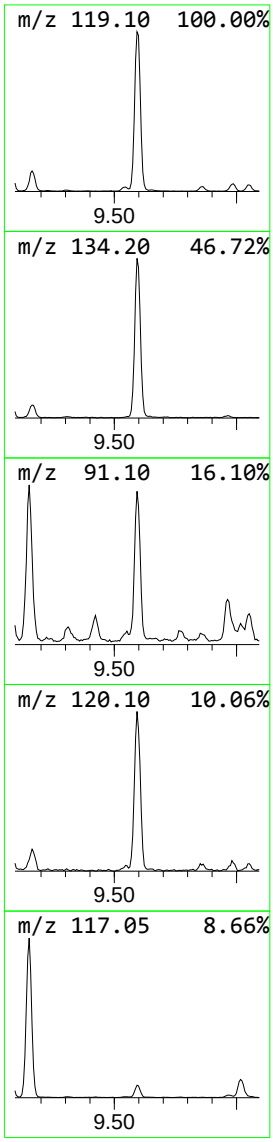
****

Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.593	4.03 ng	618553	Naphthalene-d8	10.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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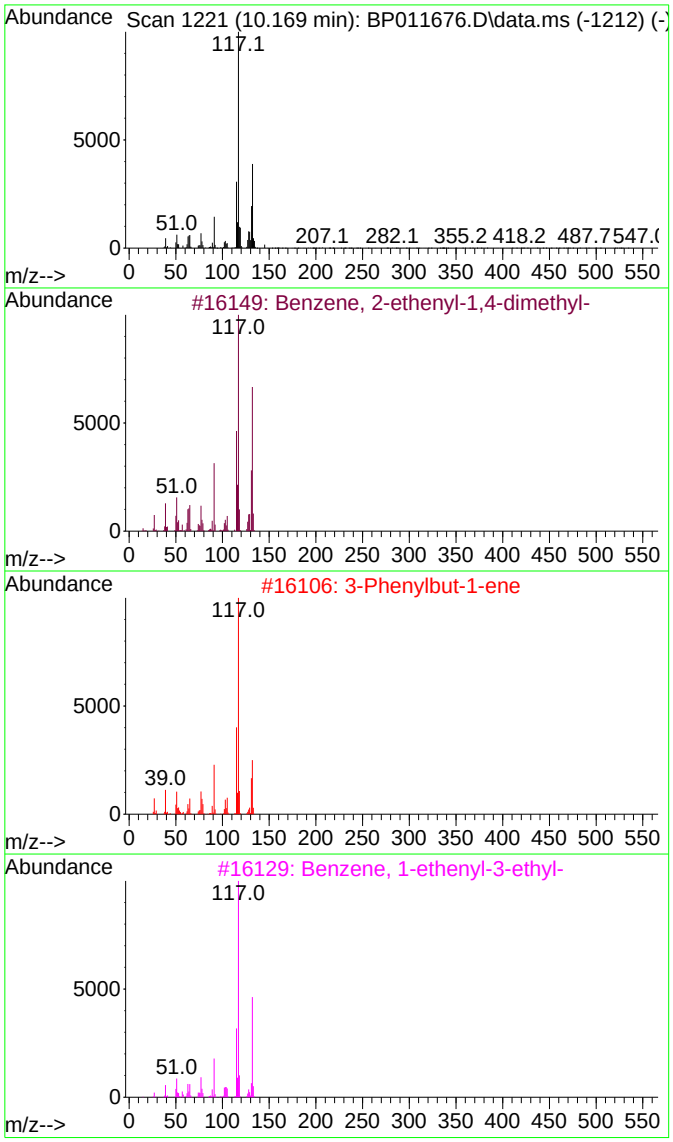
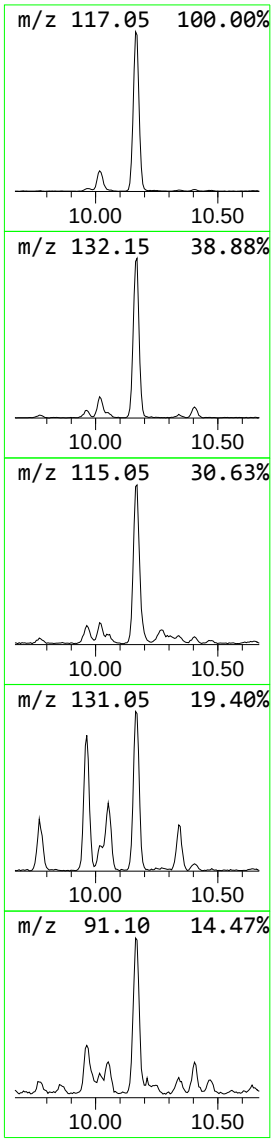
****
Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.169	5.45 ng	836440	Naphthalene-d8	10.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	81





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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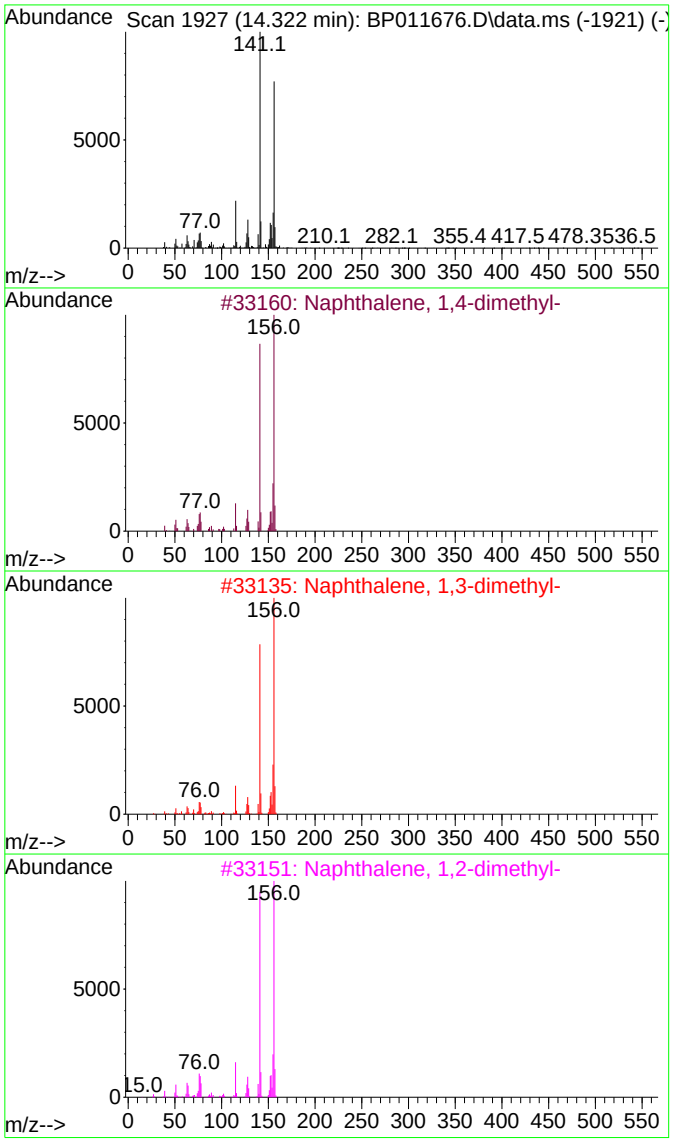
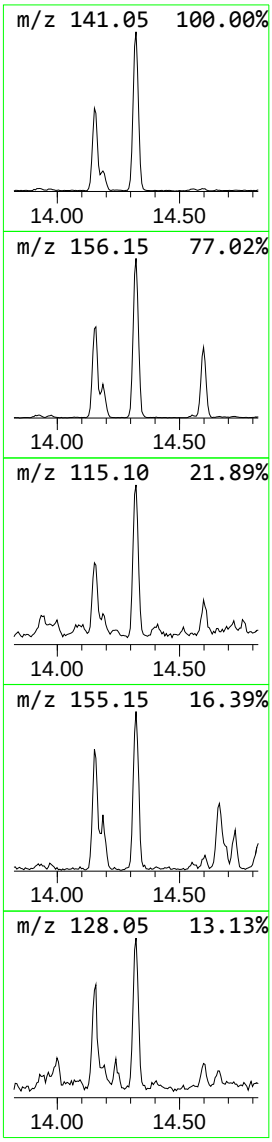
