LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005932.D
Acq On : 15 Jun 2021 16:03
Operator : CG/JU
Sample : M2672-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(60-64)

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-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005932.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	3	5	14	rVB	128754	138982	2.81%	0.608%
2	5.505	404	411	417	rBV	1324768	1954930	39.46%	8.547%
3	5.558	417	420	433	rVB	49292	106274	2.15%	0.465%
4	7.105	676	683	701	rBV	1183550	1939904	39.16%	8.482%
5	7.934	817	824	832	rBV	269894	420767	8.49%	1.840%
6	9.099	1015	1022	1032	rBV	737194	1209832	24.42%	5.290%
7	10.534	1259	1266	1276	rBV2	20869	52382	1.06%	0.229%
8	10.740	1291	1301	1314	rBV	320020	551734	11.14%	2.412%
9	13.193	1709	1718	1734	rBV	1964203	2934490	59.24%	12.830%
10	14.428	1919	1928	1931	rBV4	25937	62591	1.26%	0.274%
11	14.563	1944	1951	1961	rBV	500935	739216	14.92%	3.232%
12	15.969	2185	2190	2195	rBV	70060	89201	1.80%	0.390%
13	16.051	2197	2204	2221	rBV	1792064	2812386	56.77%	12.296%
14	17.304	2411	2417	2427	rBV	620899	911373	18.40%	3.985%
15	17.428	2433	2438	2446	rVB3	69270	97880	1.98%	0.428%
16	17.963	2524	2529	2537	rVB4	30558	51860	1.05%	0.227%
17	18.186	2563	2567	2577	rBV2	95552	149718	3.02%	0.655%
18	19.416	2772	2776	2786	rBV	65680	97863	1.98%	0.428%
19	19.851	2845	2850	2861	rVB	3933739	4953625	100.00%	21.658%
20	20.522	2960	2964	2971	rVB	148378	173700	3.51%	0.759%
21	20.592	2973	2976	2979	rBV	100386	107329	2.17%	0.469%
22	21.080	3055	3059	3064	rBV	201326	281203	5.68%	1.229%
23	21.280	3090	3093	3099	rVB	139139	151120	3.05%	0.661%
24	21.380	3105	3110	3117	rVB	985660	1288010	26.00%	5.631%
25	22.257	3257	3259	3264	rVB3	80525	97267	1.96%	0.425%
26	23.792	3514	3520	3530	rVB2	721136	1498220	30.24%	6.550%

Sum of corrected areas: 22871857

