LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
Data File : BP011673.D
Acq On : 09 Sep 2022 20:50
Operator : CG/JU
Sample : N4549-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-60

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: BP011673.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.017	3	5	13	rVB	1293310	1578766	3.59%	1.037%
2	3.093	13	18	40	rVB	12728636	16121469	36.69%	10.585%
3	5.517	423	430	439	rBV	3254610	4819700	10.97%	3.164%
4	7.111	695	701	711	rBV	1931903	3100187	7.06%	2.035%
5	7.958	837	845	853	rBV	1300554	2097417	4.77%	1.377%
6	9.128	1036	1044	1054	rBV	4341777	7315507	16.65%	4.803%
7	10.775	1316	1324	1337	rBV	1696096	3013427	6.86%	1.978%
8	12.387	1591	1598	1607	rBV	286329	521952	1.19%	0.343%
9	13.228	1733	1741	1749	rBV	11528034	17256275	39.27%	11.330%
10	14.598	1967	1974	1989	rBV	2576884	3896442	8.87%	2.558%
11	16.087	2221	2227	2236	rBV	8194453	11682309	26.59%	7.670%
12	16.840	2350	2355	2368	rBV	362656	685998	1.56%	0.450%
13	17.351	2436	2442	2454	rVB	3143952	4490204	10.22%	2.948%
14	18.234	2588	2592	2601	rBV	738958	1227386	2.79%	0.806%
15	19.463	2797	2801	2813	rBV	485546	840255	1.91%	0.552%
16	19.904	2871	2876	2881	rBV	15627482	19023006	43.29%	12.490%
17	21.145	3083	3087	3098	rVB3	392430	601574	1.37%	0.395%
18	21.433	3131	3136	3142	rBV	3568525	4734814	10.78%	3.109%
19	21.563	3151	3158	3188	rBV	25166992	43939156	100.00%	28.848%
20	21.886	3210	3213	3222	rVB	324625	487468	1.11%	0.320%
21	23.898	3549	3555	3566	rVB2	2438510	4876984	11.10%	3.202%

Sum of corrected areas: 152310296

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
Data File : BP011673.D
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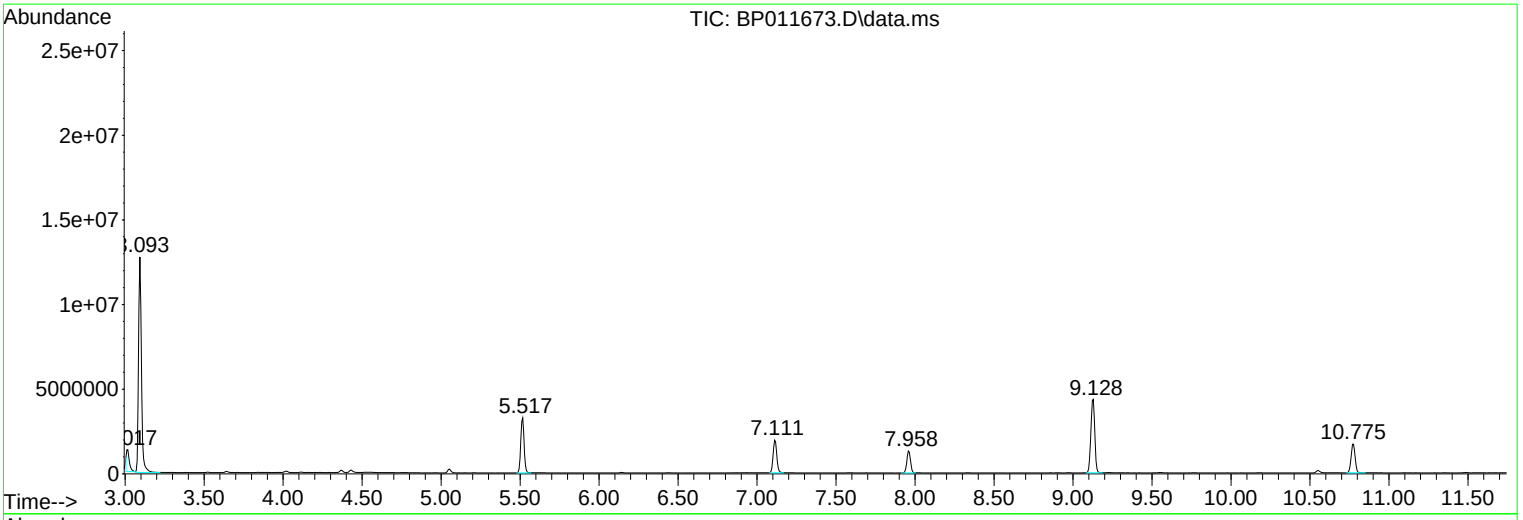
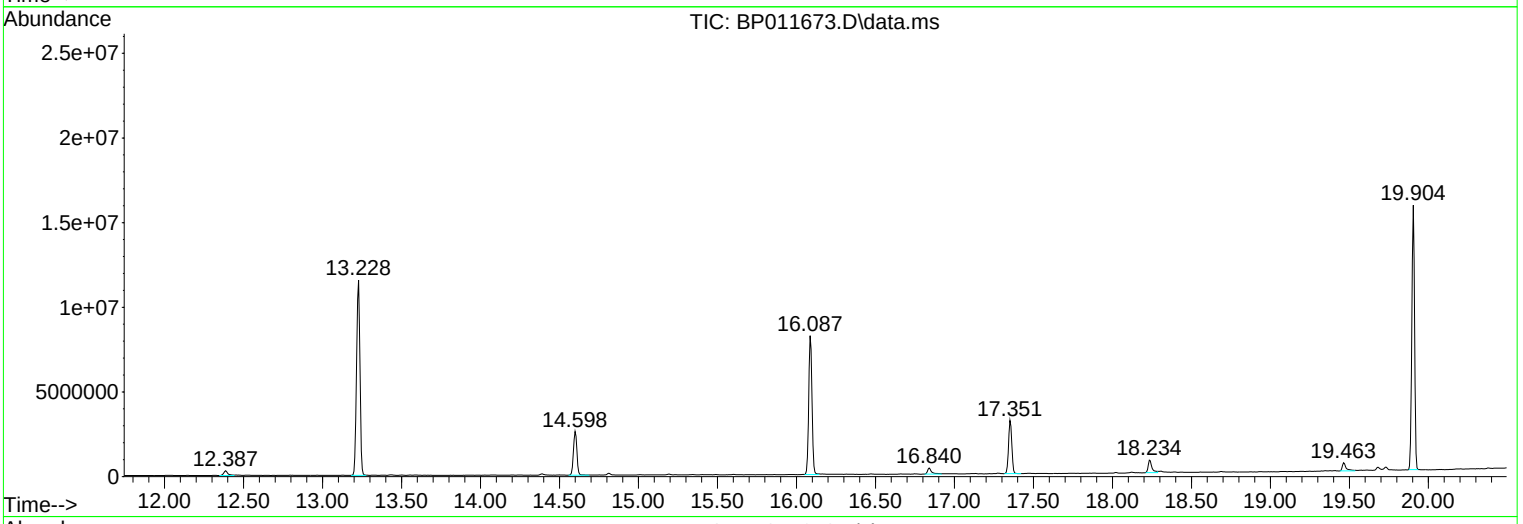
Operator : CG/JU
Sample : N4549-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

