LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090622\
Data File : BP011624.D
Acq On : 06 Sep 2022 14:21
Operator : CG/JU
Sample : N4446-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EQUIP-BLANK

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: BP011624.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	14	rVV	125766	222352	1.89%	0.488%
2	3.099	14	19	48	rVB	1313189	2444094	20.82%	5.367%
3	4.516	252	260	268	rBV2	99504	277388	2.36%	0.609%
4	5.058	346	352	359	rVB	121476	192972	1.64%	0.424%
5	5.522	425	431	442	rBV	725657	1169617	9.96%	2.569%
6	7.116	696	702	716	rBV	584726	1018311	8.67%	2.236%
7	7.969	840	847	855	rBV	222992	373510	3.18%	0.820%
8	9.134	1037	1045	1056	rBV	809459	1376116	11.72%	3.022%
9	10.787	1313	1326	1335	rBV	336959	601313	5.12%	1.321%
10	12.081	1539	1546	1562	rBV2	175076	453770	3.86%	0.996%
11	13.034	1703	1708	1719	rVB	179219	302456	2.58%	0.664%
12	13.240	1735	1743	1753	rBV	2412396	3725789	31.73%	8.182%
13	14.051	1875	1881	1894	rBV	176837	366982	3.13%	0.806%
14	14.610	1969	1976	1991	rVB	601762	929825	7.92%	2.042%
15	15.428	2106	2115	2125	rBV	70664	148430	1.26%	0.326%
16	16.098	2222	2229	2248	rBV	7883613	11198178	95.37%	24.592%
17	17.363	2438	2444	2456	rVB	950957	1405506	11.97%	3.087%
18	18.245	2590	2594	2601	rBV	205481	333456	2.84%	0.732%
19	18.322	2603	2607	2620	rVB	173514	284929	2.43%	0.626%
20	19.474	2799	2803	2812	rBV3	167501	285535	2.43%	0.627%
21	19.916	2872	2878	2885	rBV	9585112	11741319	100.00%	25.784%
22	21.439	3132	3137	3151	rBV	1929826	2516445	21.43%	5.526%
23	21.563	3154	3158	3169	rBV	598148	1144094	9.74%	2.512%
24	23.910	3551	3557	3567	rVB2	1486093	3024118	25.76%	6.641%

Sum of corrected areas: 45536505

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090622\
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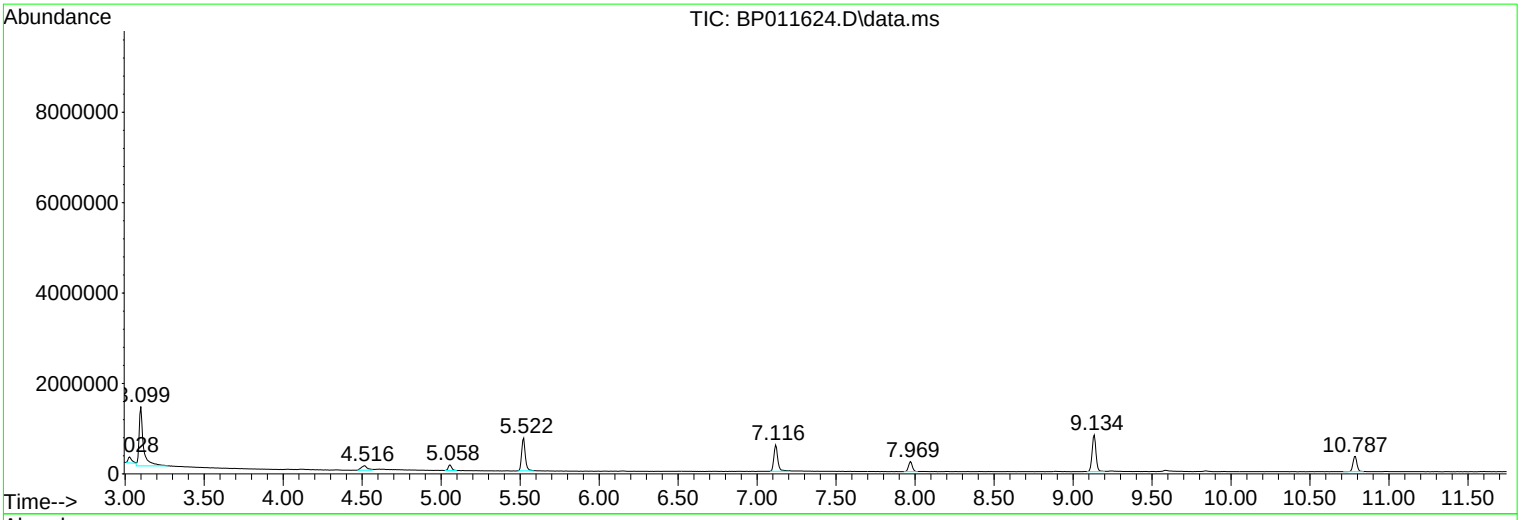
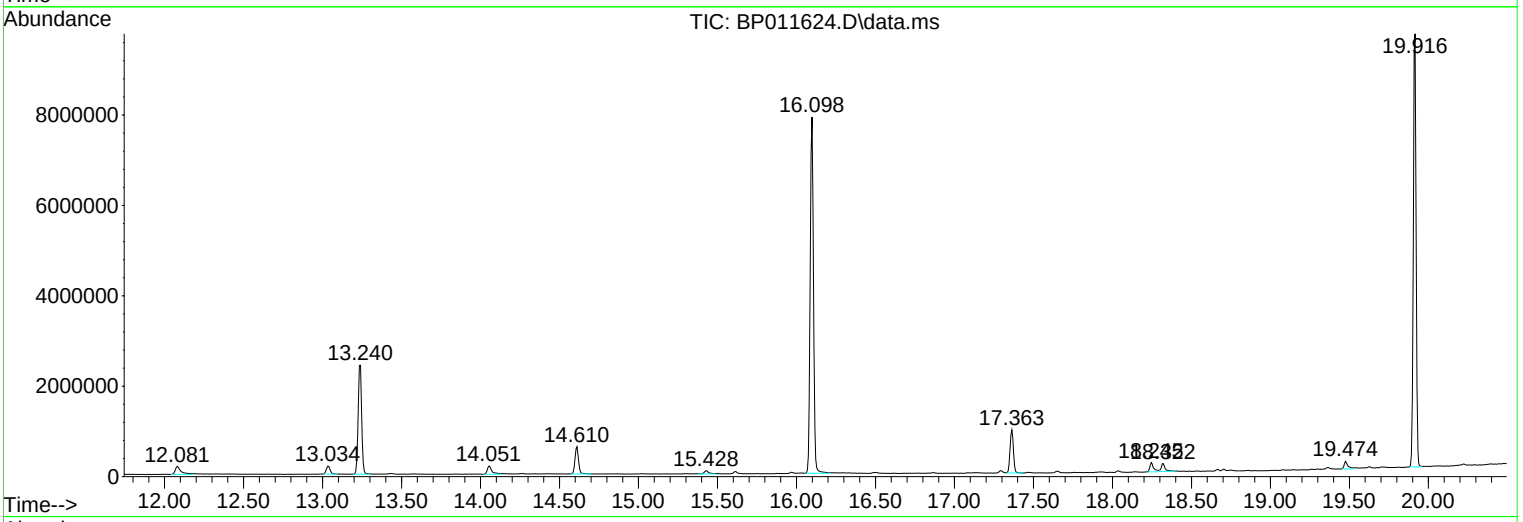
Misc :
ALS Vial : 6 Sample Multiplier: 1

