LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007103.D
Acq On : 22 Sep 2021 18:02
Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

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-BP092121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007103.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.081	163	169	176	rBV	299734	441565	2.13%	0.336%
2	4.828	275	296	300	rBV	527404	2074727	10.01%	1.579%
3	5.211	357	361	400	rVB4	307872	1102013	5.32%	0.839%
4	5.469	400	405	413	rVB	1824577	2672624	12.89%	2.034%
5	6.322	542	550	557	rVB	133335	259549	1.25%	0.197%
6	7.063	668	676	688	rBV	1039382	1767107	8.53%	1.345%
7	7.899	812	818	829	rVB	961412	1512807	7.30%	1.151%
8	8.663	941	948	961	rBV	741697	1326706	6.40%	1.010%
9	9.057	1007	1015	1024	rBV	2579056	4263904	20.57%	3.244%
10	9.440	1053	1080	1095	rBV2	1056120	5080533	24.51%	3.866%
11	10.146	1190	1200	1210	rBV	5964416	10070240	48.59%	7.663%
12	10.481	1250	1257	1268	rBV	781948	1398332	6.75%	1.064%
13	10.698	1286	1294	1298	rBV	1258422	2133141	10.29%	1.623%
14	10.746	1298	1302	1309	rVB	895255	1491827	7.20%	1.135%
15	11.251	1377	1388	1400	rBV	327022	816515	3.94%	0.621%
16	11.934	1497	1504	1514	rBV	114787	228990	1.10%	0.174%
17	12.540	1591	1607	1621	rBV	1815539	4486094	21.64%	3.414%
18	13.151	1704	1711	1722	rVB	7078701	10608883	51.19%	8.073%
19	14.334	1906	1912	1918	rBV	224338	338336	1.63%	0.257%
20	14.528	1934	1945	1954	rBV	1971345	3198071	15.43%	2.433%
21	14.945	2007	2016	2022	rBV3	148092	300037	1.45%	0.228%
22	15.733	2144	2150	2155	rBV	331165	491583	2.37%	0.374%
23	16.016	2191	2198	2208	rBV	5555468	8010680	38.65%	6.095%
24	16.204	2224	2230	2238	rBV	1254496	1978327	9.54%	1.505%
25	16.281	2238	2243	2252	rVB2	265170	441200	2.13%	0.336%
26	16.363	2252	2257	2262	rBV	452538	601906	2.90%	0.458%
27	16.675	2306	2310	2318	rBV	183809	279512	1.35%	0.213%
28	17.275	2403	2412	2417	rBV	2266133	3369761	16.26%	2.564%
29	17.422	2433	2437	2445	rBV	119169	277830	1.34%	0.211%
30	18.045	2538	2543	2551	rBV4	94918	232204	1.12%	0.177%
31	18.175	2557	2565	2591	rBV	6066360	10450101	50.42%	7.952%
32	19.280	2745	2753	2766	rBV	956388	2883490	13.91%	2.194%
33	19.410	2768	2775	2794	rVV	11692979	20726324	100.00%	15.771%
34	19.833	2841	2847	2852	rBV	11560277	14267427	68.84%	10.856%
35	21.033	3046	3051	3054	rBV	447222	700838	3.38%	0.533%
36	21.080	3054	3059	3064	rVV2	811870	1479139	7.14%	1.126%

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007103.D
Acq On : 22 Sep 2021 18:02
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Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

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-BP092121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.133	3064	3068	3076	rVV	1779655	2214567	10.68%	1.685%
38	21.357	3101	3106	3111	rBV	2803942	3535564	17.06%	2.690%
39	23.768	3509	3516	3529	rVB2	1867233	3907250	18.85%	2.973%

Sum of corrected areas: 131419704

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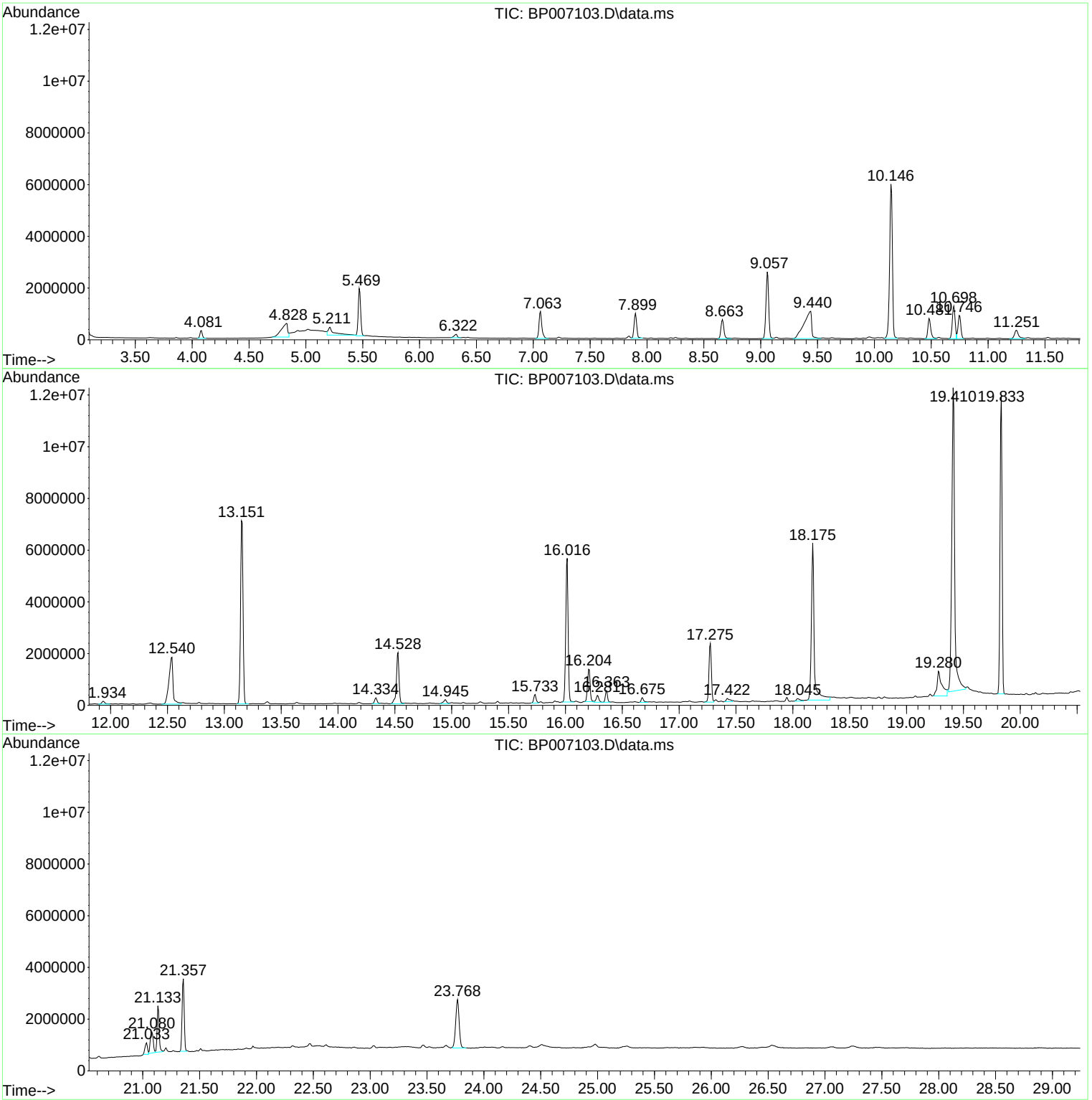
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BP007103.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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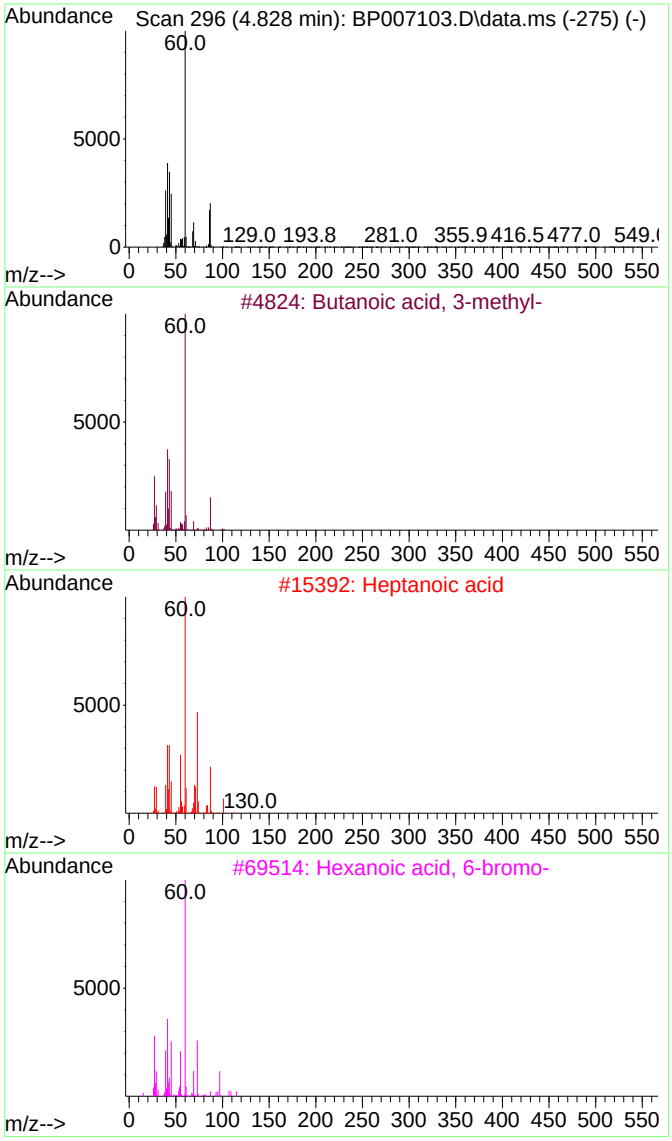
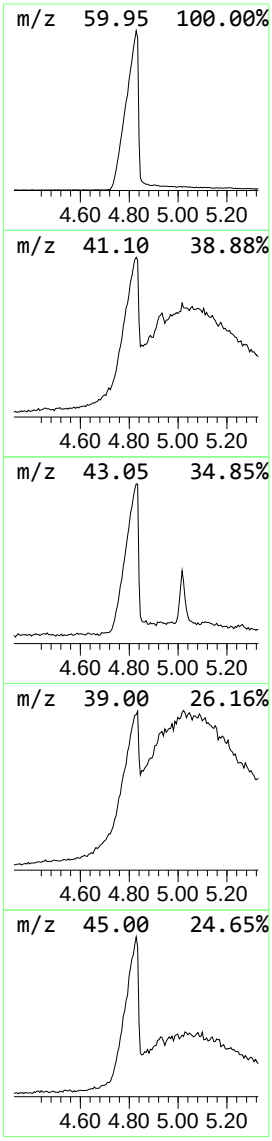
Peak Number 2 Butanoic acid, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.828	27.43 ng	2074730	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
2	Heptanoic acid	130	C7H14O2	000111-14-8	38
3	Hexanoic acid, 6-bromo-	194	C6H11BrO2	004224-70-8	38
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5	Butanoic acid	88	C4H8O2	000107-92-6	9





