LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004828.D
Acq On : 19 Feb 2021 18:30
Operator : CG/JU
Sample : M1441-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SP-234-A

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-BP020521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.358	361	369	382	rBV	785479	1142969	46.91%	9.004%
2	6.940	629	638	653	rBV	722533	1163265	47.74%	9.164%
3	7.758	769	777	784	rBV	195519	301587	12.38%	2.376%
4	8.916	967	974	986	rBV	429321	719874	29.54%	5.671%
5	10.551	1244	1252	1260	rBV	229224	385808	15.83%	3.039%
6	12.234	1526	1538	1550	rBV3	22125	74713	3.07%	0.589%
7	13.028	1665	1673	1680	rBV	1038678	1533716	62.95%	12.083%
8	13.869	1810	1816	1824	rBV	33741	50701	2.08%	0.399%
9	14.410	1899	1908	1917	rBV	316017	482627	19.81%	3.802%
10	15.904	2155	2162	2172	rBV	809723	1142363	46.88%	9.000%
11	17.163	2369	2376	2381	rBV	393866	571772	23.47%	4.504%
12	17.204	2381	2383	2388	rVB	39784	50024	2.05%	0.394%
13	18.057	2521	2528	2538	rBV3	49274	95929	3.94%	0.756%
14	19.180	2713	2719	2724	rBV	127882	174913	7.18%	1.378%
15	19.527	2774	2778	2783	rVB	110217	152311	6.25%	1.200%
16	19.727	2806	2812	2823	rBV	1969871	2436597	100.00%	19.196%
17	20.692	2972	2976	2980	rBV	128670	141909	5.82%	1.118%
18	20.963	3018	3022	3030	rVB3	98692	142271	5.84%	1.121%
19	21.251	3065	3071	3075	rBV	627316	879834	36.11%	6.931%
20	21.386	3090	3094	3100	rVB6	79733	112400	4.61%	0.885%
21	22.445	3271	3274	3279	rVB	67446	92612	3.80%	0.730%
22	22.710	3316	3319	3326	rVB3	108920	161762	6.64%	1.274%
23	23.557	3457	3463	3469	rVB2	356708	683517	28.05%	5.385%

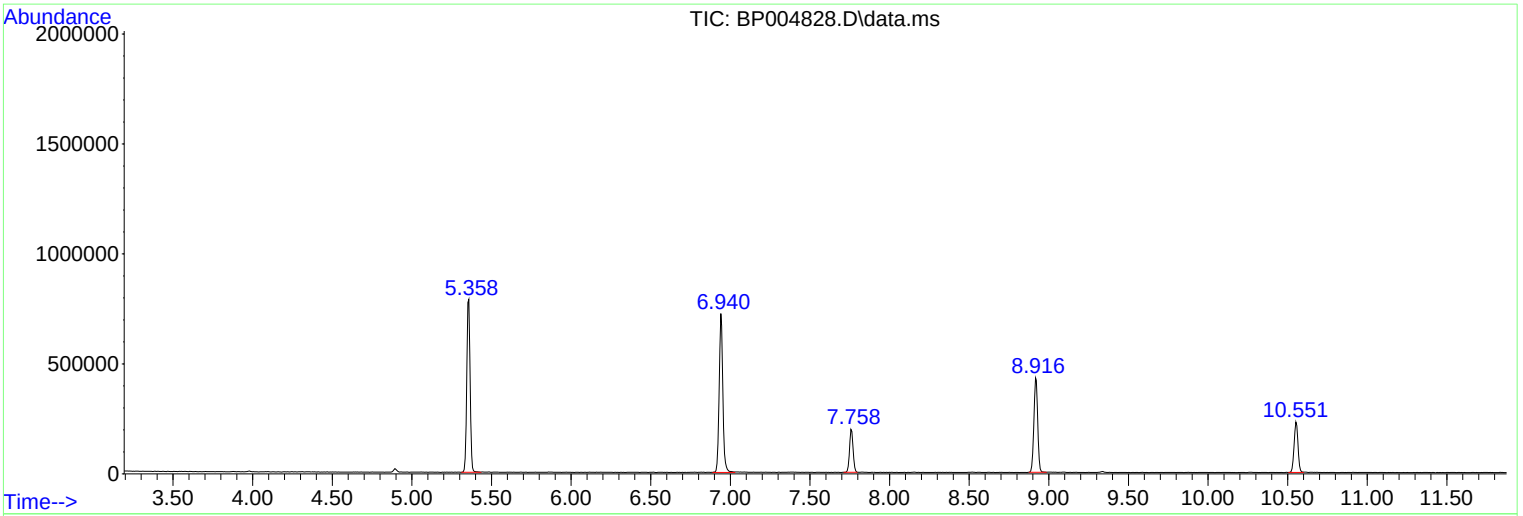
Sum of corrected areas: 12693474

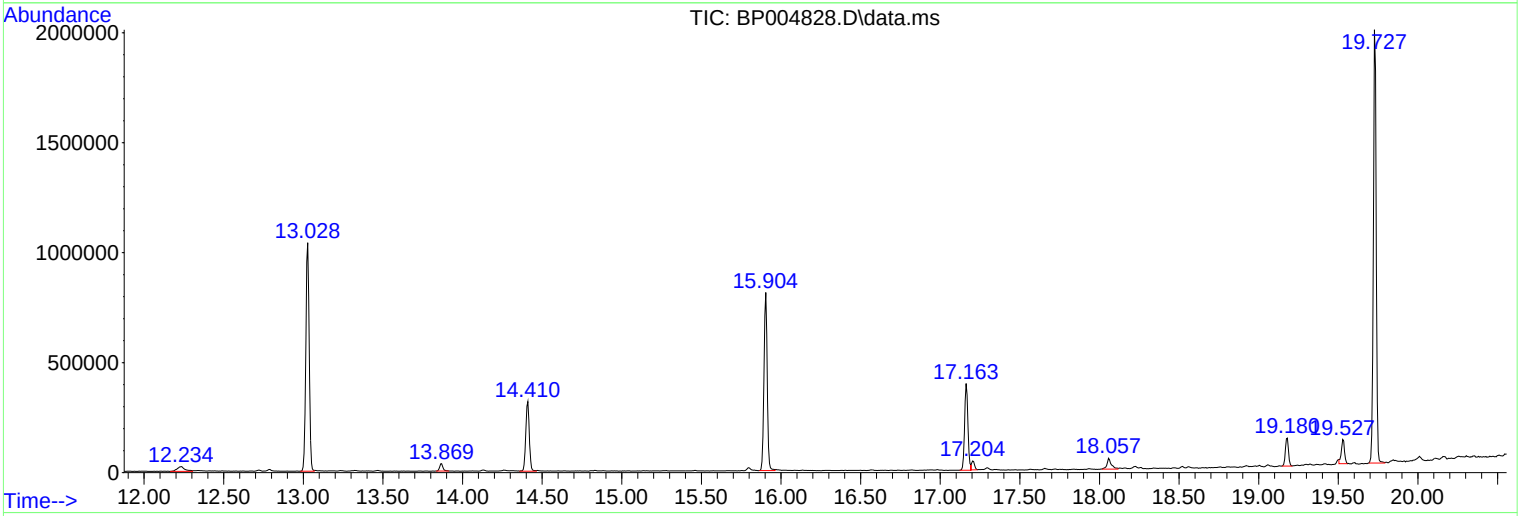
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004828.D
Acq On : 19 Feb 2021 18:30
Operator : CG/JU
Sample : M1441-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

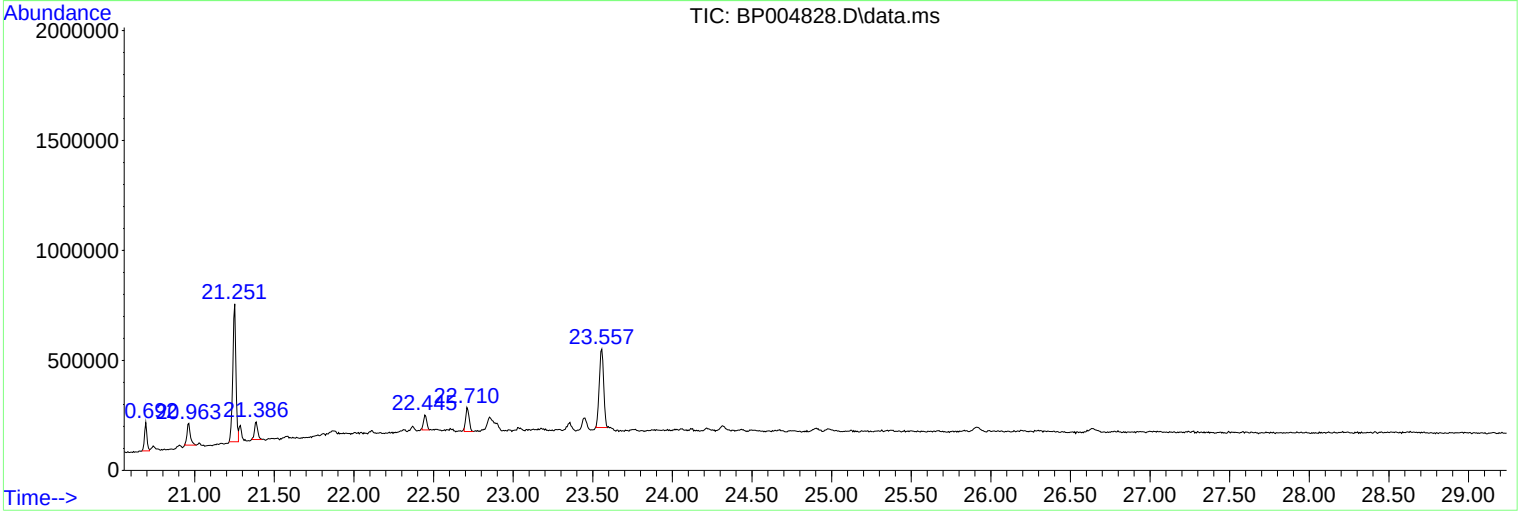
Instrument :
BNA_P
ClientSampleId :