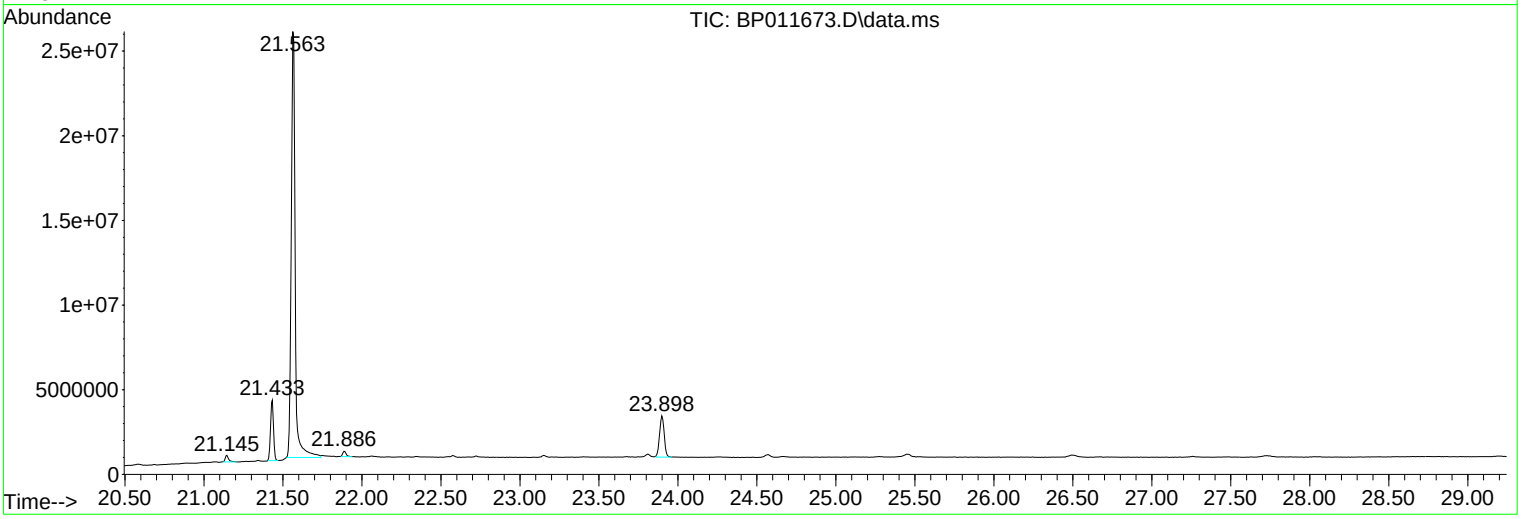
Instrument :
BNA_P
ClientSampleId :
MW-60

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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Data File : BP011673.D
Acq On : 09 Sep 2022 20:50
Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