Peak Number 8 Naphthalene, 1,4-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.322	3.11 ng	595634	Acenaphthene-d10	14.599

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
2	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
3	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
5	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	94





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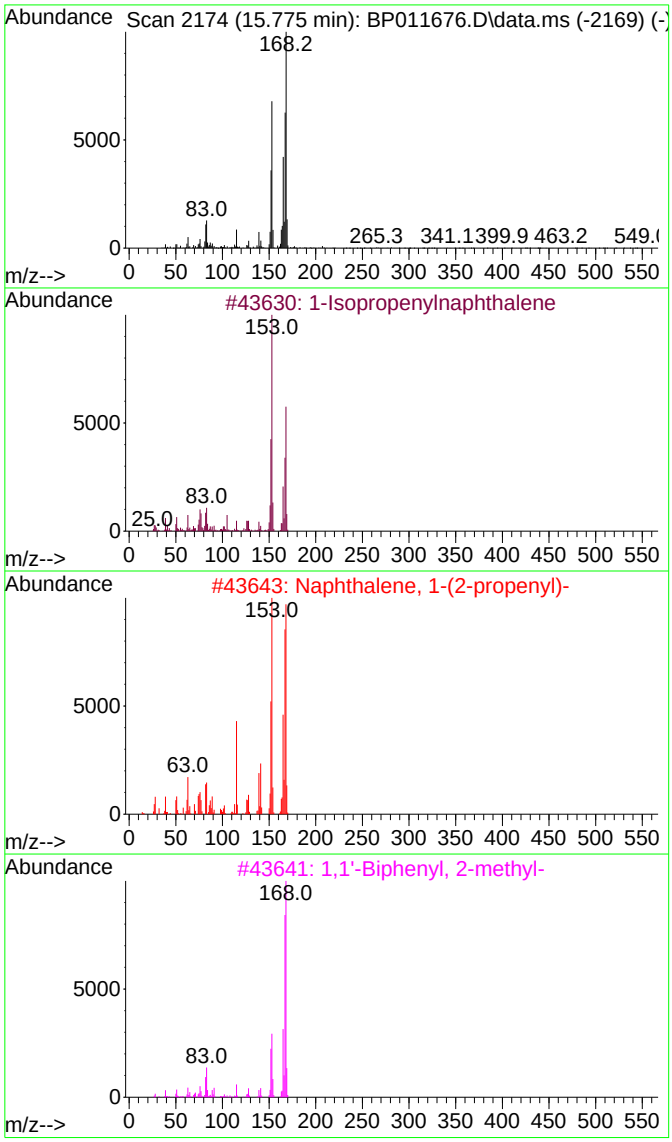
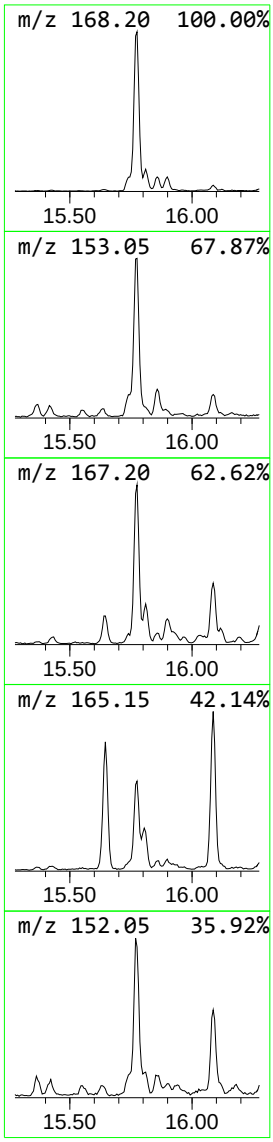
Peak Number 9 1-Isopropenylnaphthalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.775	2.80 ng	535159	Acenaphthene-d10	14.599