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Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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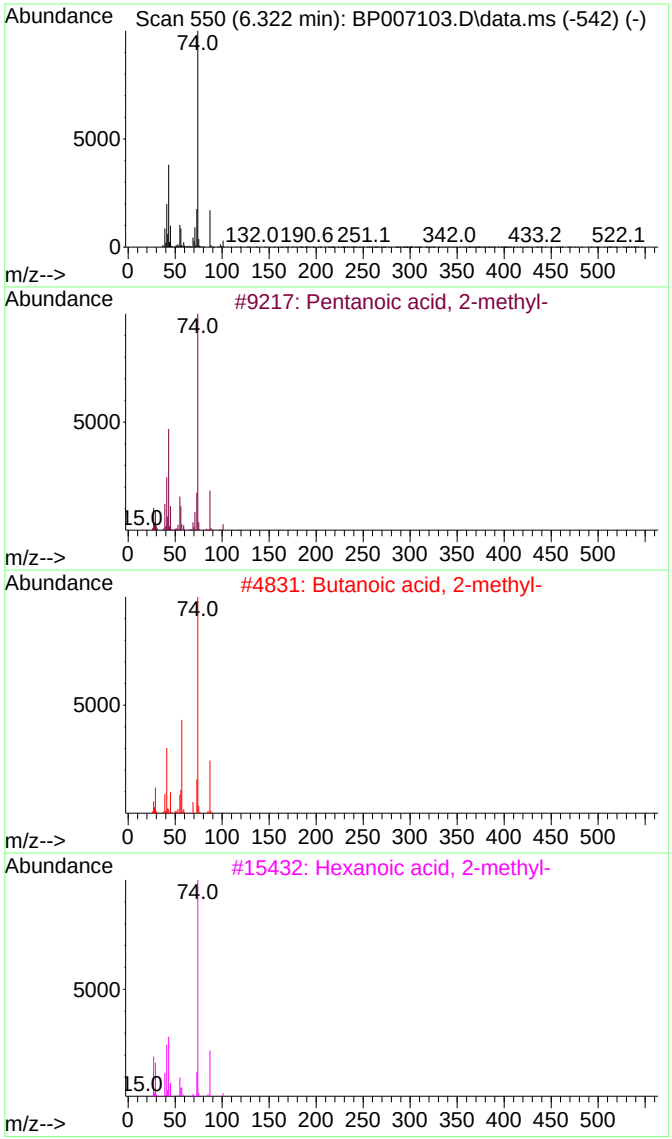
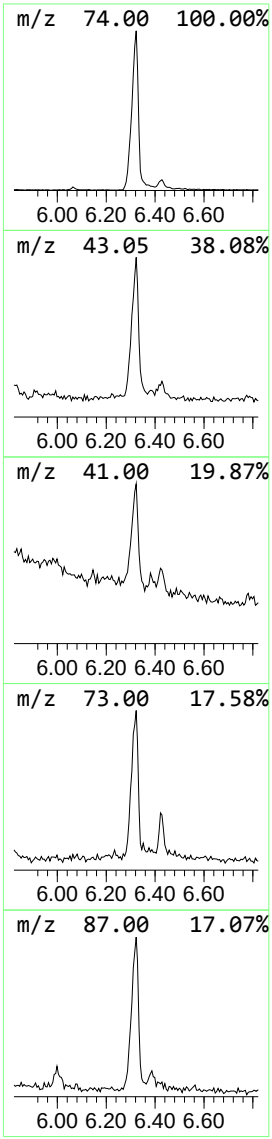
Peak Number 4 Pentanoic acid, 2-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.322	3.43 ng	259549	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	90
2	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
3	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72
4	Decanoic acid, 2-methyl-	186	C11H22O2	024323-23-7	45
5	3-(Dioxolan-2-yl)-1,1-dimethyl-2...	251	C14H21NO3	1000305-98-1	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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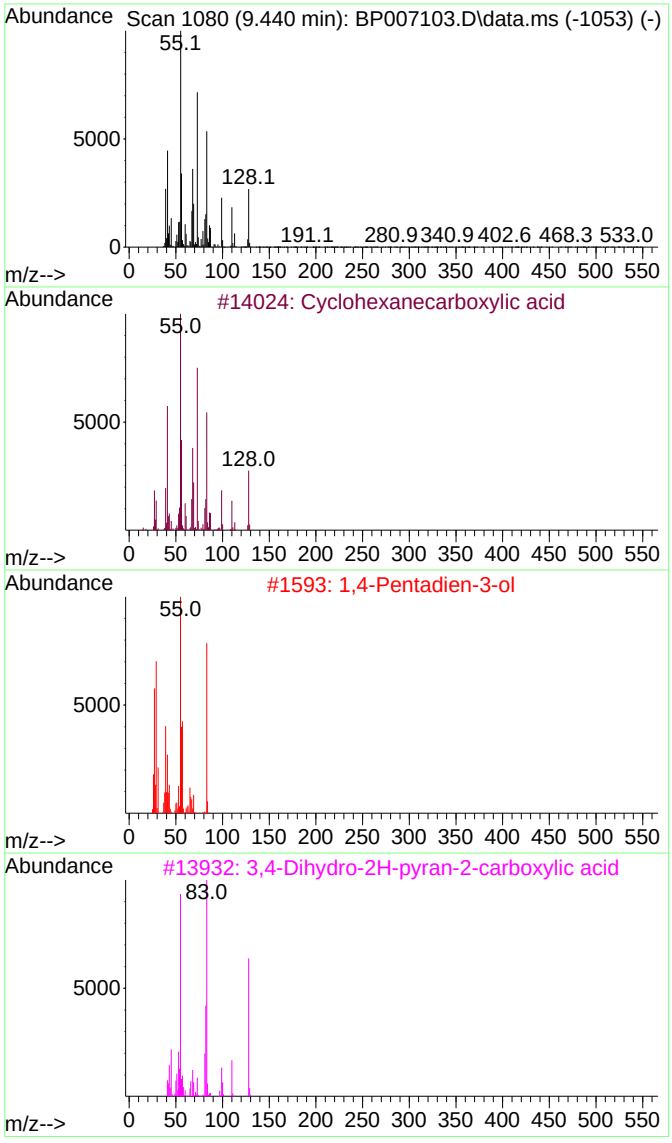
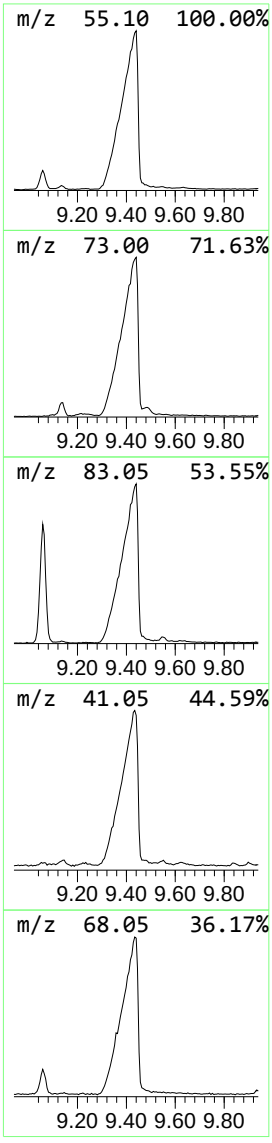
Peak Number 5 Cyclohexanecarboxylic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.440	47.63 ng	5080530	Naphthalene-d8	10.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	96
2	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	35
3	3,4-Dihydro-2H-pyran-2-carboxyli...	128	C6H8O3	1010132-10-4	25
4	Cyclohexanecarboxaldehyde	112	C7H12O	002043-61-0	25
5	Trichloroacetic acid, 6-chlorohe...	280	C8H12Cl4O2	1000330-89-2	22