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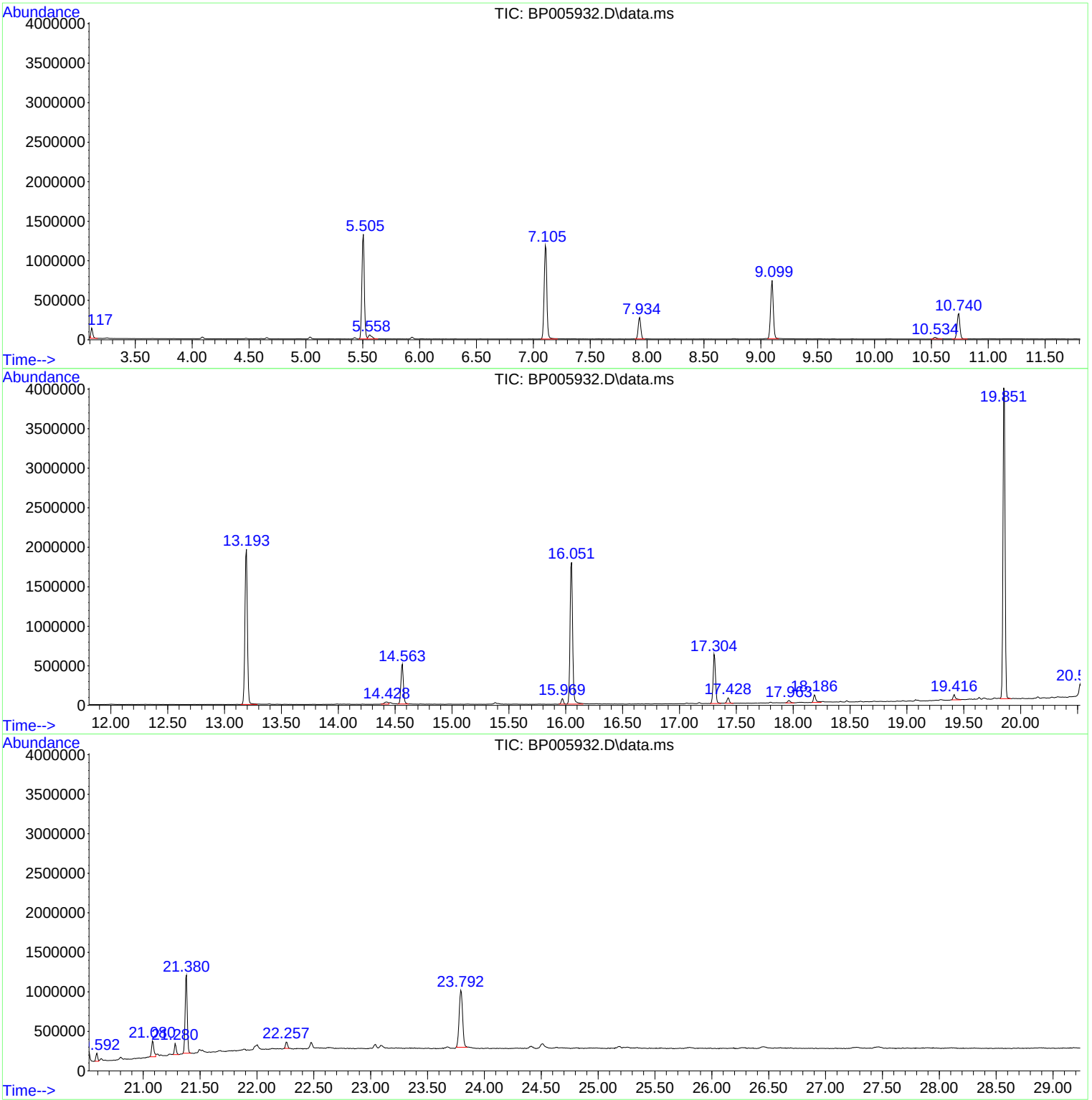
BNA_P
ClientSampleId :
17-B6(60-64)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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 : BP005932.D
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Operator : CG/JU
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
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17-B6(60-64)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

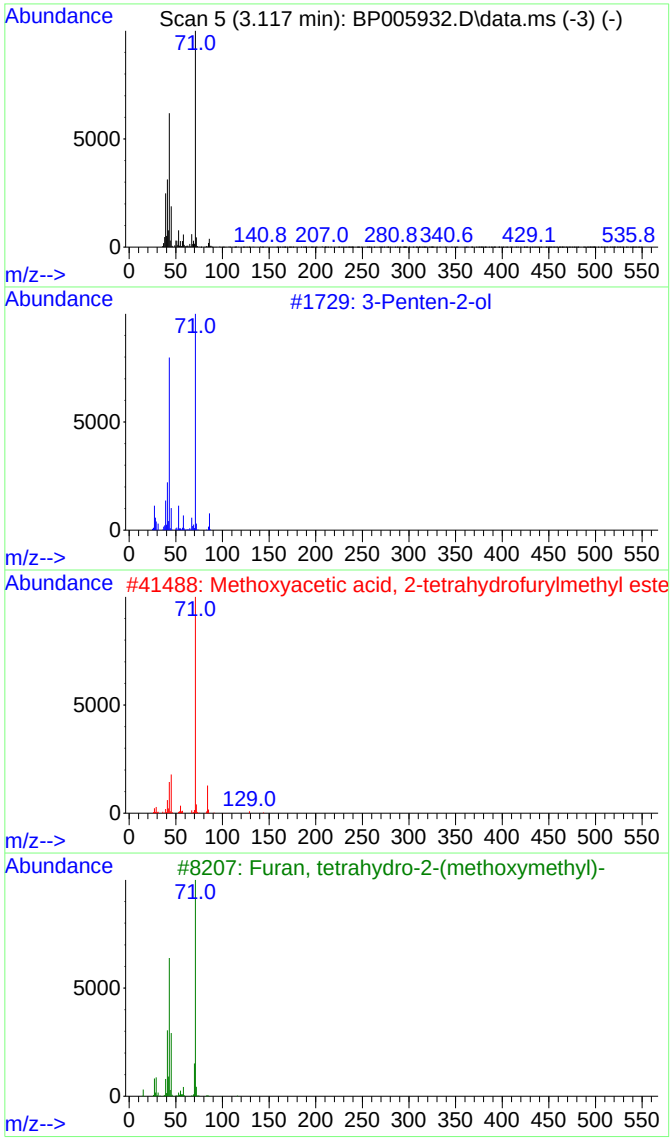
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

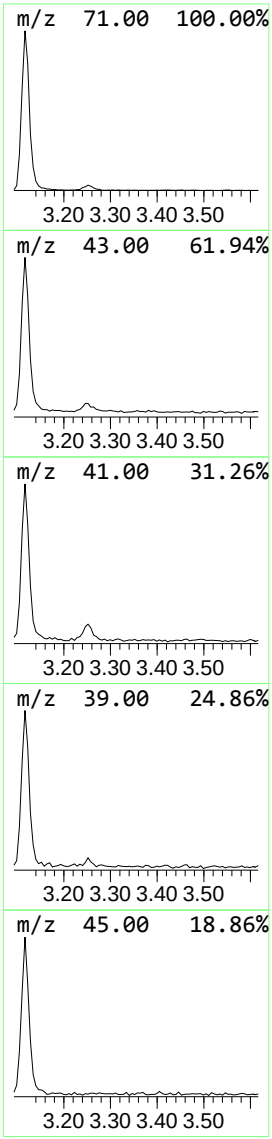
****

Peak Number 1 3-Penten-2-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.117	6.61 ng	138982	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	80
2	Methoxyacetic acid, 2-tetrahydro...	174	C8H14O4	1000282-41-3	64
3	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	59