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Isopropenylnaphthalene	168	C13H12	001855-47-6	81
2	Naphthalene, 1-(2-propenyl)-	168	C13H12	002489-86-3	74
3	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	64
4	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	58
5	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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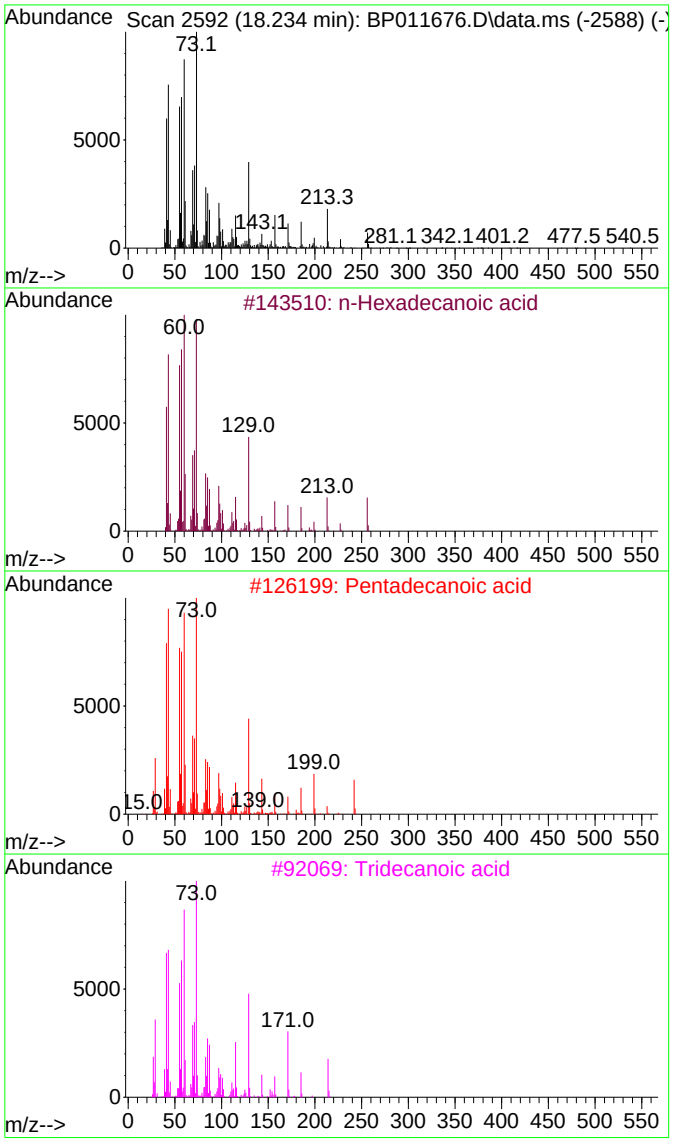
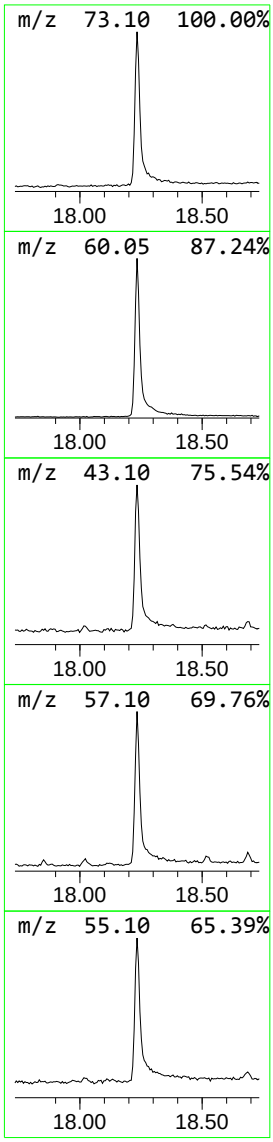
Peak Number 10 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.234	8.12 ng	1709860	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	64





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Data File : BP011676.D
Acq On : 09 Sep 2022 22:34