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SW-RR-02-(1.0)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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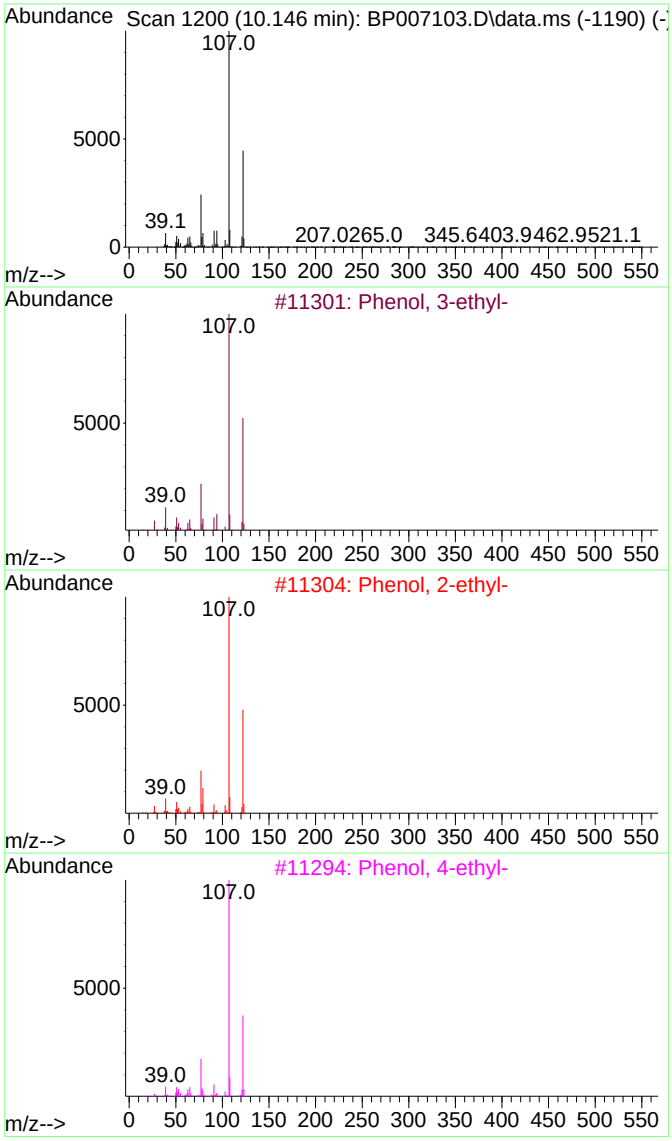
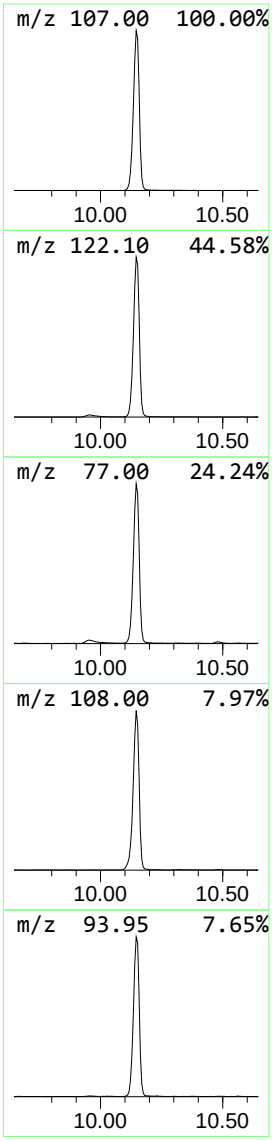
Peak Number 6 Phenol, 3-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.146	94.42 ng	10070200	Naphthalene-d8	10.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-ethyl-	122	C8H10O	000620-17-7	97
2	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	91
3	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	90
4	Phenol, 2,3-dimethyl-	122	C8H10O	000526-75-0	78
5	2-Isopropylpyrazine	122	C7H10N2	029460-90-0	59