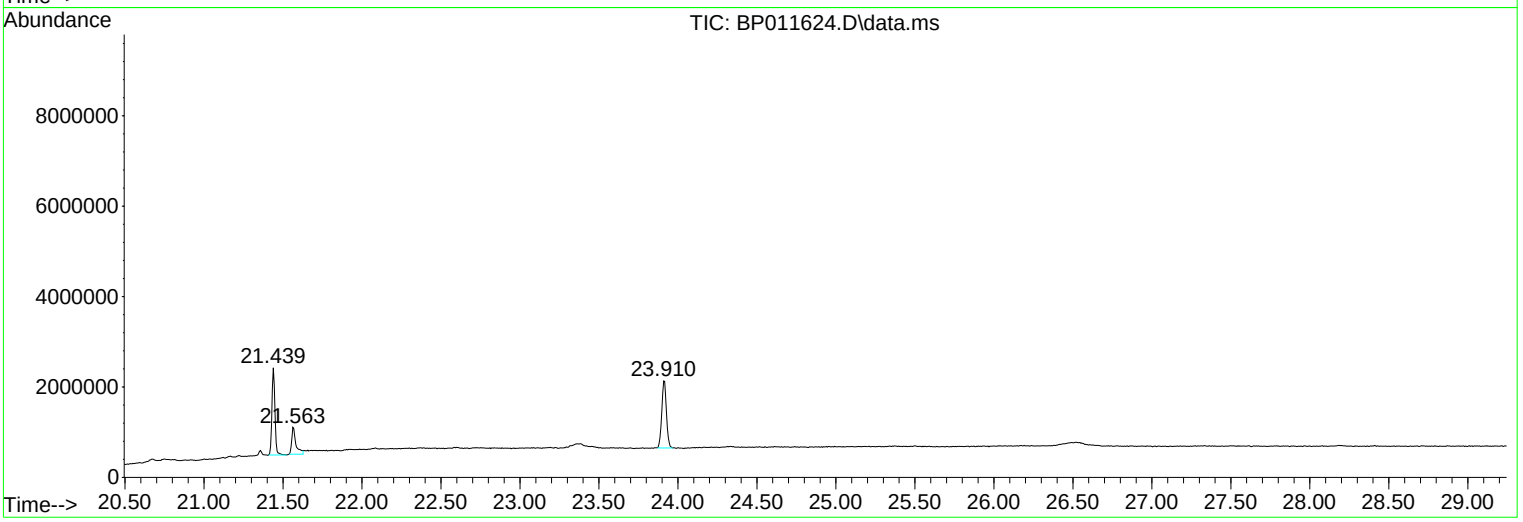
Instrument :
BNA_P
ClientSampleId :
EQUIP-BLANK

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 : BP011624.D
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Operator : CG/JU
Sample : N4446-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

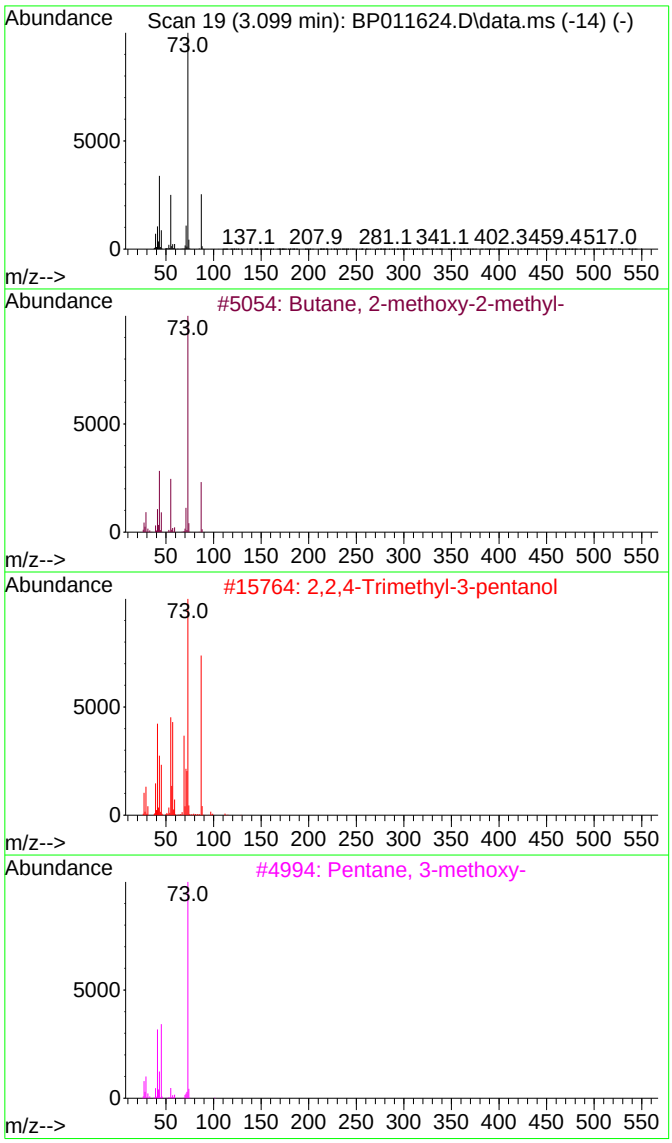
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