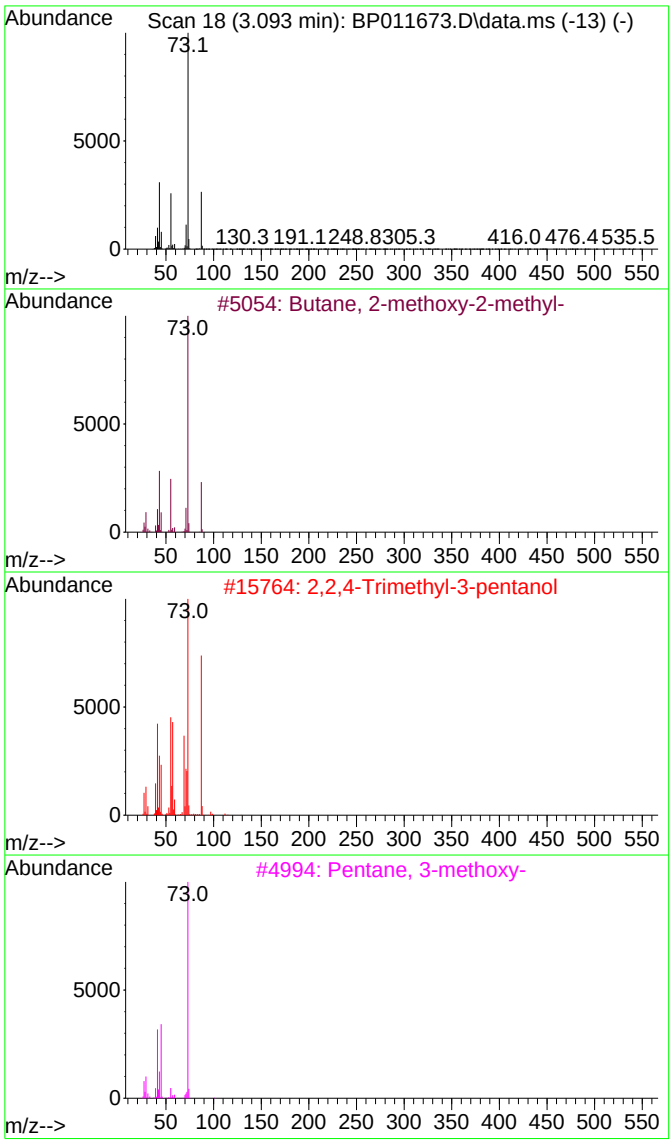
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

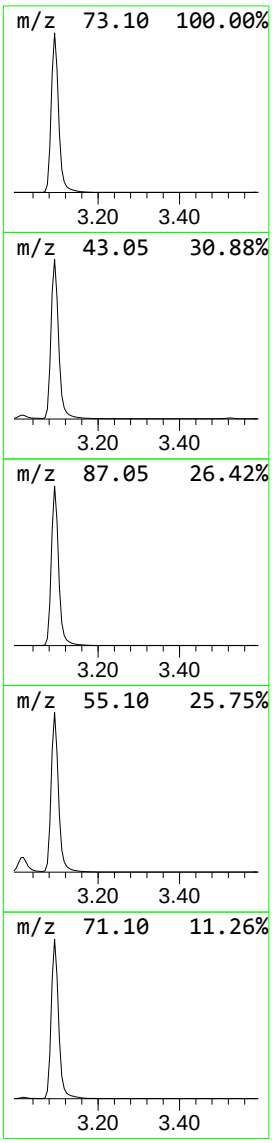
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.093	153.73 ng	16121500	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Data File : BP011673.D
Acq On : 09 Sep 2022 20:50
Operator : CG/JU
Sample : N4549-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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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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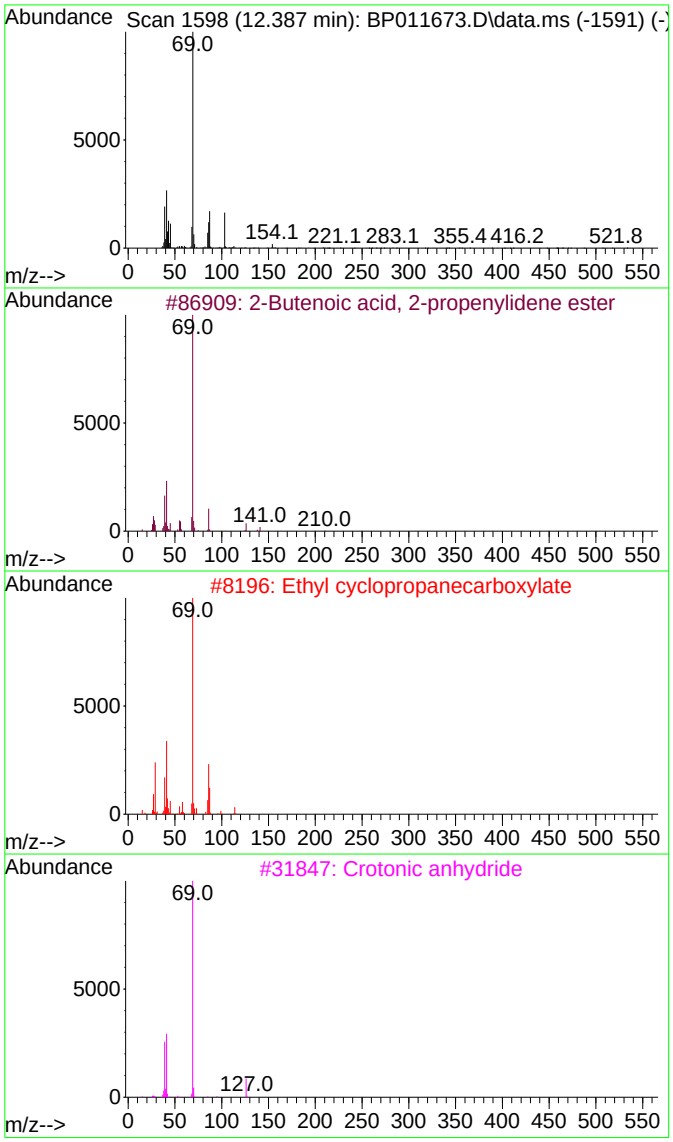
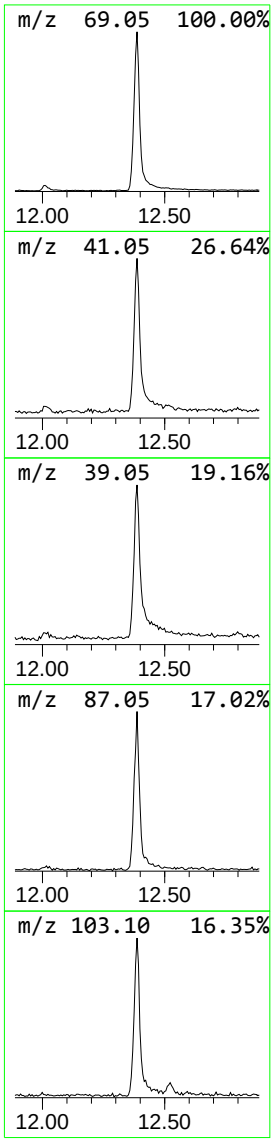
Peak Number 3 unknown12.387 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.387	3.46 ng	521952	Naphthalene-d8	10.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	45
2	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
3	Crotonic anhydride	154	C8H10O3	000623-68-7	38
4	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	33
5	Oxazole	69	C3H3NO	000288-42-6	9