SP-234-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Data File : BP004828.D
Acq On : 19 Feb 2021 18:30
Operator : CG/JU
Sample : M1441-01
Misc :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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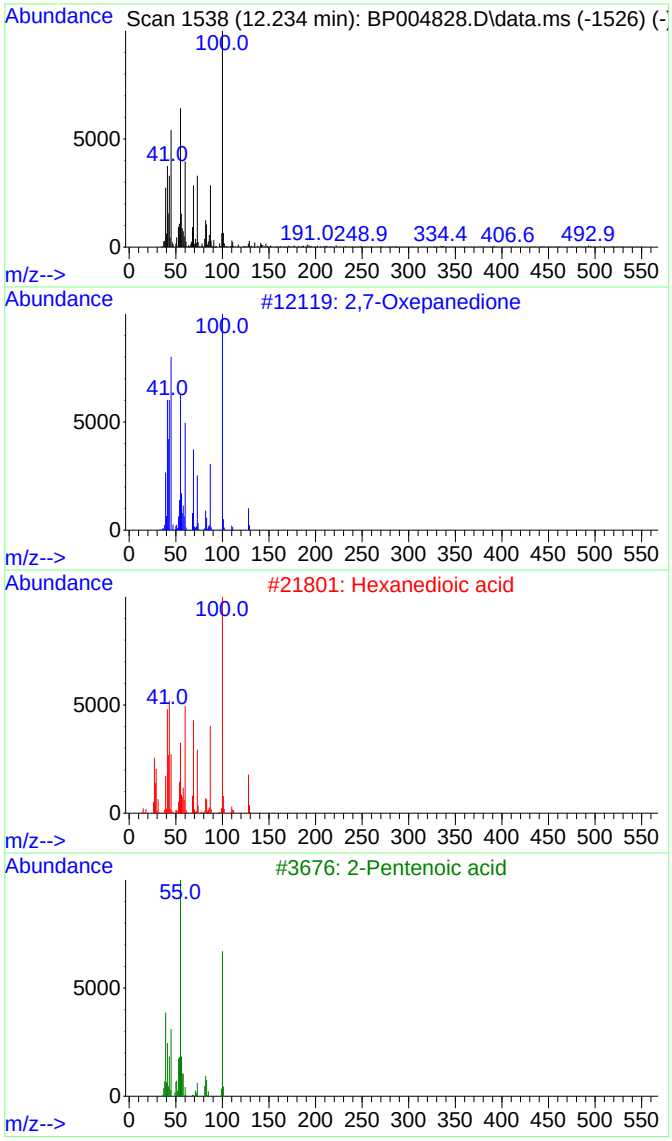
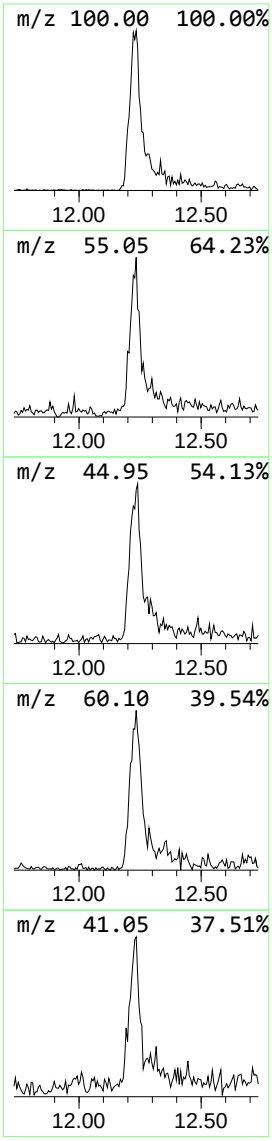
Peak Number 1 2,7-Oxepanedione Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.234	3.87 ng	74713	Naphthalene-d8	10.552

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,7-Oxepanedione	128	C6H8O3	002035-75-8	52
2	Hexanedioic acid	146	C6H10O4	000124-04-9	43
3	2-Pentenoic acid	100	C5H8O2	000626-98-2	41
4	1-Morpholinopropan-2-ol, tert-bu...	259	C13H29NO2Si	1000373-40-9	35
5	2-Butenoic acid, 2-methyl-	100	C5H8O2	013201-46-2	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004828.D
Acq On : 19 Feb 2021 18:30
Operator : CG/JU