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Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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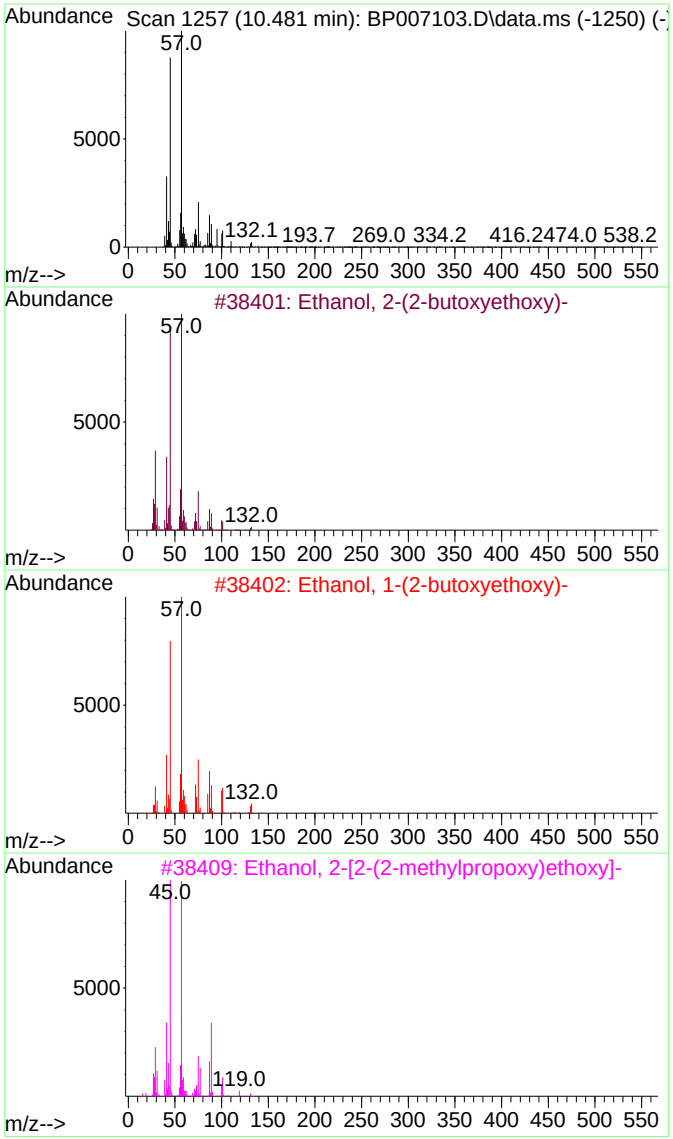
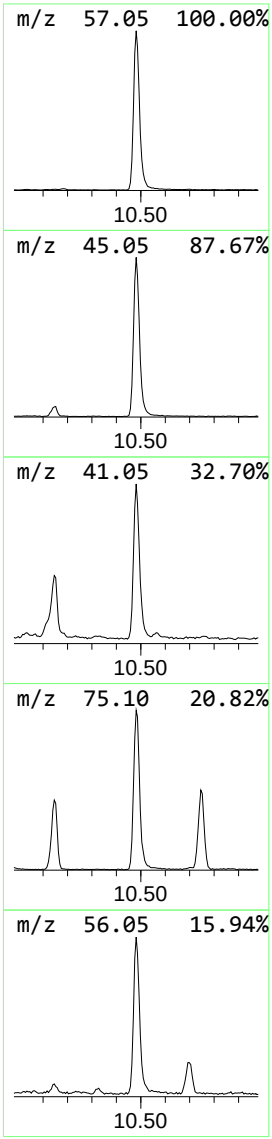
Peak Number 7 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.481	13.11 ng	1398330	Naphthalene-d8	10.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50





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SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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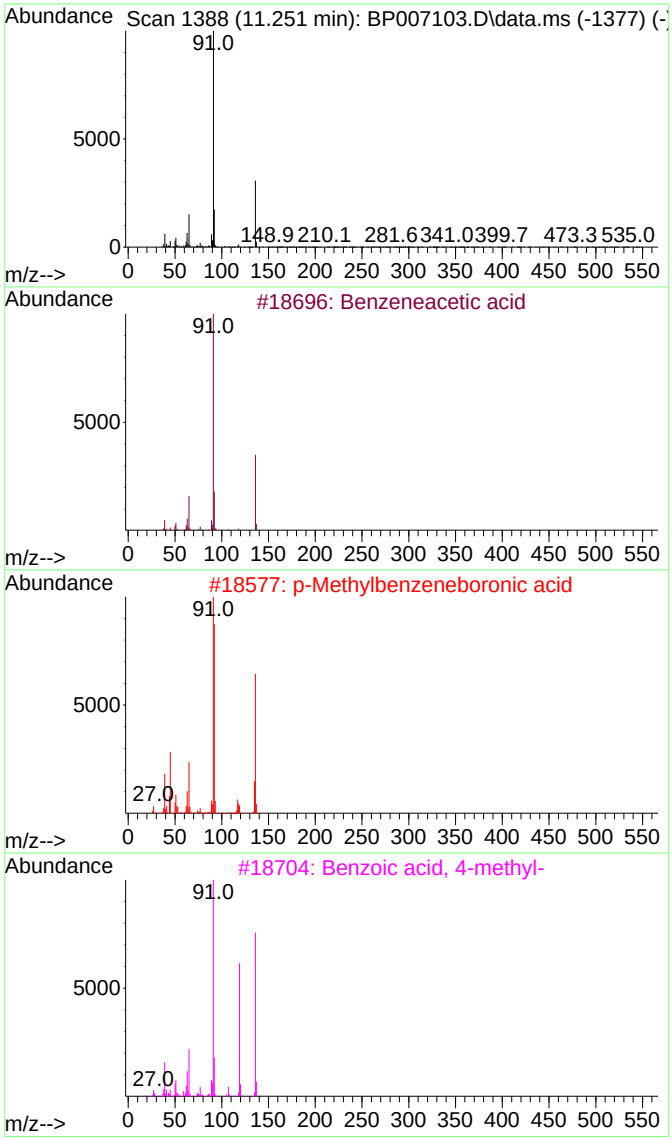
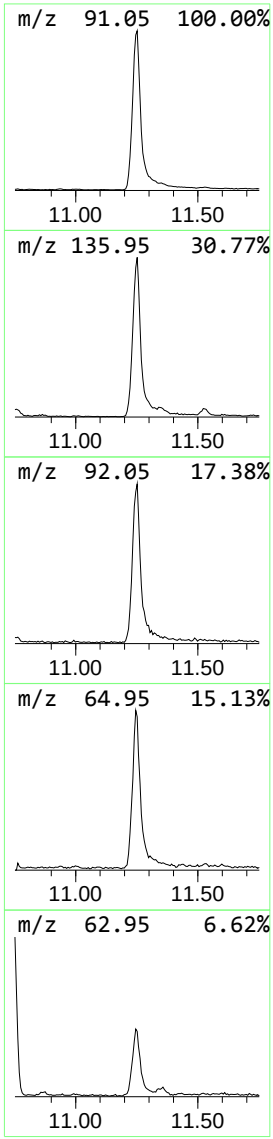
Peak Number 8 Benzeneacetic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.251	7.66 ng	816515	Naphthalene-d8	10.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	94
2	p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	64
3	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	58
4	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	53
5	Benzene, (iodomethyl)-	218	C7H7I	000620-05-3	50