Operator : CG/JU
Sample : N4549-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-62

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.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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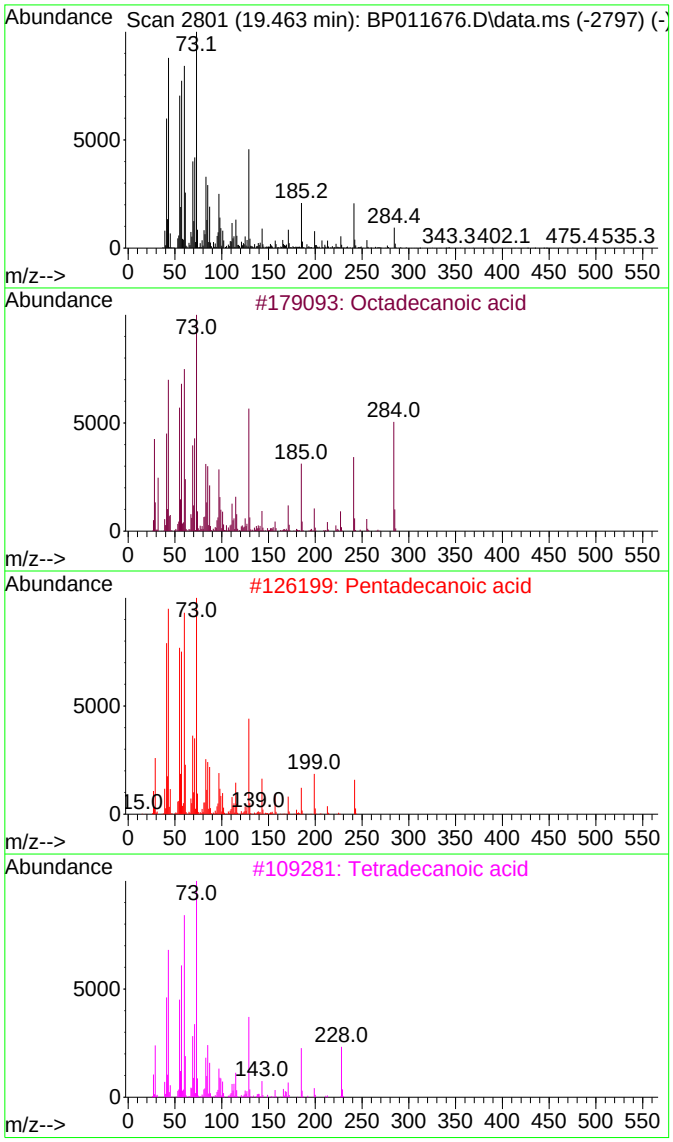
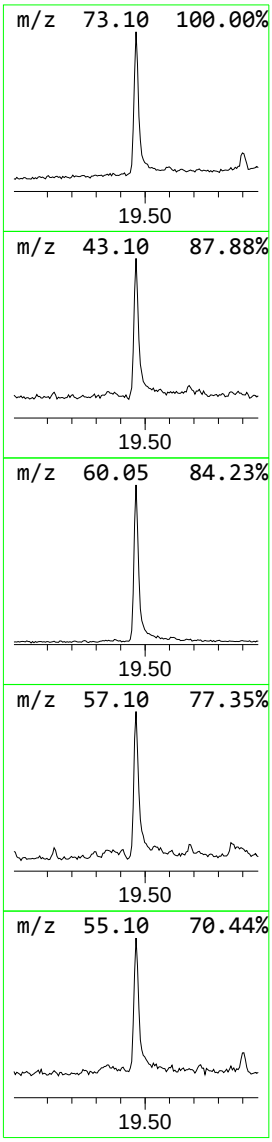
Peak Number 11 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.463	4.22 ng	989299	Chrysene-d12	21.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
Data File : BP011676.D
Acq On : 09 Sep 2022 22:34
Operator : CG/JU
Sample : N4549-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-62