Sample : M1441-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SP-234-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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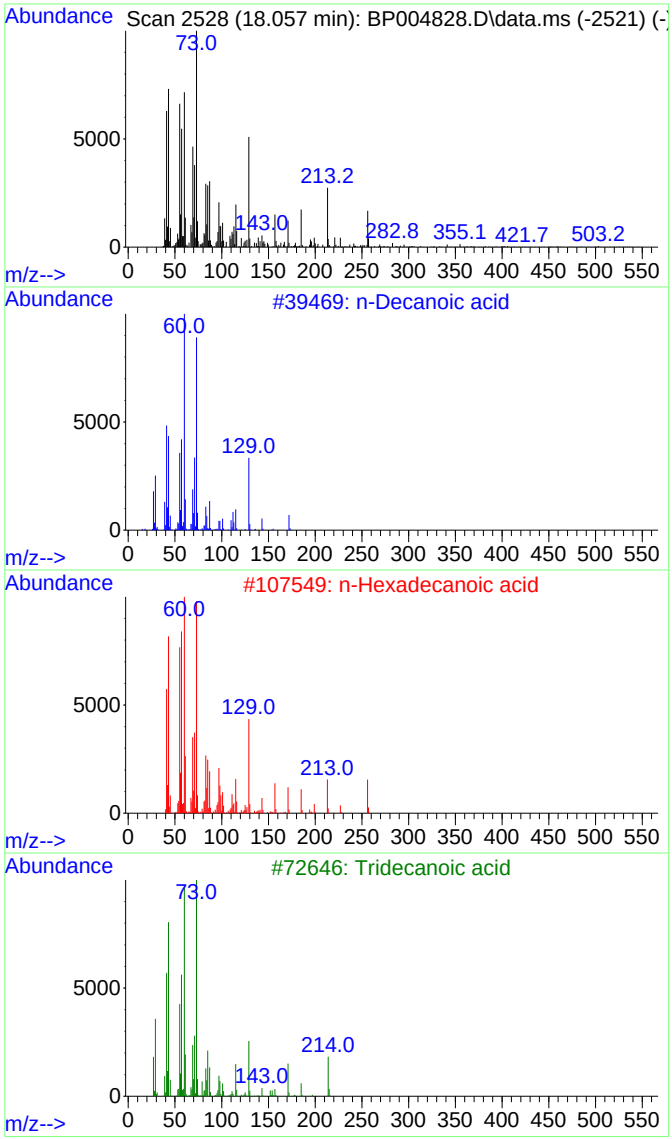
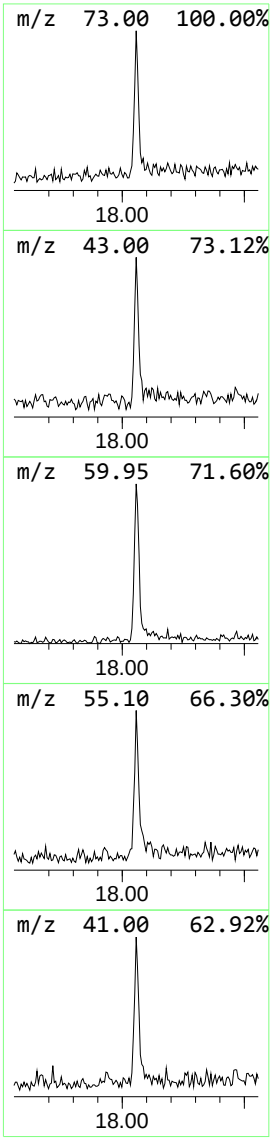
Peak Number 2 n-Decanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.057	3.36 ng	95929	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	60
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
3	Tridecanoic acid	214	C13H26O2	000638-53-9	38
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	38
5	Adipic acid, butyl hexyl ester	286	C16H30O4	1000324-10-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004828.D
Acq On : 19 Feb 2021 18:30
Operator : CG/JU
Sample : M1441-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-234-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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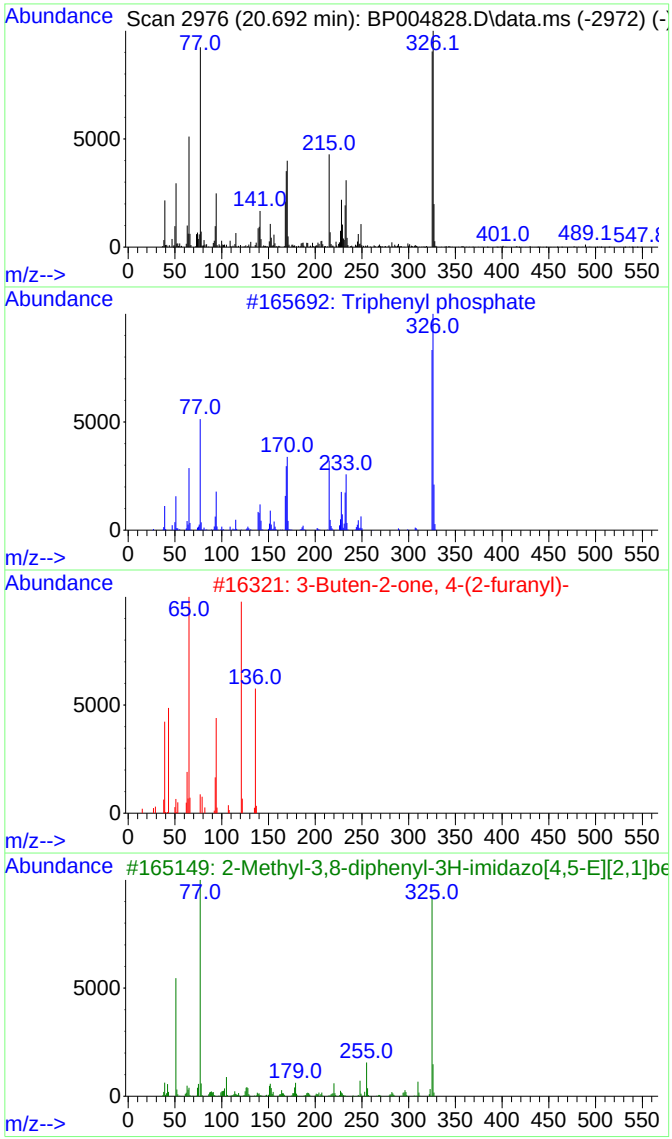
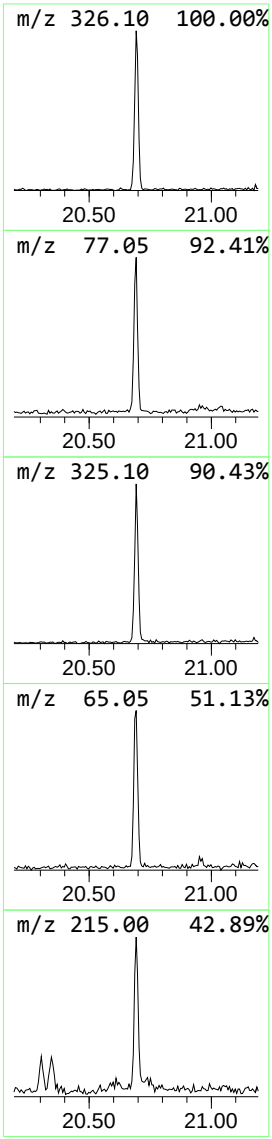