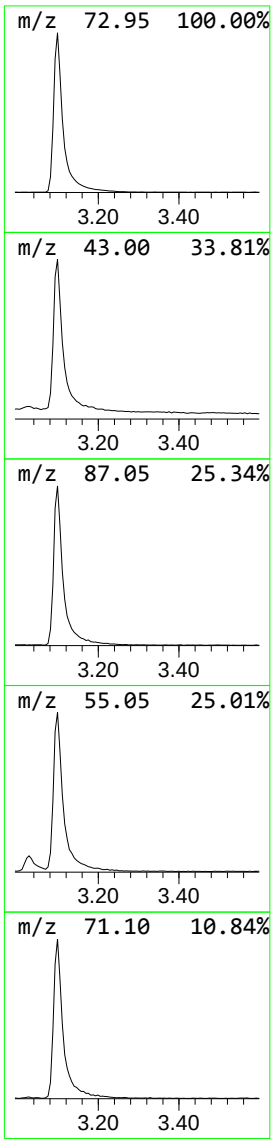
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.099	130.87 ng	2444090	1,4-Dichlorobenzene-d4	7.969

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BP011624.D
Acq On : 06 Sep 2022 14:21
Operator : CG/JU
Sample : N4446-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EQUIP-BLANK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

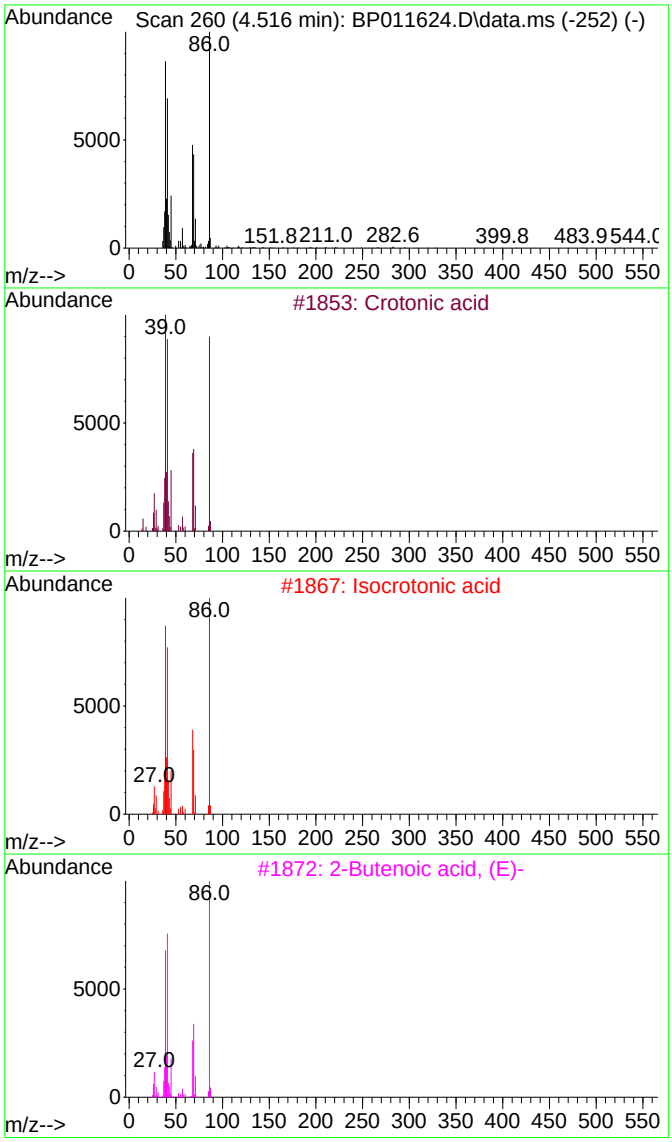
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

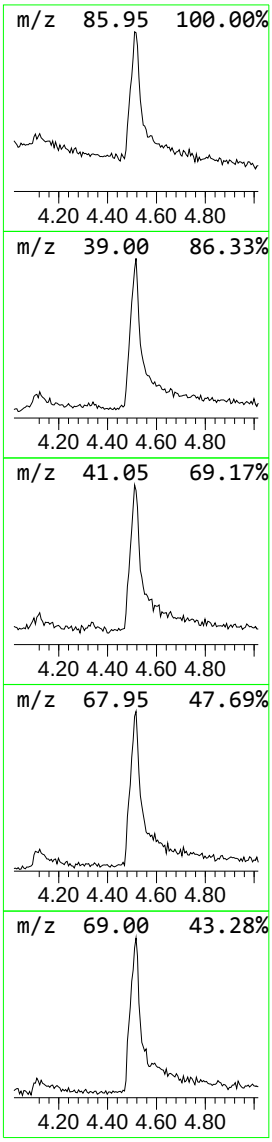
****

Peak Number 3 Crotonic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.516	14.85 ng	277388	1,4-Dichlorobenzene-d4	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Crotonic acid	86	C4H6O2	003724-65-0	97
2	Isocrotonic acid	86	C4H6O2	000503-64-0	95
3	2-Butenoic acid, (E)-	86	C4H6O2	000107-93-7	93
4	2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	87
5	Furan	68	C4H4O	000110-00-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090622\
Data File : BP011624.D
Acq On : 06 Sep 2022 14:21
Operator : CG/JU
Sample : N4446-11
Misc :
ALS Vial : 6 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