4	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	50
5	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	50





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Data File : BP005932.D
Acq On : 15 Jun 2021 16:03
Operator : CG/JU
Sample : M2672-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(60-64)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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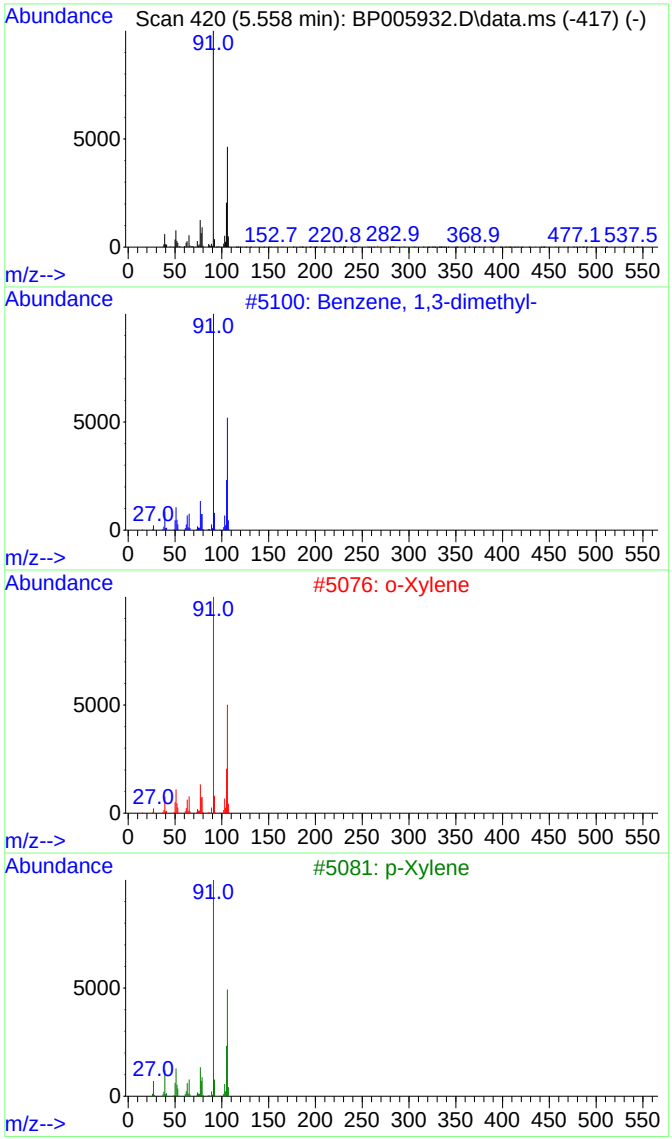
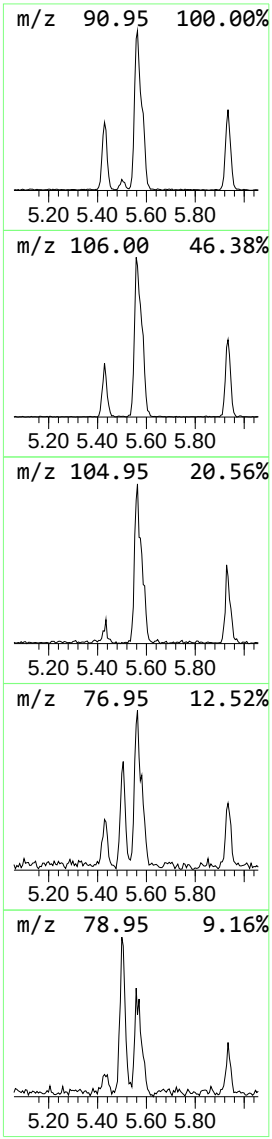
Peak Number 2 Benzene, 1,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.558	5.05 ng	106274	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	93
2	o-Xylene	106	C8H10	000095-47-6	93
3	p-Xylene	106	C8H10	000106-42-3	90
4	Benzeneethanol, .alpha.,.beta.-d...	150	C10H14O	052089-32-4	78
5	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005932.D
Acq On : 15 Jun 2021 16:03
Operator : CG/JU