Peak Number 3 Triphenyl phosphate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.692	3.23 ng	141909	Chrysene-d12	21.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenyl phosphate	326	C18H15O4P	000115-86-6	99
2	3-Buten-2-one, 4-(2-furanyl)-	136	C8H8O2	000623-15-4	14
3	2-Methyl-3,8-diphenyl-3H-imidazo...	325	C21H15N3O	089174-96-9	14
4	Dichloroacetic acid, pent-2-en-4...	192	C7H6Cl2O2	1000299-43-1	14
5	trans-6-Carboxy-2-(p-chlorostyry...	326	C18H11ClO4	076808-23-6	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004828.D
Acq On : 19 Feb 2021 18:30
Operator : CG/JU
Sample : M1441-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SP-234-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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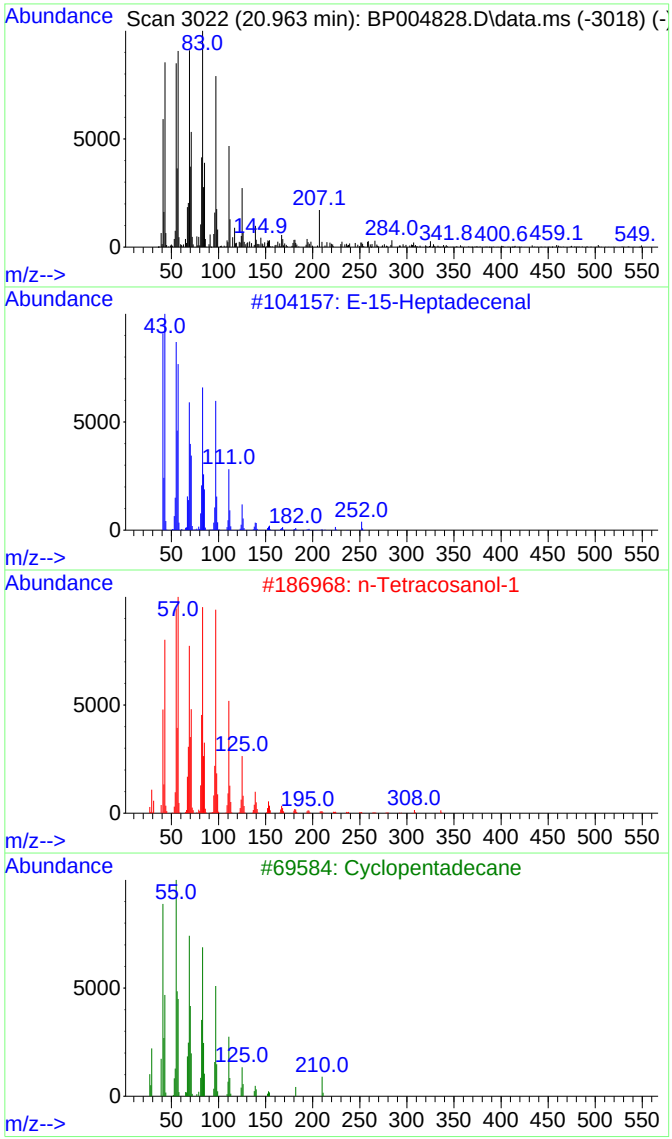
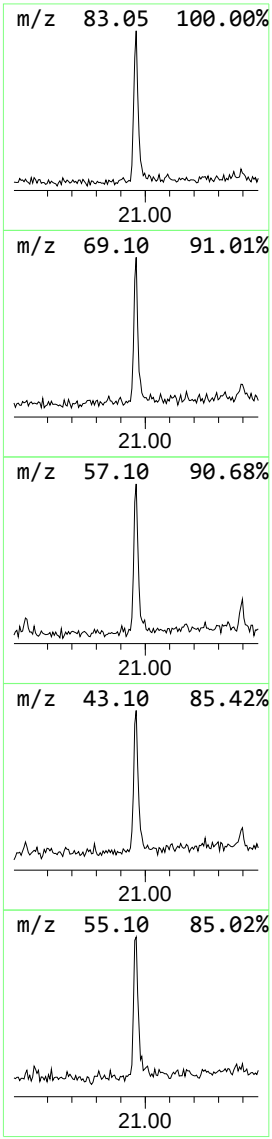
Peak Number 4 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.963	3.23 ng	142271	Chrysene-d12	21.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	97
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Cyclopentadecane	210	C15H30	000295-48-7	90