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Operator : CG/JU
Sample : N4549-16
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Instrument :
BNA_P
ClientSampleId :
MW-60

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
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TIC Integration Parameters: LSCINT.P

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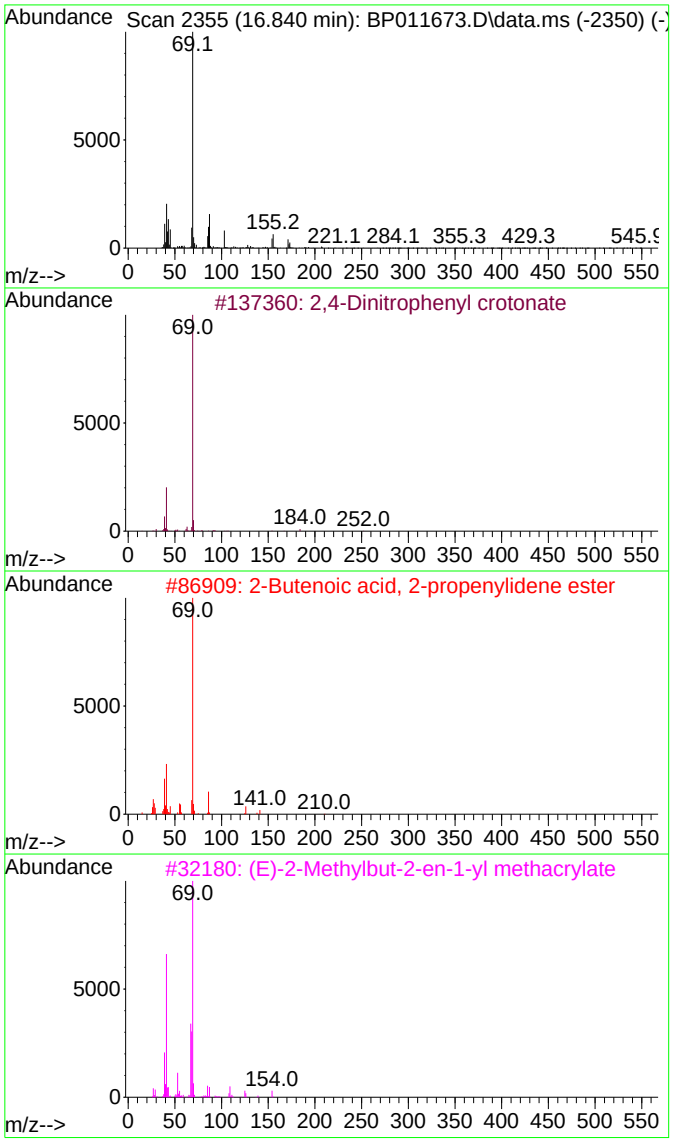
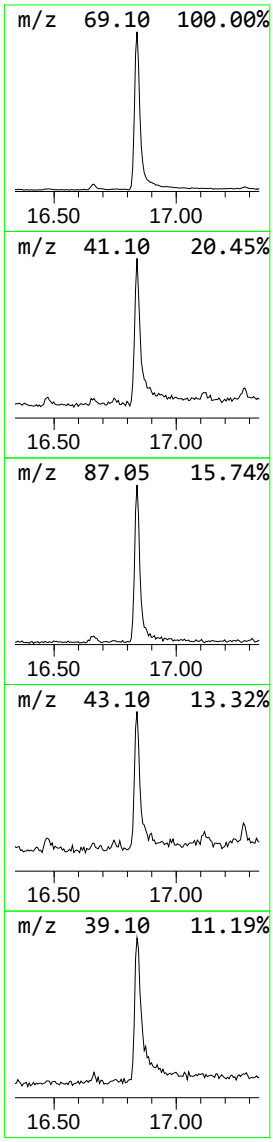
Peak Number 4 unknown16.480 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.840	3.06 ng	685998	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dinitrophenyl crotonate	252	C10H8N2O6	069817-88-5	47
2	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
3	(E)-2-Methylbut-2-en-1-yl methac...	154	C9H14O2	088142-95-4	42
4	Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1010156-45-5	38
5	Succinic acid, 3-methylbut-2-en-...	296	C15H17ClO4	1000389-79-8	36