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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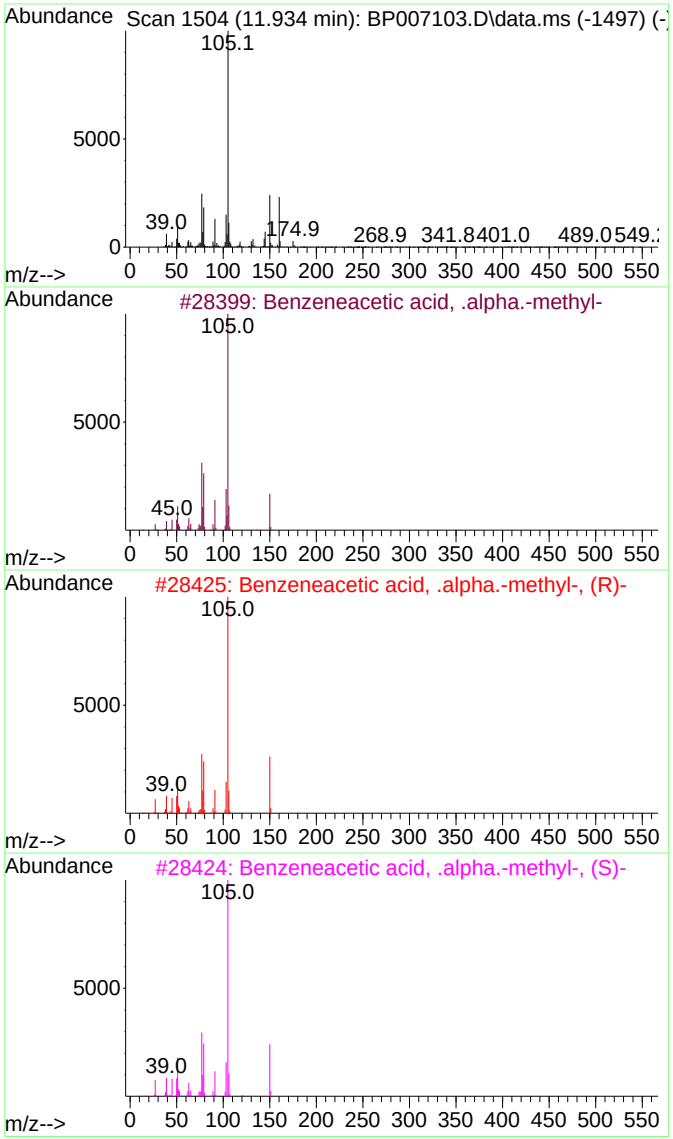
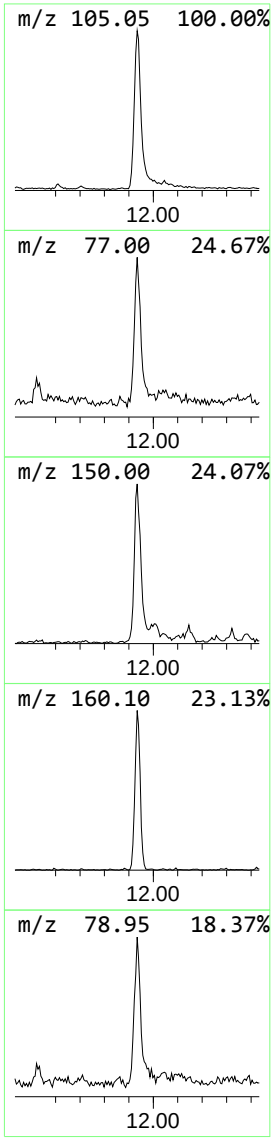
Peak Number 9 Benzeneacetic acid, .alpha.... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.934	2.15 ng	228990	Naphthalene-d8	10.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid, .alpha.-methyl-	150	C9H10O2	000492-37-5	93
2	Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-26-5	64
3	Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-24-3	64
4	p-Tolylacetic acid	150	C9H10O2	000622-47-9	58
5	Benzene, 1-methyl-4-(3-methyl-3-...	160	C12H16	056818-01-0	47





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Data File : BP007103.D
Acq On : 22 Sep 2021 18:02
Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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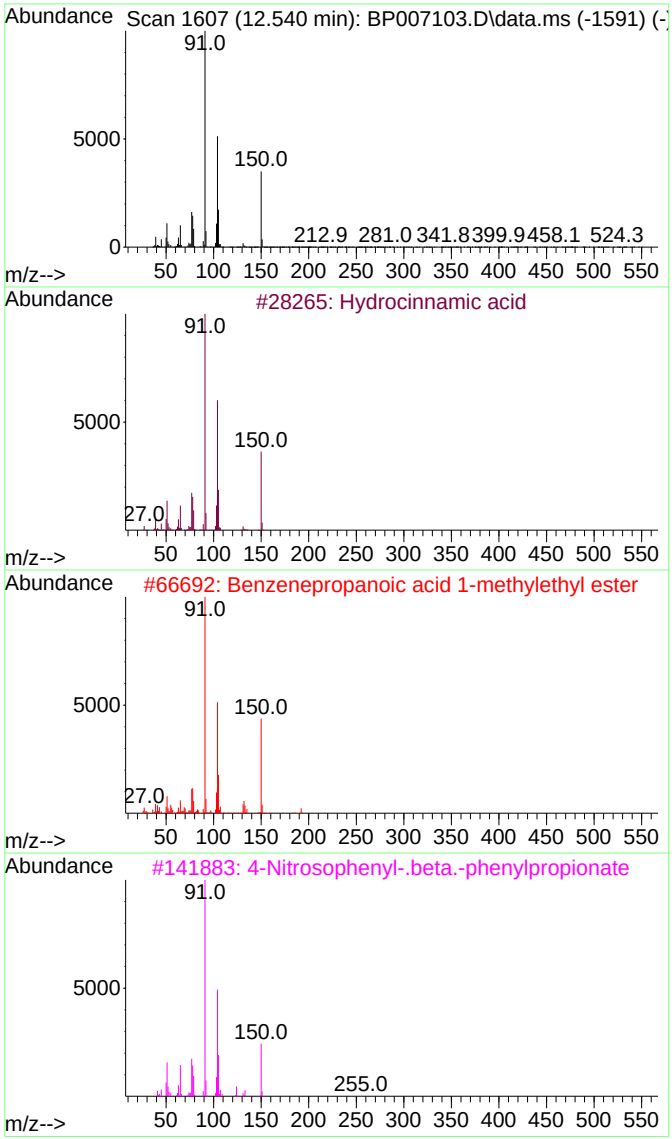
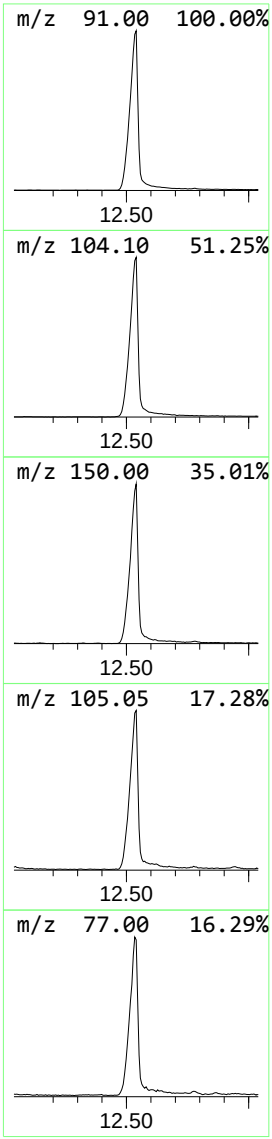
Peak Number 10 Hydrocinnamic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.540	42.06 ng	4486090	Naphthalene-d8	10.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrocinnamic acid	150	C9H10O2	000501-52-0	96
2	Benzenepropanoic acid 1-methylet...	192	C12H16O2	022767-95-9	78
3	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	64
4	Benzenepropanoic acid, silver(1+...	256	C9H9AgO2	075112-79-7	53
5	Acetic acid, trifluoro-, 2-pheny...	218	C10H9F3O2	055419-66-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007103.D
Acq On : 22 Sep 2021 18:02
Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