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004828.D
Acq On : 19 Feb 2021 18:30
Operator : CG/JU
Sample : M1441-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-234-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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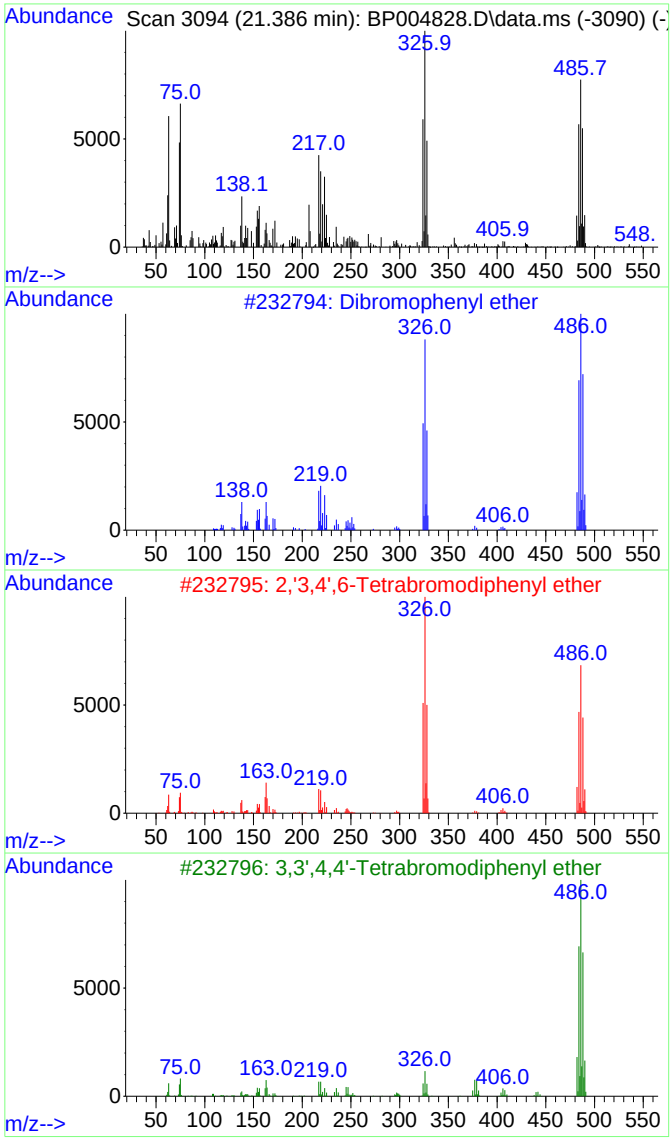
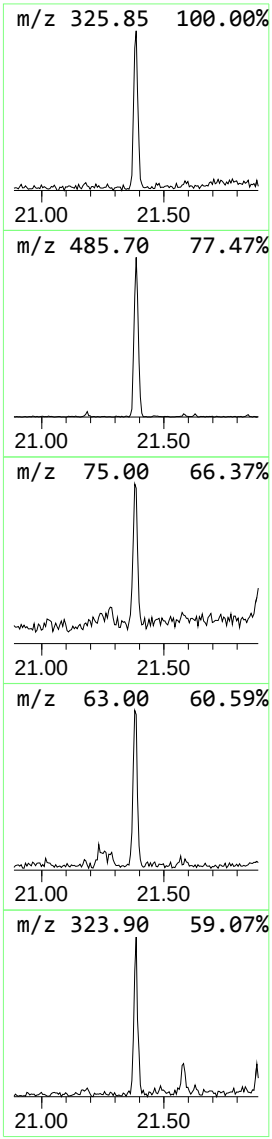
Peak Number 5 Dibromophenyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.386	2.56 ng	112400	Chrysene-d12	21.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibromophenyl ether	482	C12H6Br4O	005436-43-1	99
2	2,'3,4',6-Tetrabromodiphenyl ether	482	C12H6Br4O	189084-62-6	95
3	3,3',4,4'-Tetrabromodiphenyl ether	482	C12H6Br4O	093703-48-1	49
4	2,3,3',4',5-Pentachloro-1,1'-bip...	324	C12H5Cl5	070424-68-9	41
5	2,3,3,',5',6-Pentachloro-1,1'-bi...	324	C12H5Cl5	068194-10-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004828.D