Sample : M2672-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(60-64)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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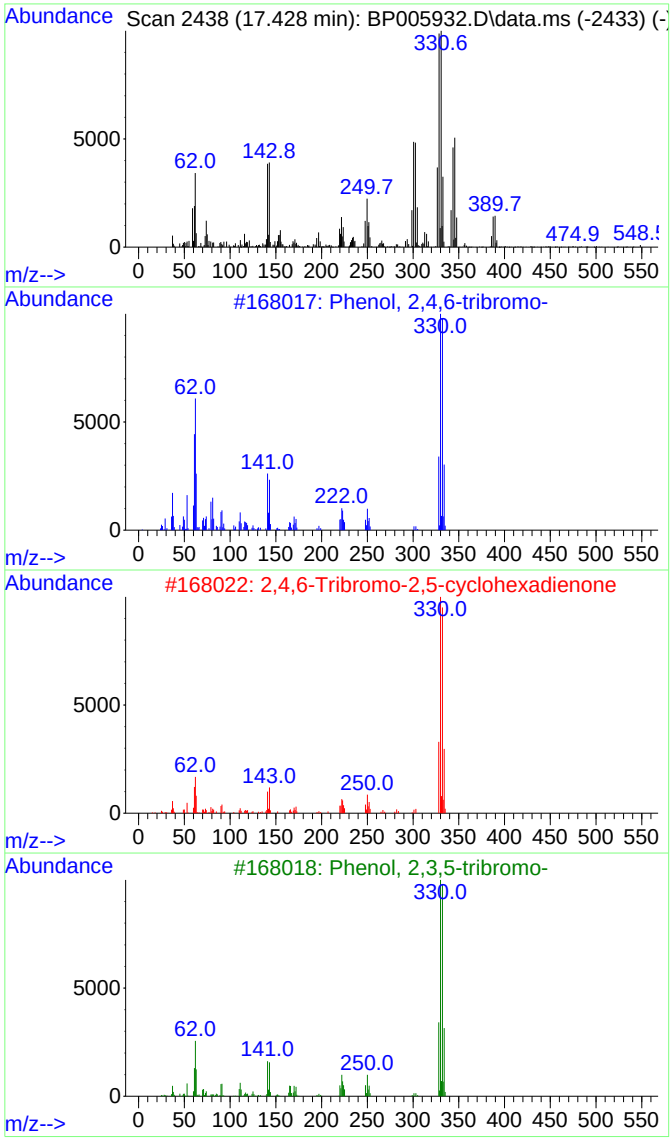
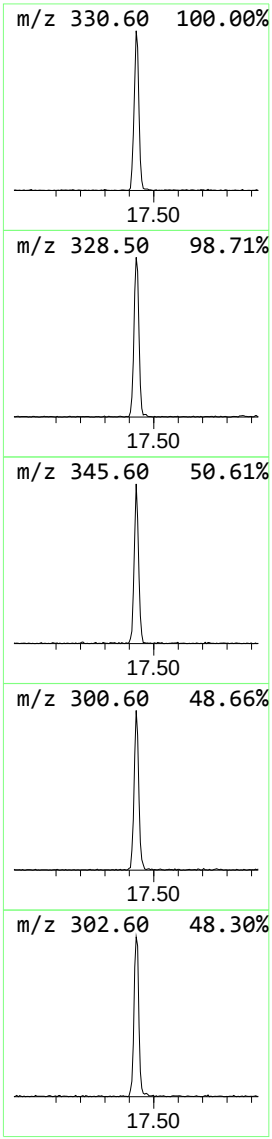
Peak Number 3 Phenol, 2,4,6-tribromo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.428	2.15 ng	97880	Phenanthrene-d10	17.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	53
2	2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	53
3	Phenol, 2,3,5-tribromo-	328	C6H3Br3O	057383-81-0	22
4	4-[p-Chlorophenoxy]-6-methoxy-8-...	330	C16H11ClN2O4	063456-77-9	14
5	Ketone, 11-bromotricyclo[8.2.2.2...	328	C18H17BrO	018931-44-7	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005932.D
Acq On : 15 Jun 2021 16:03
Operator : CG/JU
Sample : M2672-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(60-64)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