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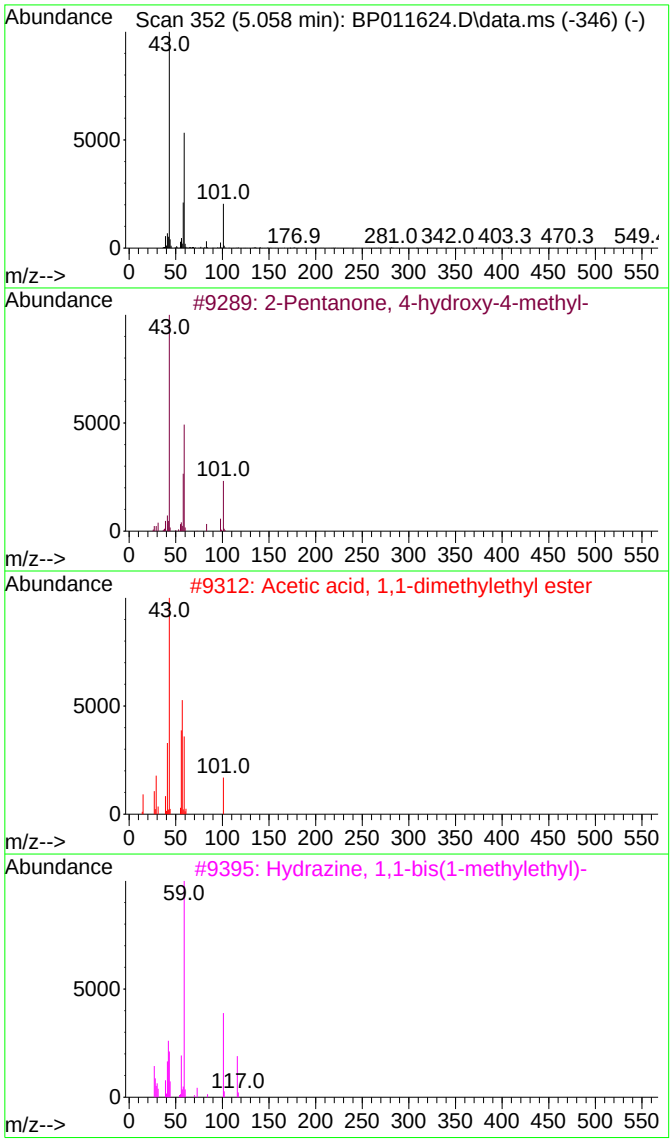
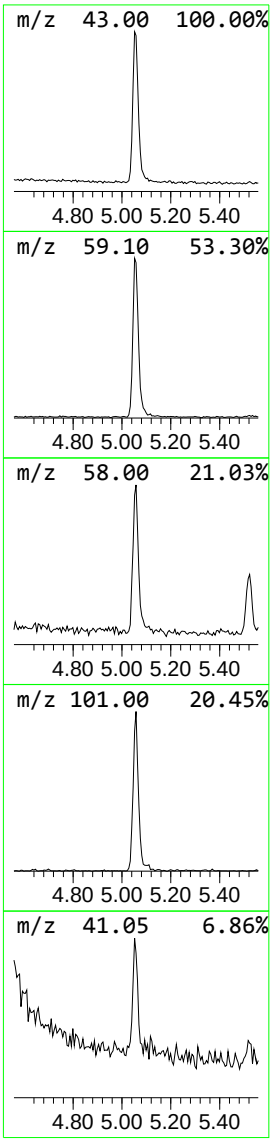
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.058	10.33 ng	192972	1,4-Dichlorobenzene-d4	7.969

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	38
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
4	3-Octanol	130	C8H18O	000589-98-0	25
5	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	25





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Misc :
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Instrument :
BNA_P
ClientSampleId :
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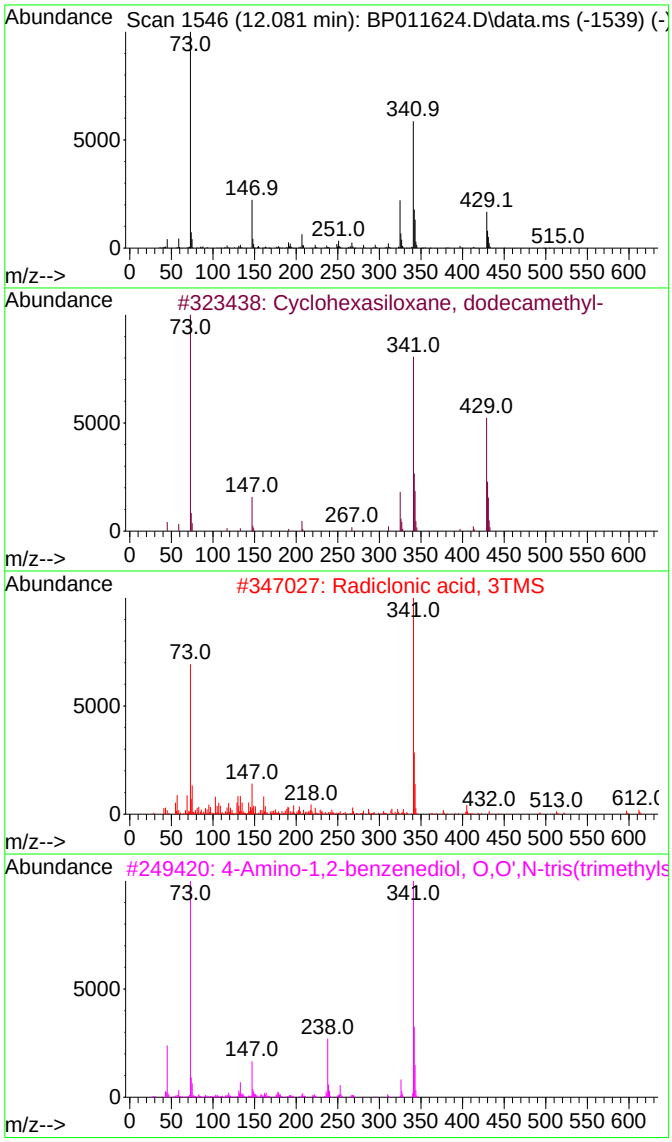
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