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Operator : CG/JU
Sample : M1441-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-234-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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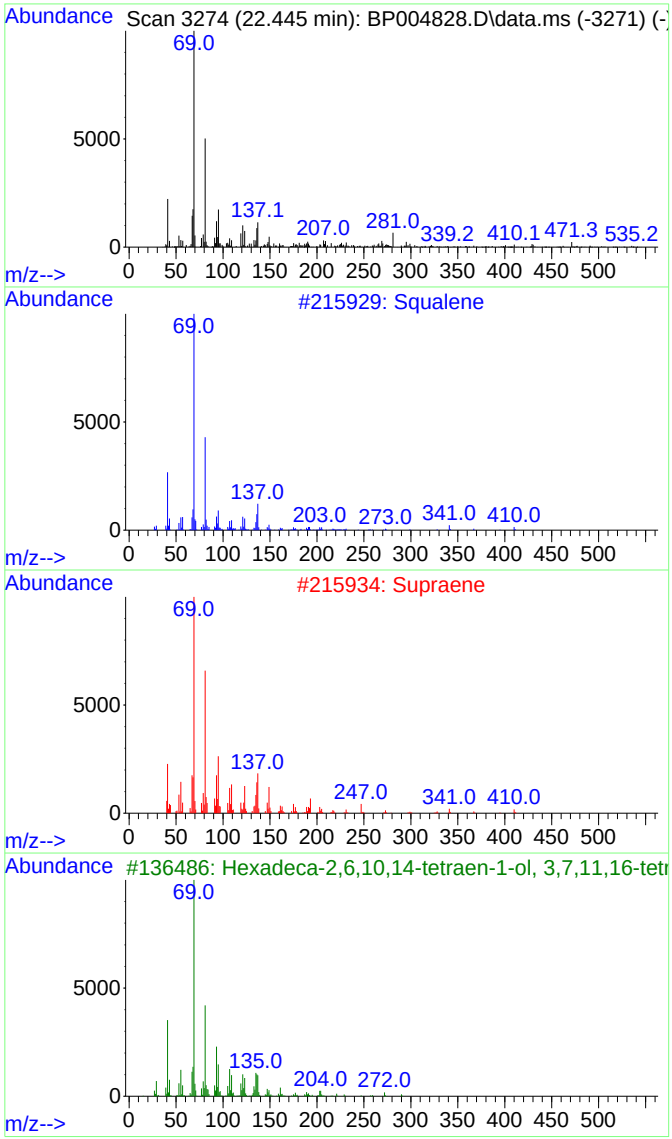
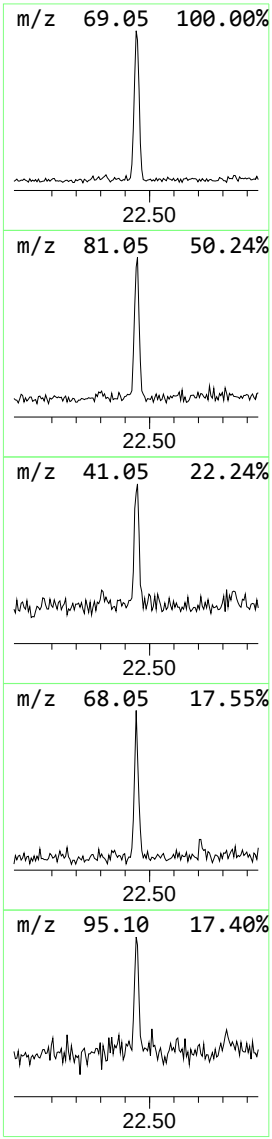
Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.445	2.71 ng	92612	Perylene-d12	23.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	81
2	Supraene	410	C30H50	007683-64-9	74
3	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	72
4	trans-Geranylgeraniol	290	C20H34O	024034-73-9	72
5	(3,7-Dimethylocta-2,6-dienylthio...	246	C16H22S	1000190-11-8	64





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Operator : CG/JU
Sample : M1441-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-234-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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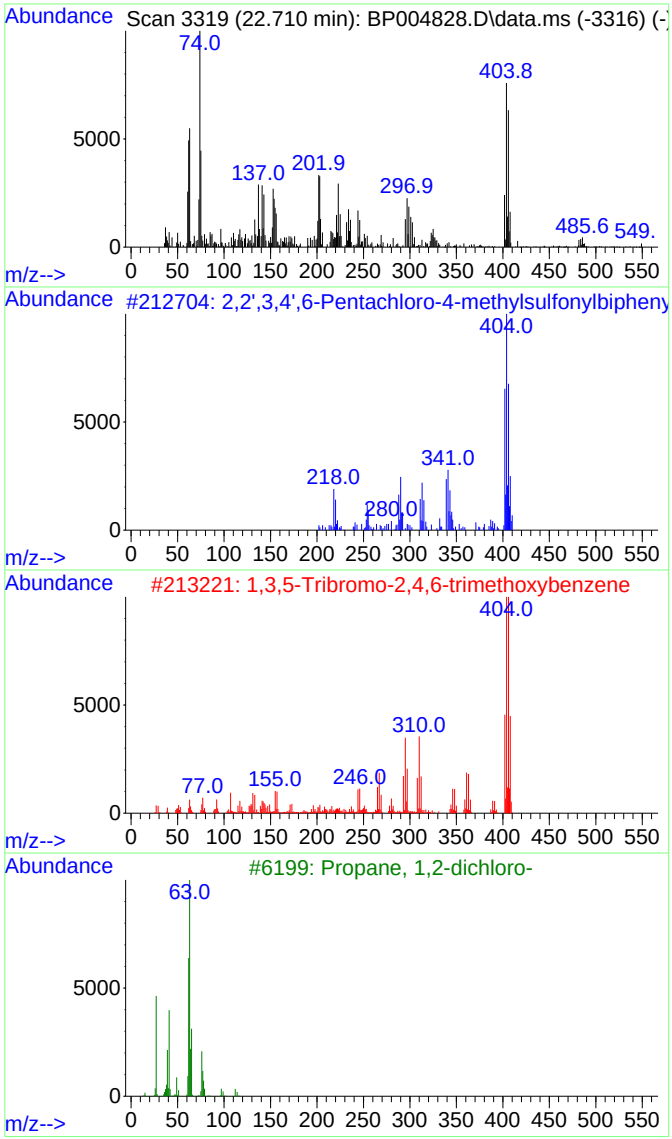