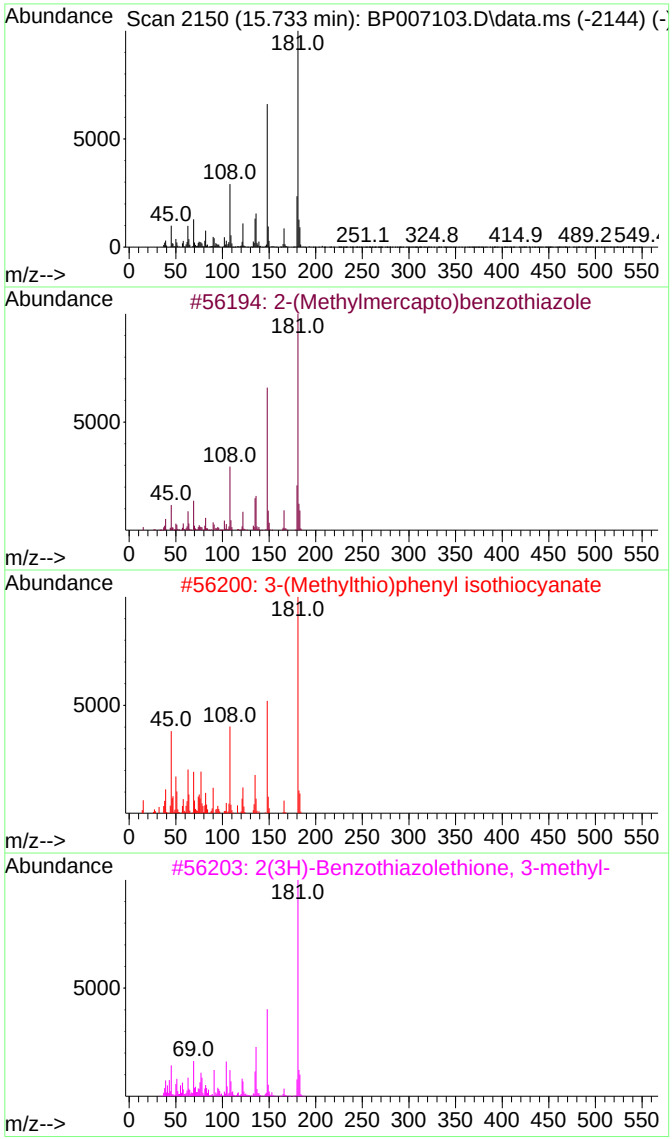
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

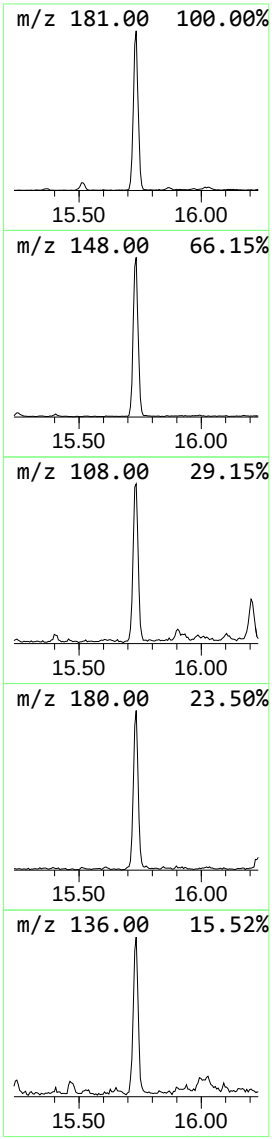
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2-(Methylmercapto)benzothia... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	3.07 ng	491583	Acenaphthene-d10	14.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	99
2	3-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-80-3	87
3	2(3H)-Benzothiazolethione, 3-met...	181	C8H7NS2	002254-94-6	80
4	Acetonitrile, (3-chloro-5,5-dime...	181	C10H12ClN	076399-17-2	42
5	9-Amino-6-[methylthio]-9H-purine	181	C6H7N5S	020914-61-8	37





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Data File : BP007103.D
Acq On : 22 Sep 2021 18:02
Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

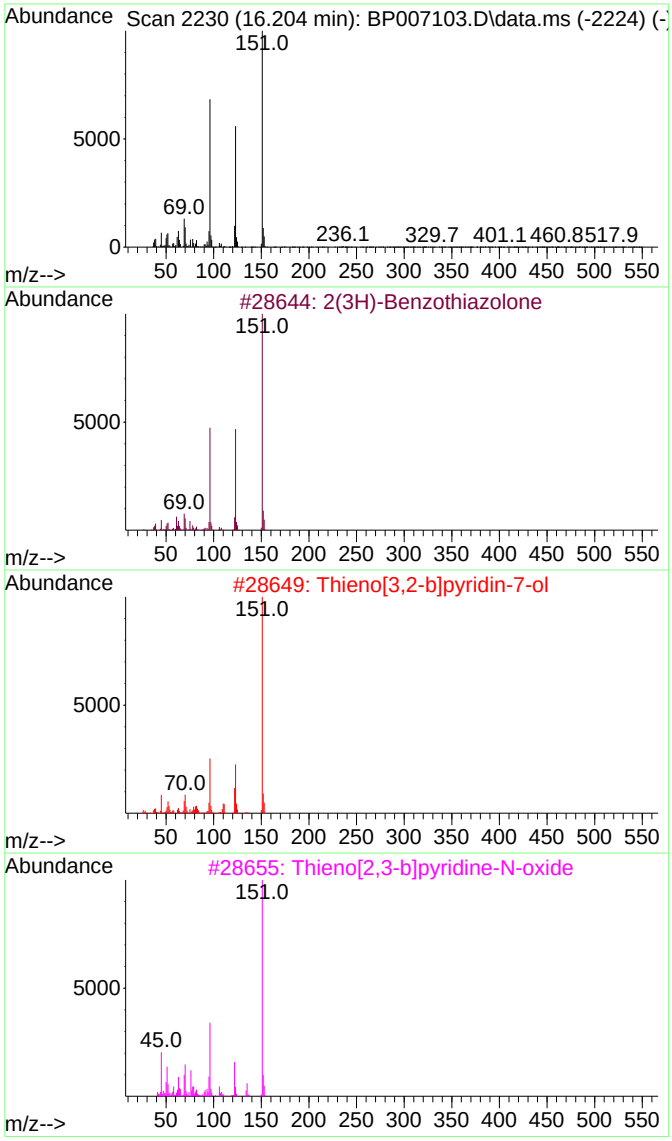
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

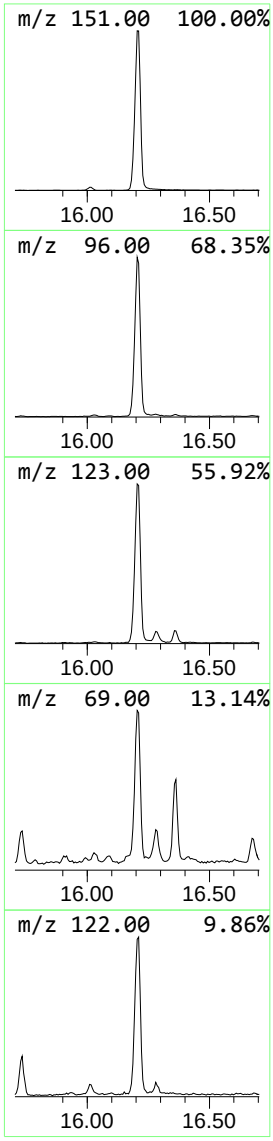
****

Peak Number 12 2(3H)-Benzothiazolone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.204	11.74 ng	1978330	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94
2	Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	64
3	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	53
4	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	52
5	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50