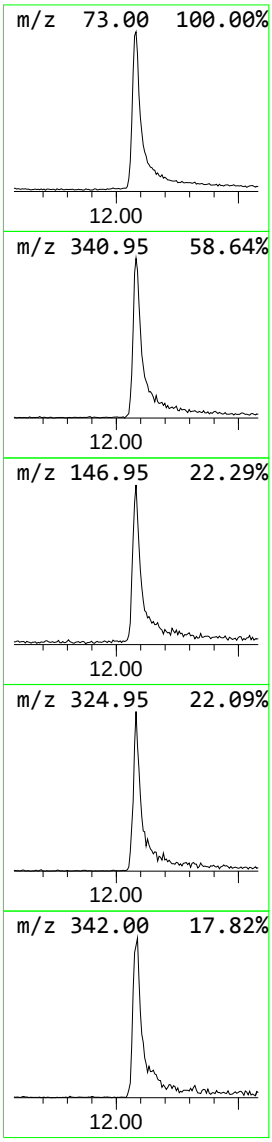
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexasiloxane, dodecame... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.081	15.09 ng	453770	Naphthalene-d8	10.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	87
2	Radiclonic acid, 3TMS	612	C32H64O5Si3	1000506-01-9	53
3	4-Amino-1,2-benzenediol, O,O',N-...	341	C15H31NO2Si3	1000493-87-4	49
4	4',6'-Dimethoxy-2'-(tert.-butyld...	398	C23H30O4Si	1000453-95-4	35
5	4',6'-Dimethoxy-2'-(tert.-bytuld...	398	C23H30O4Si	1000453-93-0	35





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Sample : N4446-11
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
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TIC Library : C:\Database\NIST20.L
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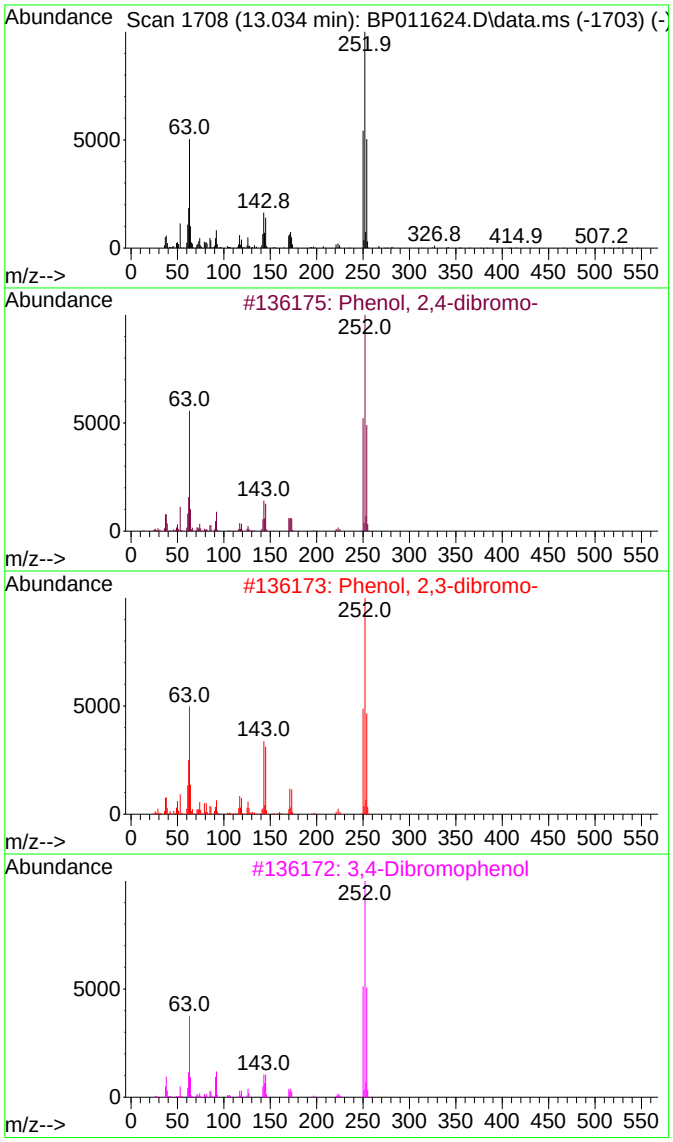
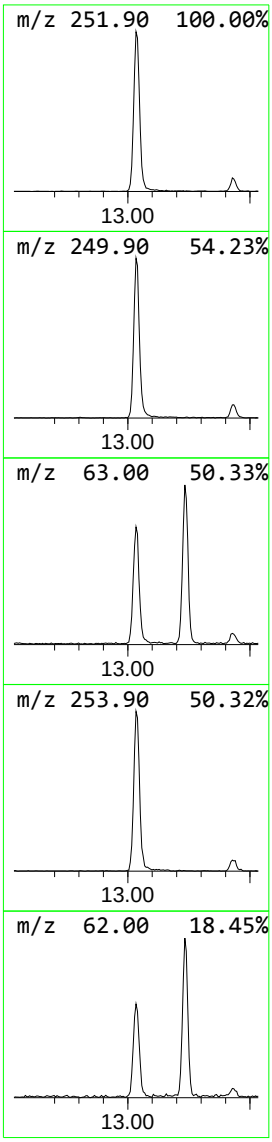
****