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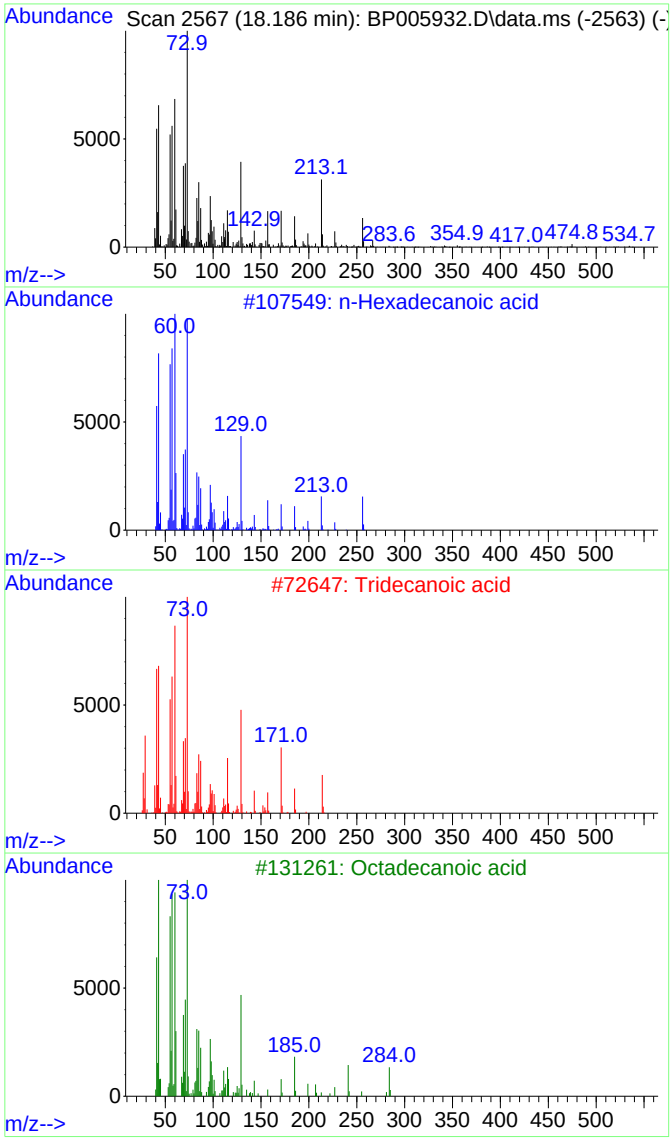
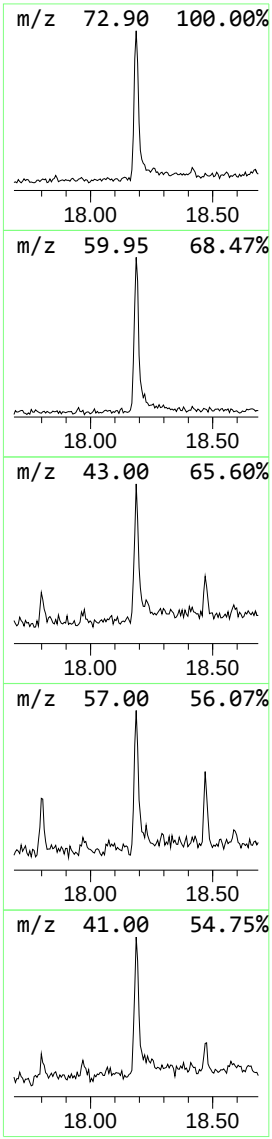
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	3.29 ng	149718	Phenanthrene-d10	17.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Octadecanoic acid	284	C18H36O2	000057-11-4	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64





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Data File : BP005932.D
Acq On : 15 Jun 2021 16:03
Operator : CG/JU
Sample : M2672-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(60-64)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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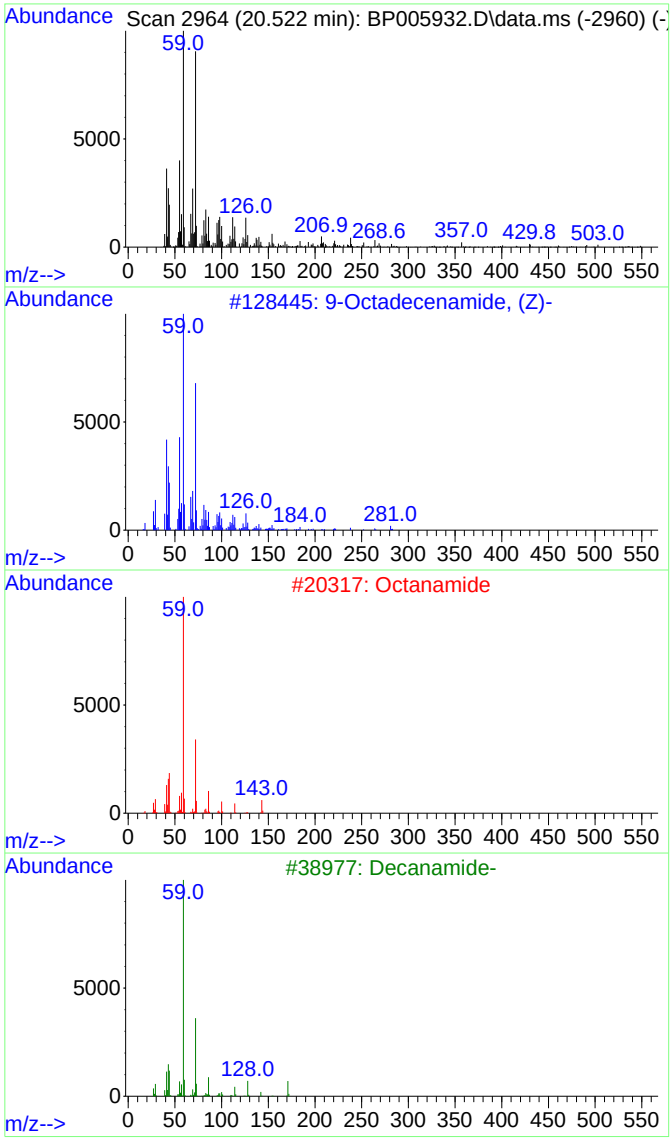
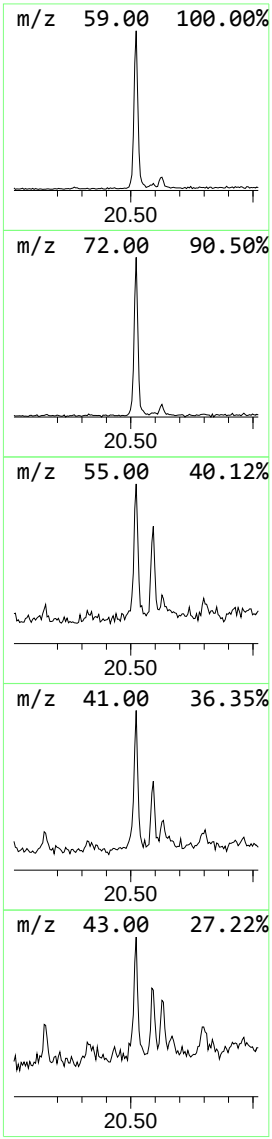
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.522	2.70 ng	173700	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	Octanamide	143	C8H17NO	000629-01-6	43