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.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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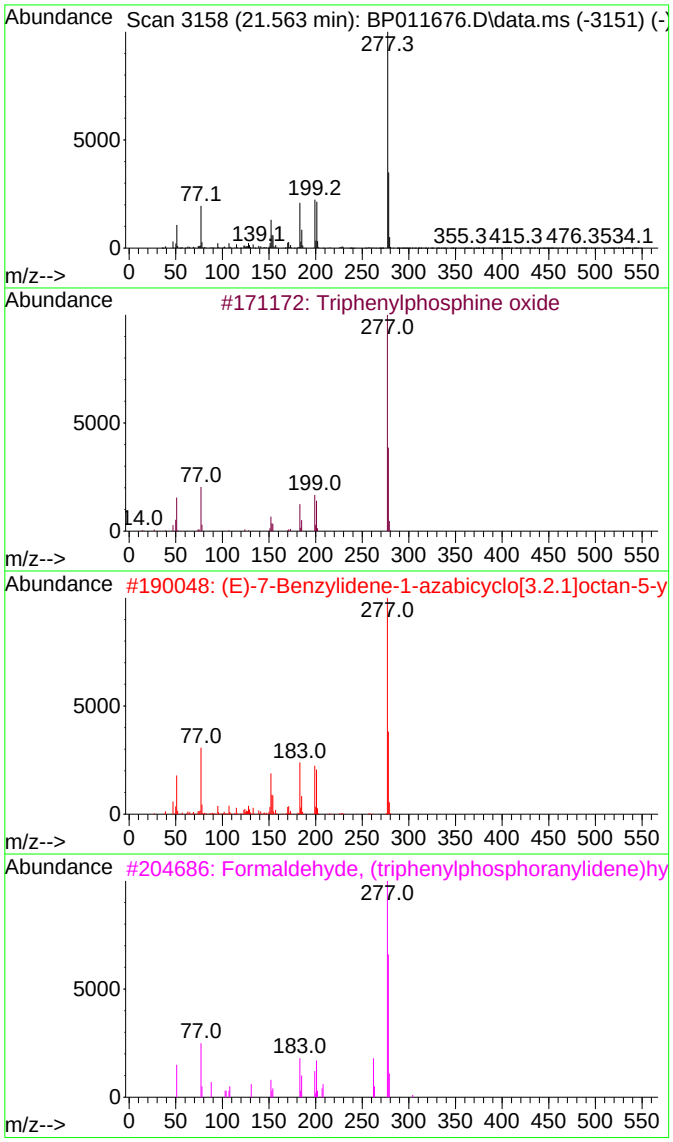
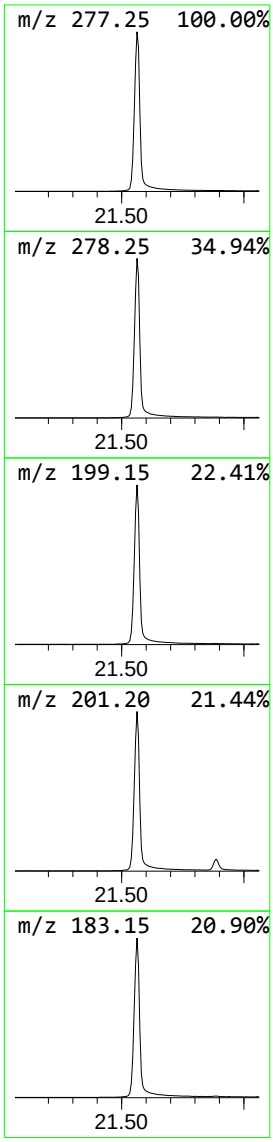
Peak Number 12 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.563	164.56 ng	38560700	Chrysene-d12	21.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	17





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
Data File : BP011676.D
Acq On : 09 Sep 2022 22:34
Operator : CG/JU
Sample : N4549-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-62

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.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
Butane, 2-metho...	3.093	148.1	ng	15228100	1	7.958	2056560	20.0
Propylene Glycol	3.634	14.3	ng	1466200	1	7.958	2056560	20.0
Indane	8.334	14.9	ng	1526570	1	7.958	2056560	20.0
Benzene, 1-ethy...	9.075	3.9	ng	403540	1	7.958	2056560	20.0
Benzene, 1,2,4,...	9.593	4.0	ng	618553	2	10.769	3068510	20.0
Benzene, 2-ethe...	10.169	5.5	ng	836440	2	10.769	3068510	20.0
Naphthalene, 1,...	14.322	3.1	ng	595634	3	14.599	3827110	20.0
1-Isopropenylna...	15.775	2.8	ng	535159	3	14.599	3827110	20.0
n-Hexadecanoic ...	18.234	8.1	ng	1709860	4	17.351	4210830	20.0
Octadecanoic acid	19.463	4.2	ng	989299	5	21.427	4686420	20.0
Triphenylphosph...	21.563	164.6	ng	38560700	5	21.427	4686420	20.0