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Data File : BP011673.D
Acq On : 09 Sep 2022 20:50
Operator : CG/JU
Sample : N4549-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-60

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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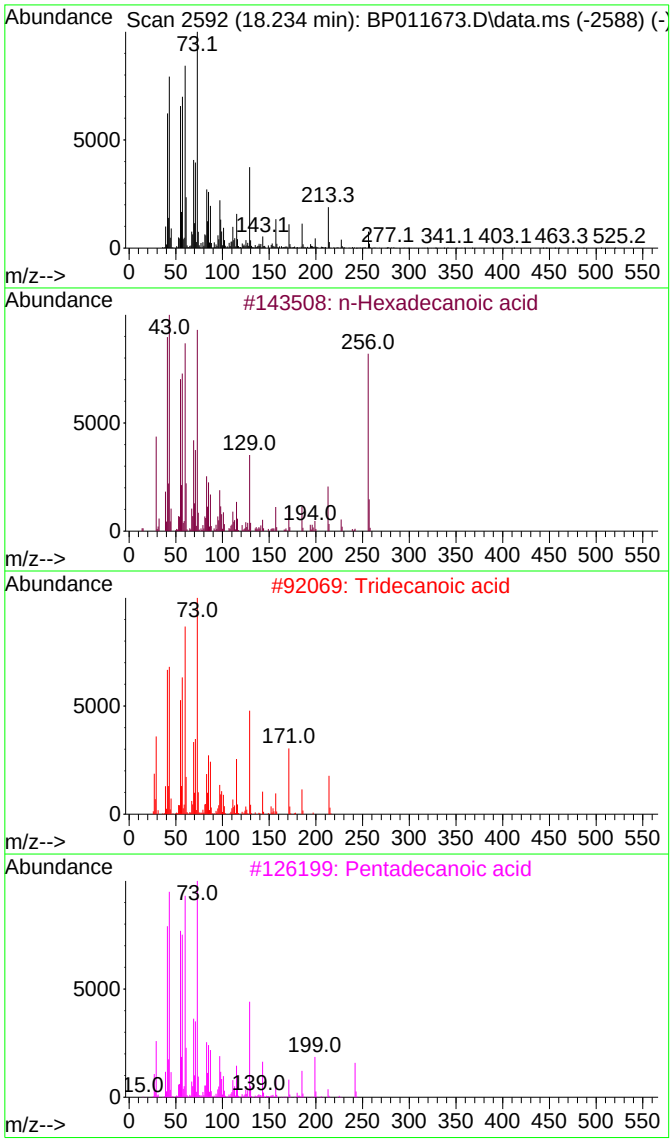
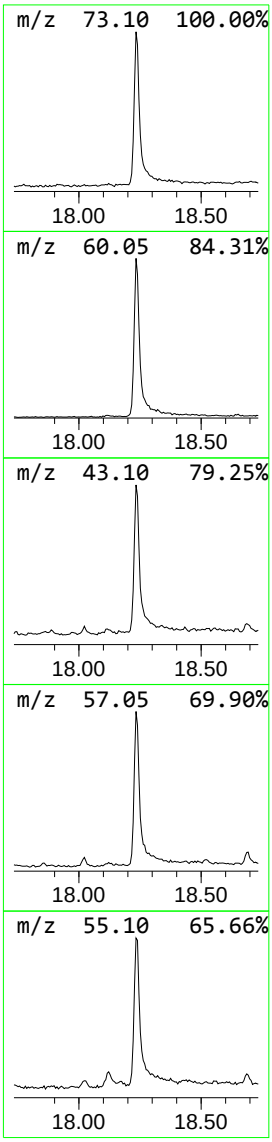
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.234	5.47 ng	1227390	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
Data File : BP011673.D
Acq On : 09 Sep 2022 20:50
Operator : CG/JU
Sample : N4549-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-60