Peak Number 6 Phenol, 2,4-dibromo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.034	6.51 ng	302456	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	99
2	Phenol, 2,3-dibromo-	250	C6H4Br2O	057383-80-9	97
3	3,4-Dibromophenol	250	C6H4Br2O	1010487-11-5	95
4	Phenol, 2,6-dibromo-	250	C6H4Br2O	000608-33-3	95
5	Phenol, 2,5-dibromo-	250	C6H4Br2O	028165-52-8	81





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Data File : BP011624.D
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Sample : N4446-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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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
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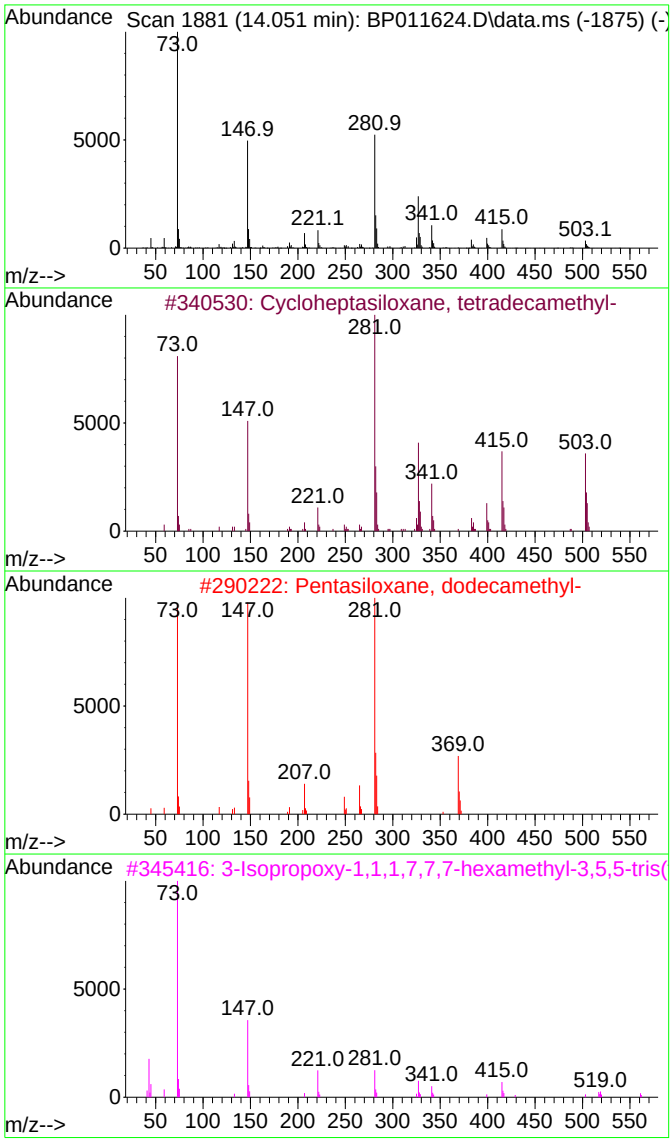
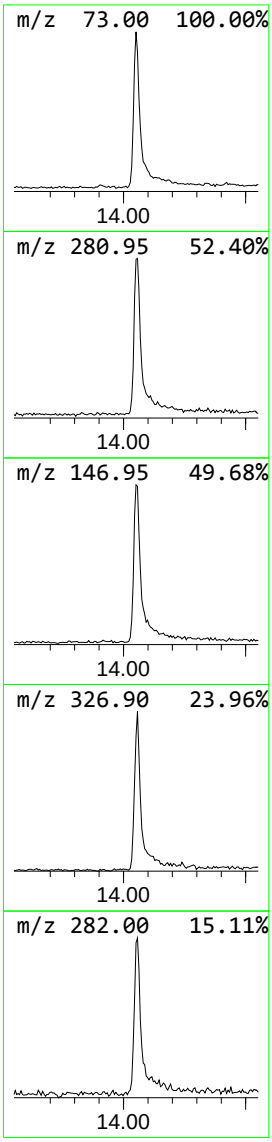
Peak Number 7 Cycloheptasiloxane, tetrade... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.051	7.89 ng	366982	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptasiloxane, tetradecamet...	518	C14H42O7Si7	000107-50-6	90
2	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	50
3	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	38
4	2,6-Dihydroxyacetophenone, 2TMS ...	296	C14H24O3Si2	1000352-81-3	30
5	14.alpha.-Morphinan, 7,8-didehyd...	281	C19H23NO	017939-34-3	27