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Data File : BP007103.D
Acq On : 22 Sep 2021 18:02
Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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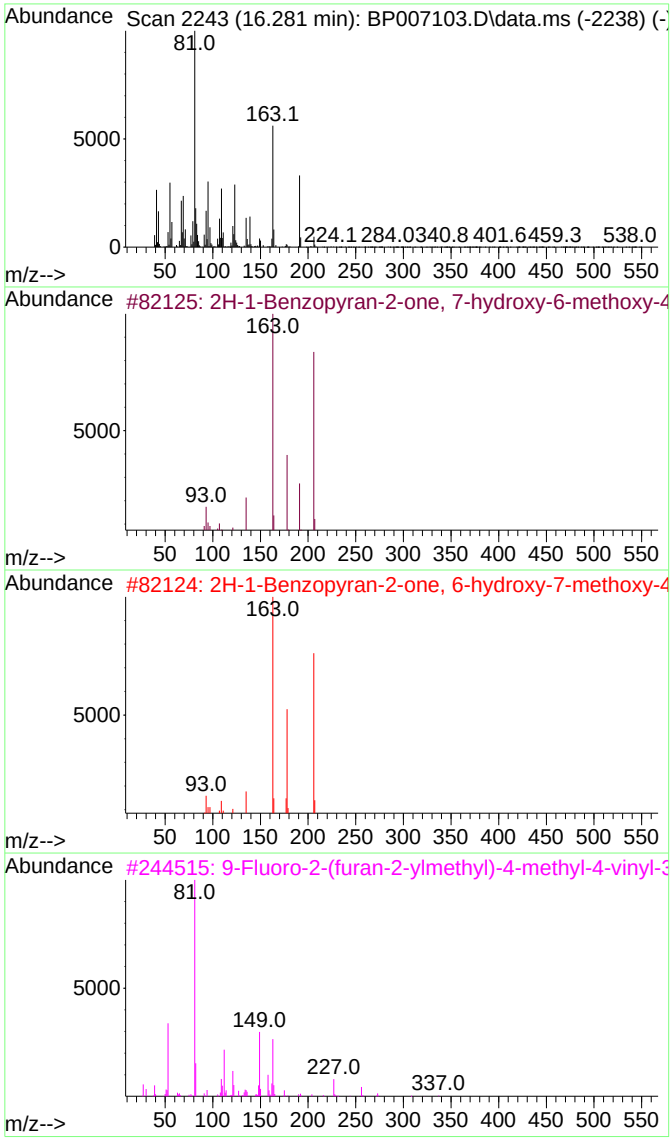
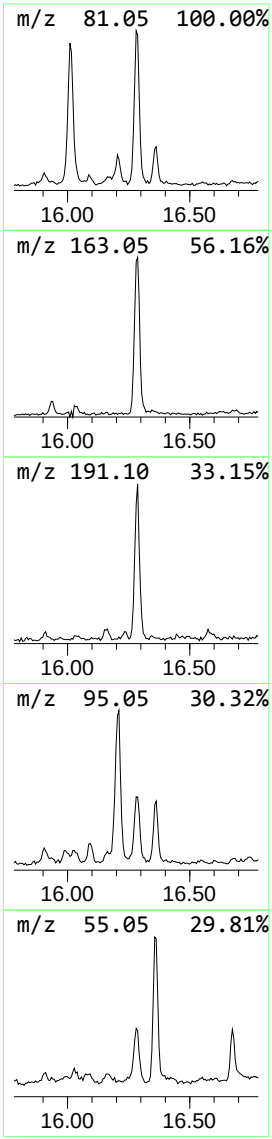
Peak Number 13 unknown16.281 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.281	2.62 ng	441200	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1-Benzopyran-2-one, 7-hydroxy...	206	C11H10O4	003374-03-6	38
2	2H-1-Benzopyran-2-one, 6-hydroxy...	206	C11H10O4	006345-62-6	27
3	9-Fluoro-2-(furan-2-ylmethyl)-4-...	337	C16H16FNO4S	1000458-16-7	25
4	1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3NO2	1000301-43-3	22
5	Isomyocorene	136	C10H16	006876-07-9	22





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Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

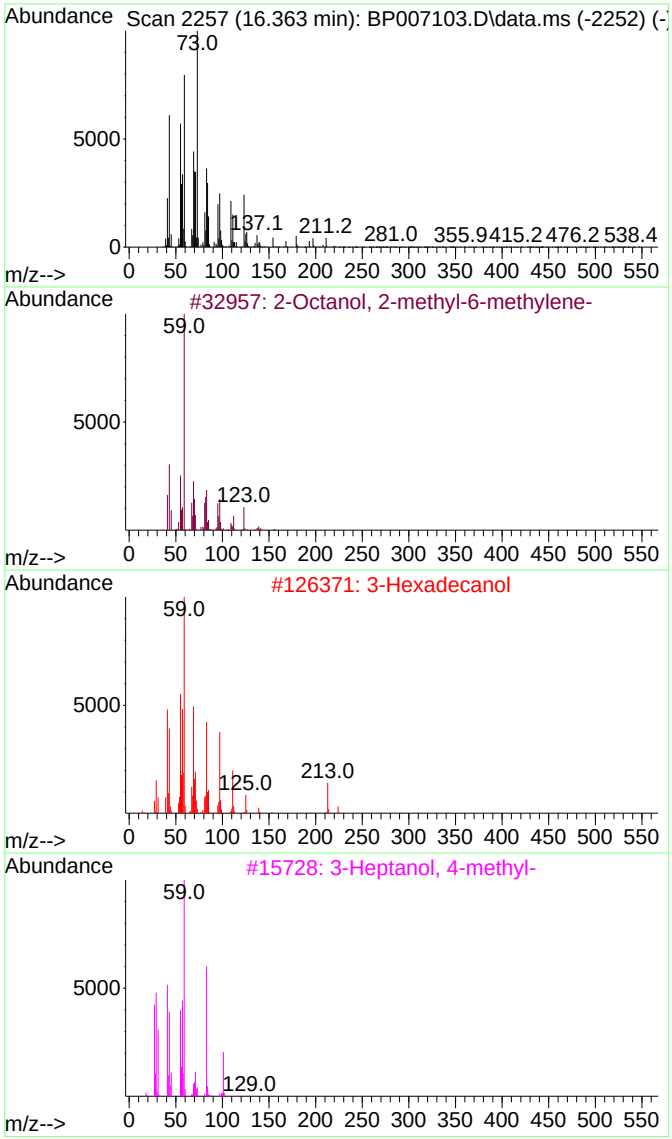
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

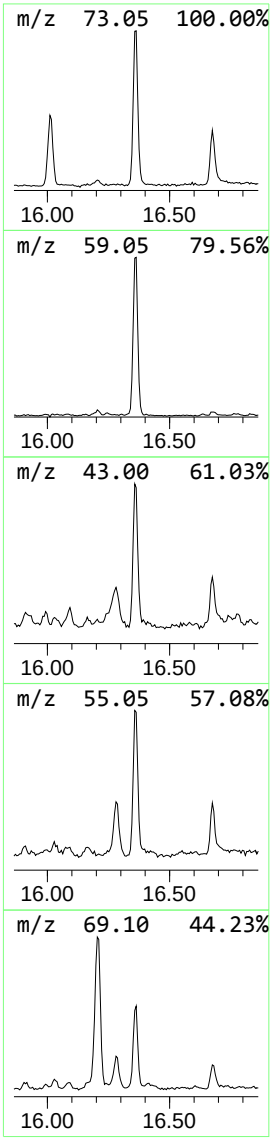
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2-Octanol, 2-methyl-6-methy... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.363	3.57 ng	601906	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	53
2	3-Hexadecanol	242	C16H34O	000593-03-3	49
3	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	27
4	Bromoacetic acid, tridecyl ester	320	C15H29BrO2	1000281-85-0	27
5	3-Hexanol	102	C6H14O	000623-37-0	27