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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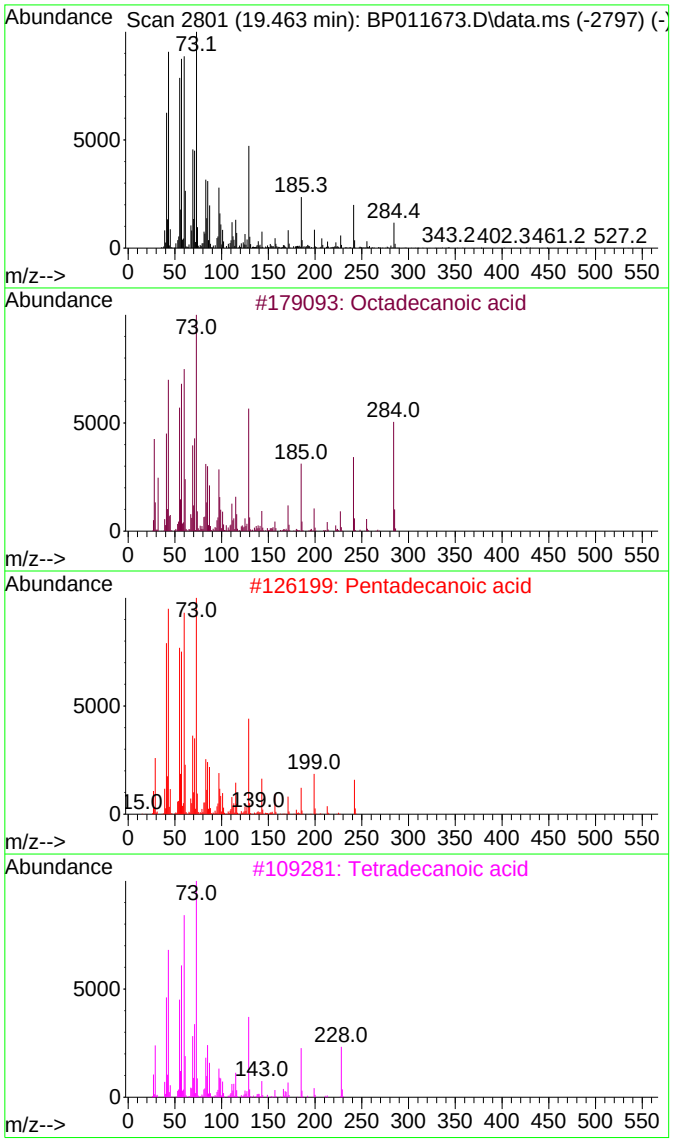
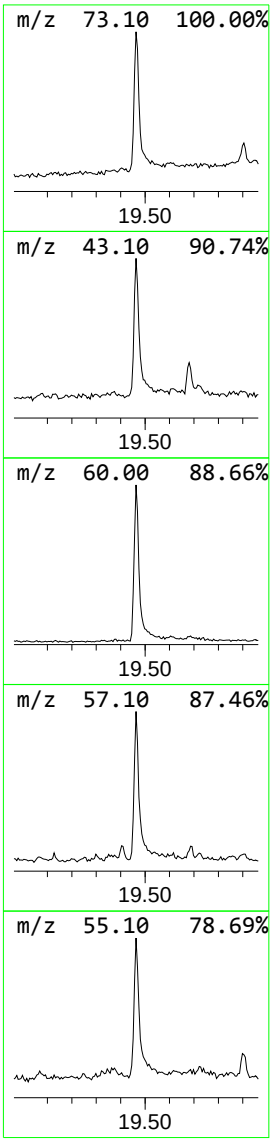
Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.463	3.55 ng	840255	Chrysene-d12	21.433

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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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ALS Vial : 14 Sample Multiplier: 1

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BNA_P
ClientSampleId :
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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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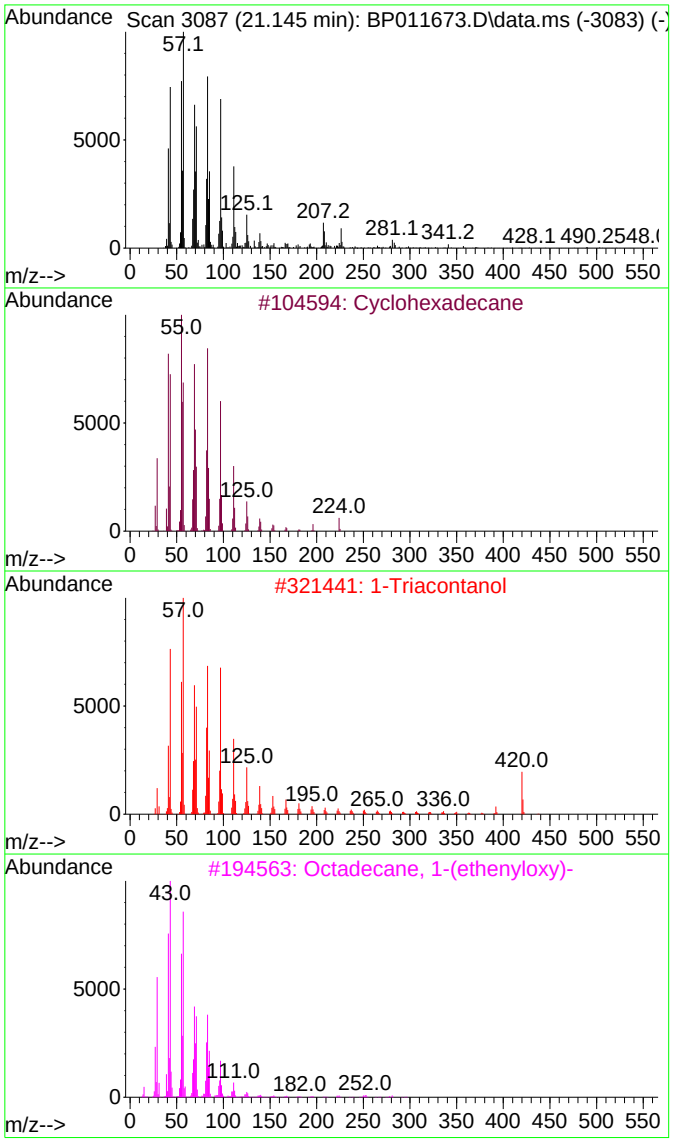
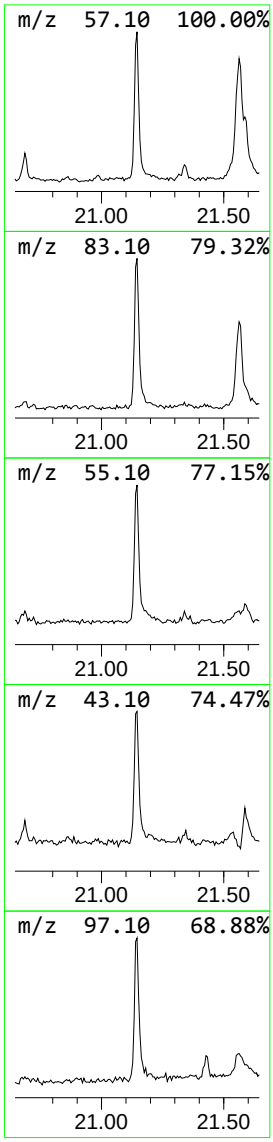
Peak Number 7 Cyclohexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.145	2.54 ng	601574	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	94
2	1-Triacontanol	438	C30H62O	000593-50-0	91
3	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	87
4	9-Tricosanol, acetate	382	C25H50O2	039754-92-2	87
5	1-Hexacosene	364	C26H52	018835-33-1	87