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Data File : BP011624.D
Acq On : 06 Sep 2022 14:21
Operator : CG/JU
Sample : N4446-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
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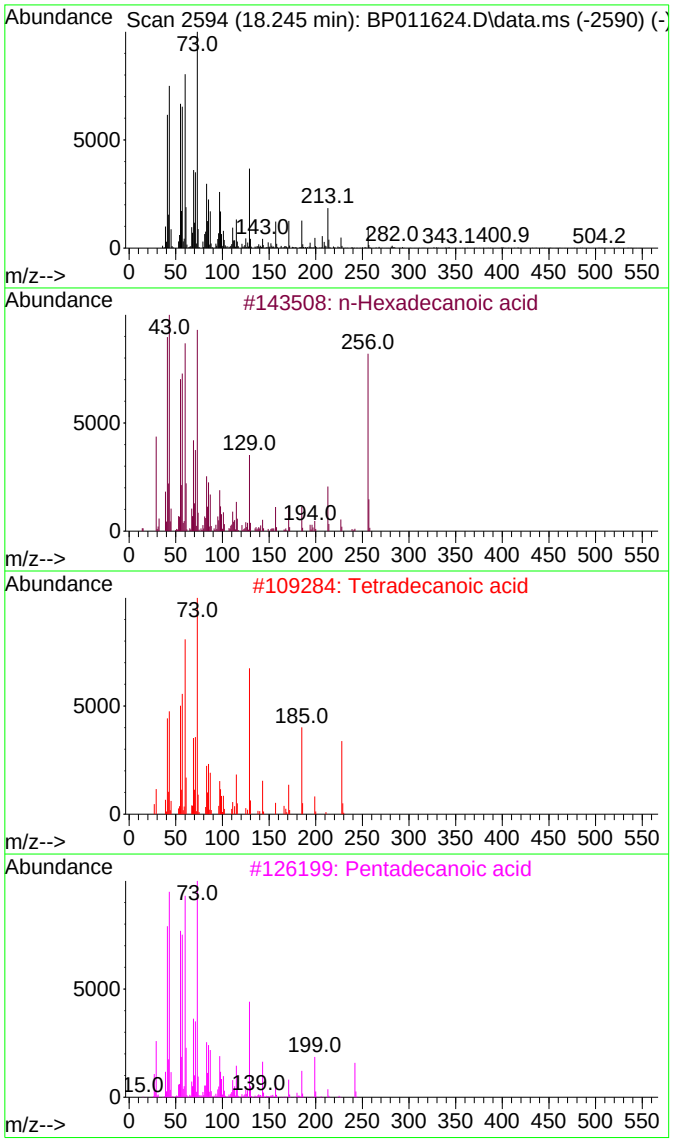
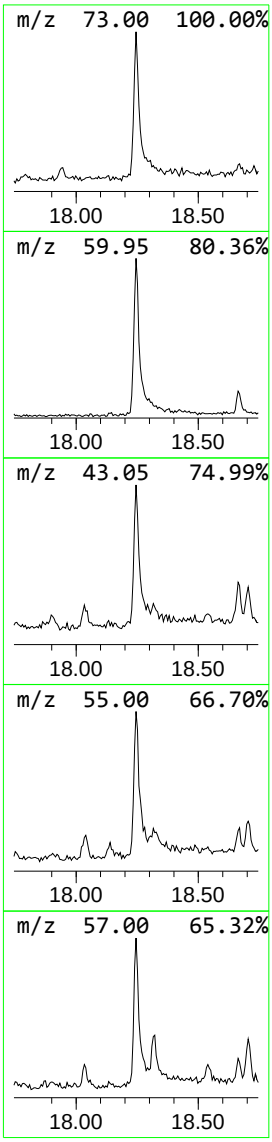
Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.245	4.75 ng	333456	Phenanthrene-d10	17.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Octadecanoic acid	284	C18H36O2	000057-11-4	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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TIC Library : C:\Database\NIST20.L
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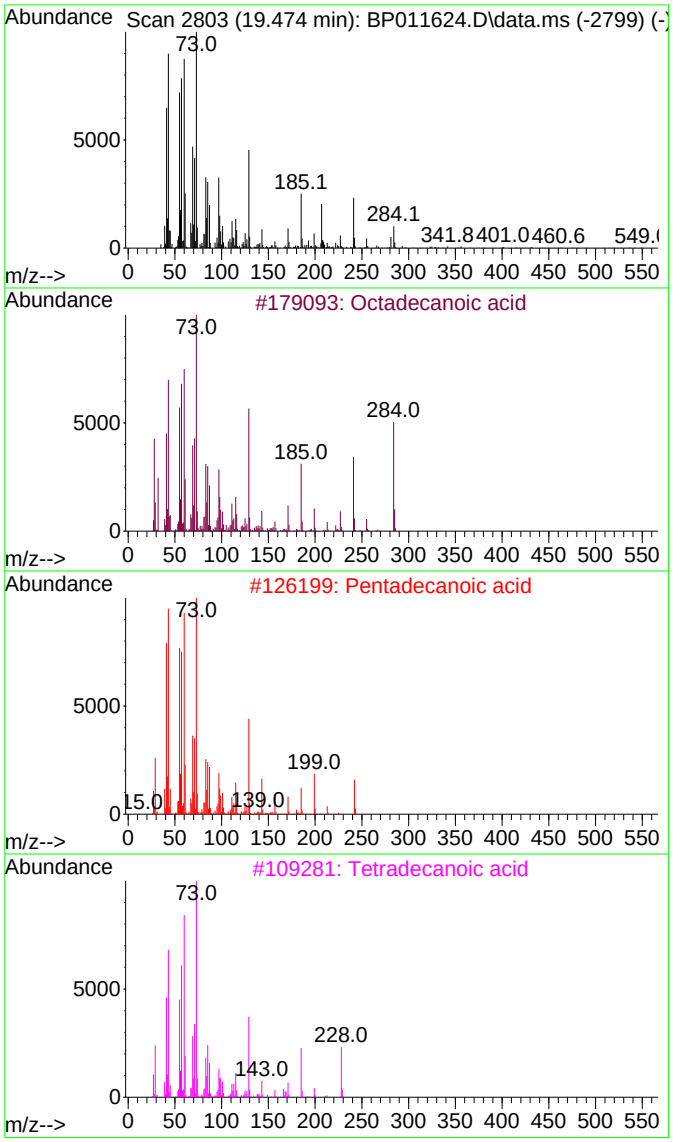
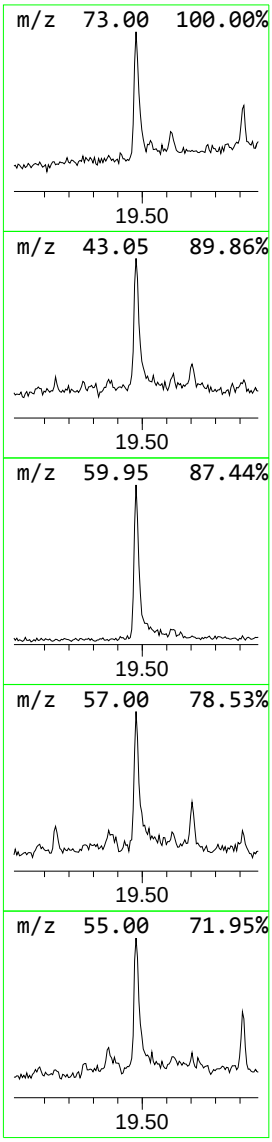
Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.474	2.27 ng	285535	Chrysene-d12	21.439