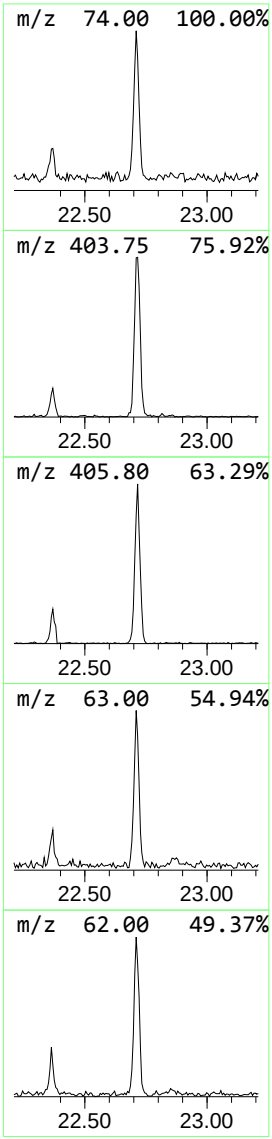
Peak Number 7 unknown22.710 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.710	4.73 ng	161762	Perylene-d12	23.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2',3,4',6-Pentachloro-4-methyl...	402	C13H7Cl5O2S	149949-87-1	45
2	1,3,5-Tribromo-2,4,6-trimethoxyb...	402	C9H9Br3O3	105404-90-8	25
3	Propane, 1,2-dichloro-	112	C3H6Cl2	000078-87-5	20
4	Thiocyanic acid, 2,4-dinitrophen...	225	C7H3N3O4S	001594-56-5	17
5	1,3-Bis(2-chloroethyl)-1,3-bis(t...	376	C9H8Cl2F6N2O3	1000144-02-5	12





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2,7-Oxepanedione	12.234	3.9	ng	74713	2	10.552	385808	20.0
n-Decanoic acid	18.057	3.4	ng	95929	4	17.163	571772	20.0
Triphenyl phosp...	20.692	3.2	ng	141909	5	21.251	879834	20.0
E-15-Heptadecenal	20.963	3.2	ng	142271	5	21.251	879834	20.0
Dibromophenyl e...	21.386	2.6	ng	112400	5	21.251	879834	20.0
Squalene	22.445	2.7	ng	92612	6	23.557	683517	20.0
unknown22.710	22.710	4.7	ng	161762	6	23.557	683517	20.0