3	Decanamide-	171	C10H21NO	002319-29-1	35
4	N-tert-Butylmethylamine	87	C5H13N	014610-37-8	30
5	Butanal, 3-methyl-, oxime	101	C5H11NO	000626-90-4	30





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

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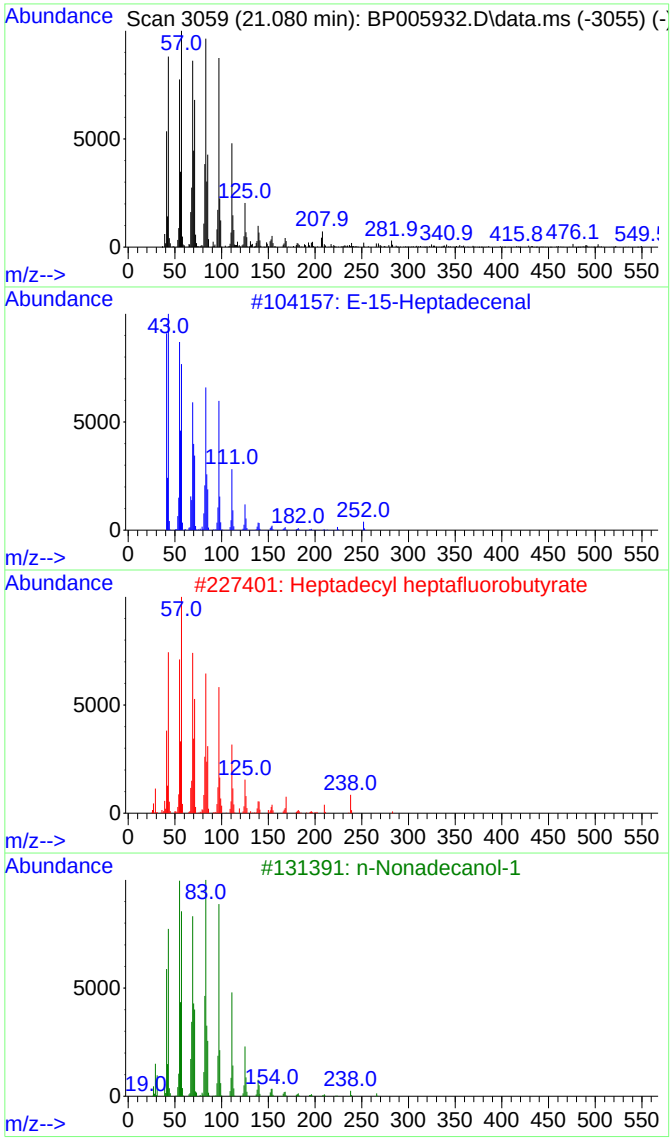
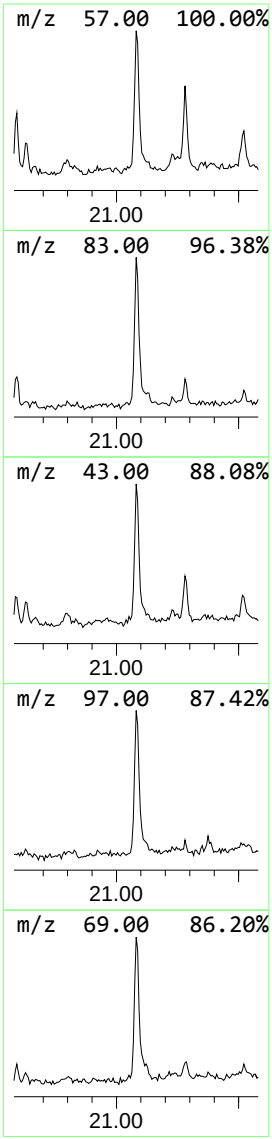
Peak Number 6 E-15-Heptadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.081	4.37 ng	281203	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





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
3-Penten-2-ol	3.117	6.6	ng	138982	1	7.934	420767	20.0
Benzene, 1,3-di...	5.558	5.0	ng	106274	1	7.934	420767	20.0
Phenol, 2,4,6-t...	17.428	2.1	ng	97880	4	17.304	911373	20.0
n-Hexadecanoic ...	18.186	3.3	ng	149718	4	17.304	911373	20.0
9-Octadecenamid...	20.522	2.7	ng	173700	5	21.380	1288010	20.0
E-15-Heptadecenal	21.081	4.4	ng	281203	5	21.380	1288010	20.0