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	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090622\
Data File : BP011624.D
Acq On : 06 Sep 2022 14:21
Operator : CG/JU
Sample : N4446-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EQUIP-BLANK

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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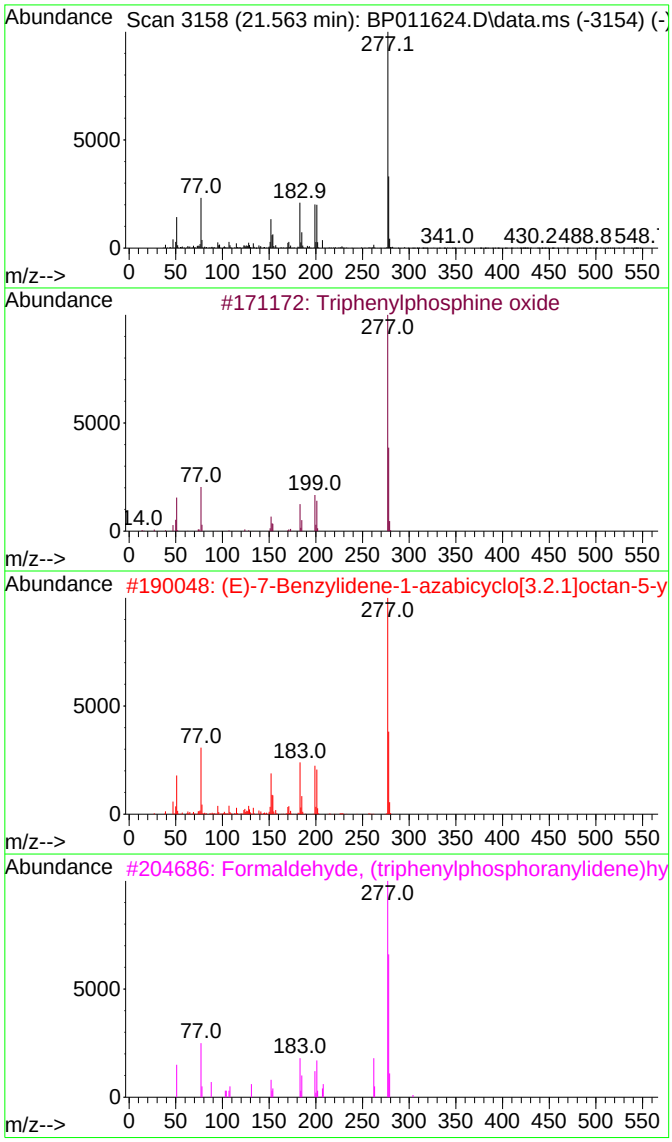
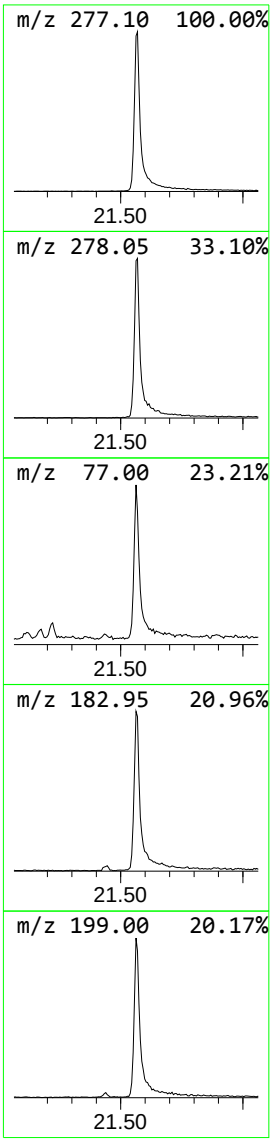
Peak Number 10 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.563	9.09 ng	1144090	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	81
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
4	5-quinolinol, 8-[2-(3,5-dimethyl...	277	C17H15N3O	1000397-10-2	32
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	23





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090622\
Data File : BP011624.D
Acq On : 06 Sep 2022 14:21
Operator : CG/JU
Sample : N4446-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EQUIP-BLANK

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...	3.099	130.9	ng	2444090	1	7.969	373510	20.0
Crotonic acid	4.516	14.9	ng	277388	1	7.969	373510	20.0
2-Pentanone, 4-...	5.058	10.3	ng	192972	1	7.969	373510	20.0
Cyclohexasiloxa...	12.081	15.1	ng	453770	2	10.787	601313	20.0
Phenol, 2,4-dib...	13.034	6.5	ng	302456	3	14.610	929825	20.0
Cycloheptasilox...	14.051	7.9	ng	366982	3	14.610	929825	20.0
n-Hexadecanoic ...	18.245	4.8	ng	333456	4	17.363	1405510	20.0
Octadecanoic acid	19.474	2.3	ng	285535	5	21.439	2516450	20.0
Triphenylphosph...	21.563	9.1	ng	1144090	5	21.439	2516450	20.0