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Instrument :
BNA_P
ClientSampleId :
MW-60

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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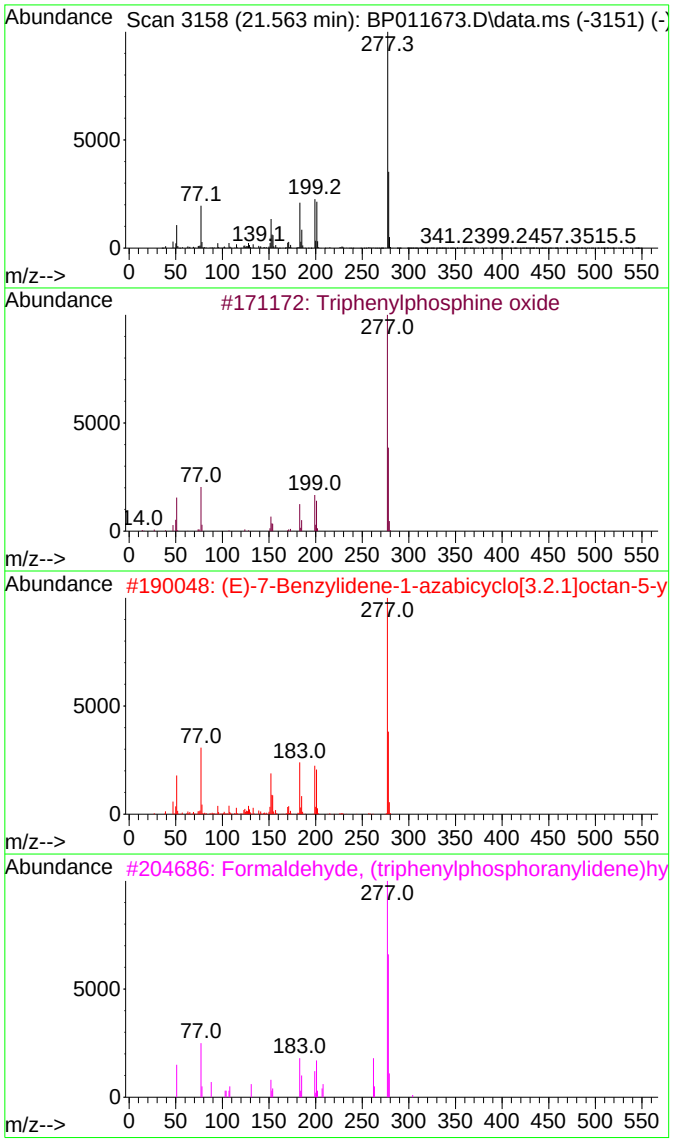
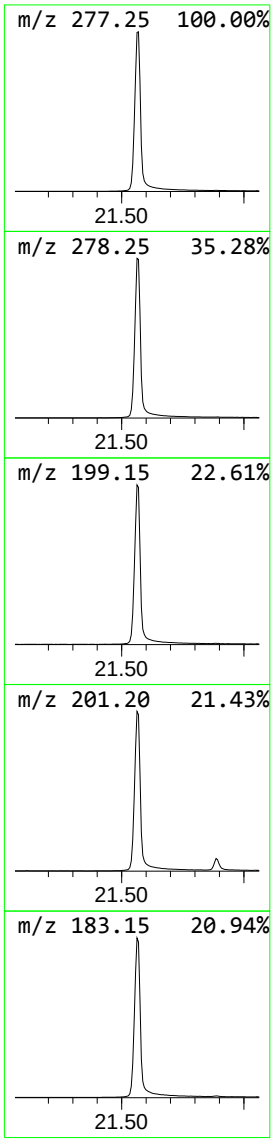
Peak Number 8 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.563	185.60 ng	43939200	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
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





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TIC Library : C:\Database\NIST20.L
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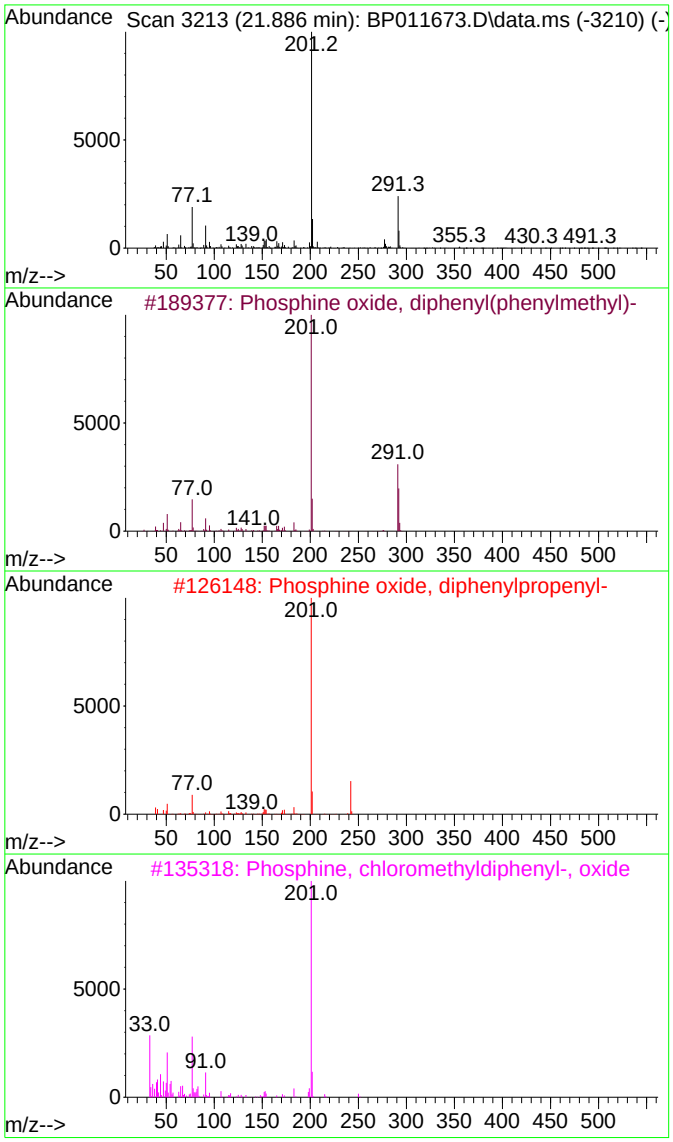
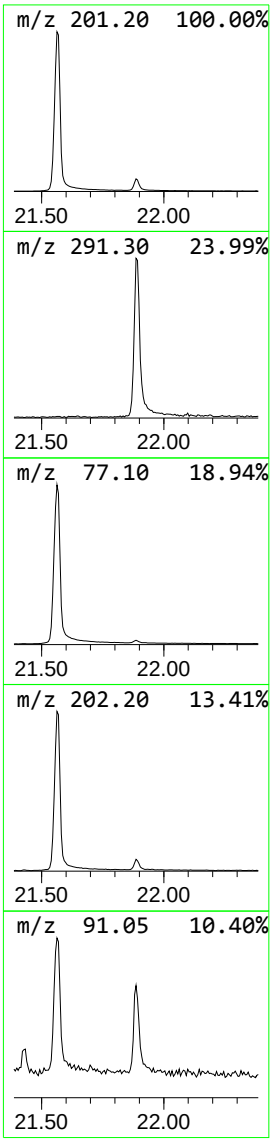
Peak Number 9 unknown21.886 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.886	2.06 ng	487468	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphine oxide, diphenyl(phenyl...	292	C19H17OP	002959-74-2	46
2	Phosphine oxide, diphenylpropenyl-	242	C15H15OP	004252-89-5	45
3	Phosphine, chloromethyldiphenyl-...	250	C13H12ClOP	001806-49-1	42
4	2,3-Dihydro-7-methoxyfuro(2,3-b)...	201	C12H11NO2	073863-58-8	40
5	1,4-Bis[2-[N-[6-methoxy-8-quinol...	542	C30H34N6O4	050823-62-6	40





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...	3.093	153.7	ng	16121500	1	7.958	2097420	20.0
unknown12.387	12.387	3.5	ng	521952	2	10.775	3013430	20.0
unknown16.480	16.840	3.1	ng	685998	4	17.351	4490200	20.0
n-Hexadecanoic ...	18.234	5.5	ng	1227390	4	17.351	4490200	20.0
Octadecanoic acid	19.463	3.5	ng	840255	5	21.433	4734810	20.0
Cyclohexadecane	21.145	2.5	ng	601574	5	21.433	4734810	20.0
Triphenylphosph...	21.563	185.6	ng	43939200	5	21.433	4734810	20.0
unknown21.886	21.886	2.1	ng	487468	5	21.433	4734810	20.0