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Acq On : 22 Sep 2021 18:02
Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

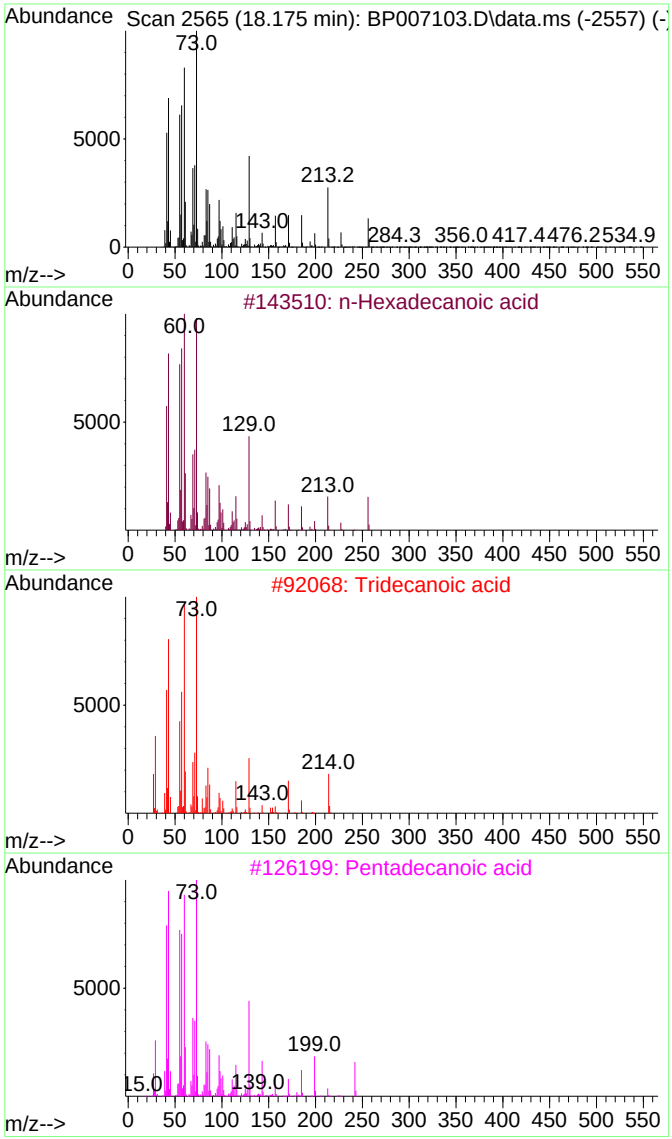
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

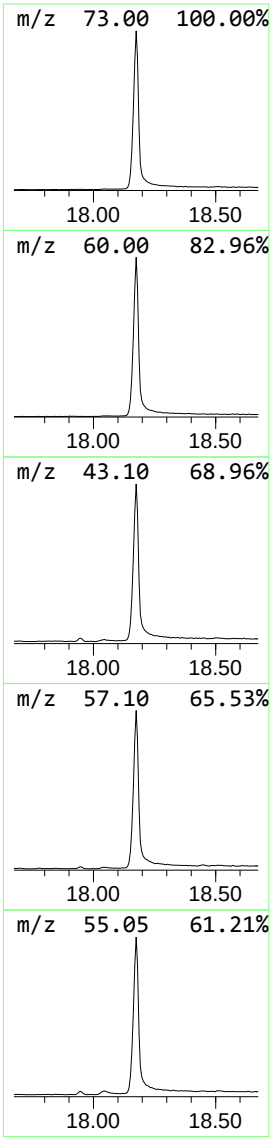
****

Peak Number 15 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	62.02 ng	10450100	Phenanthrene-d10	17.275

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Data File : BP007103.D
Acq On : 22 Sep 2021 18:02
Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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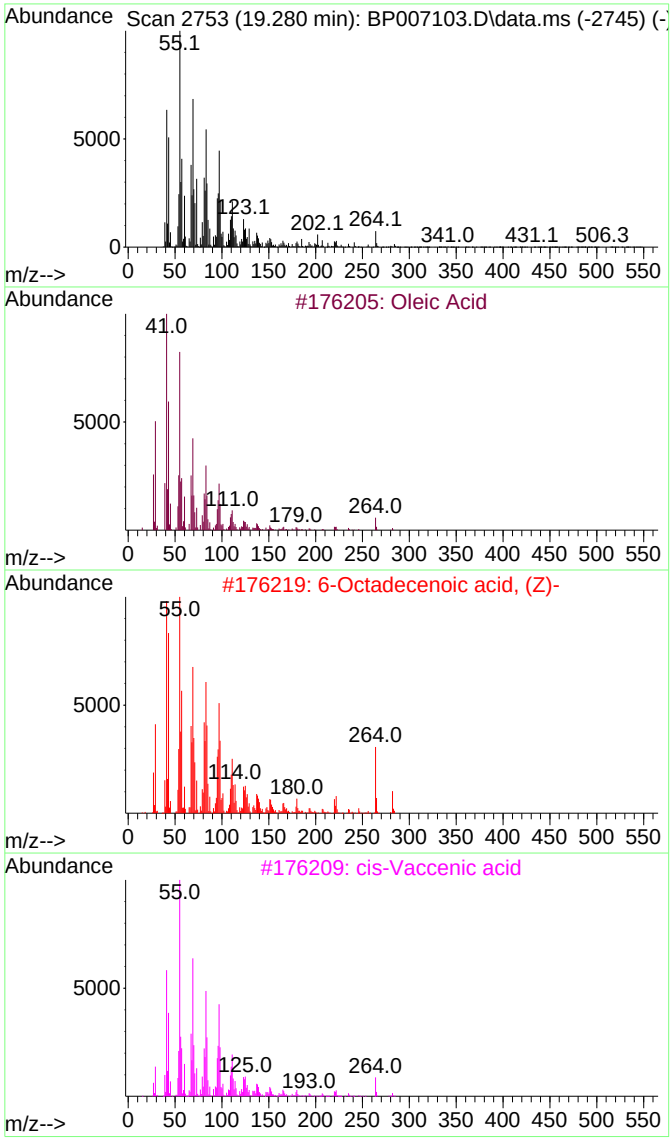
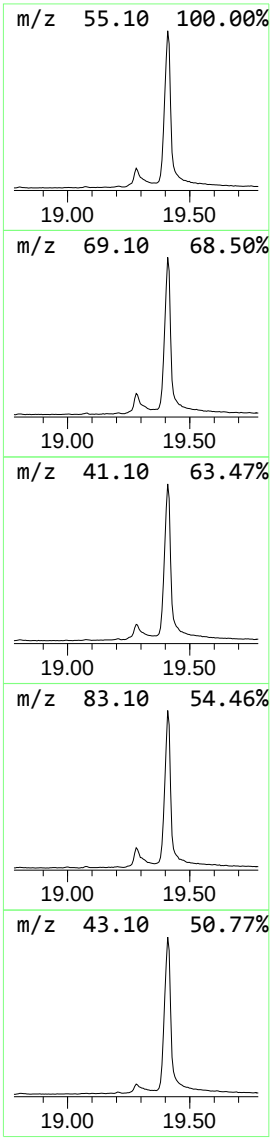
Peak Number 16 Oleic Acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.280	17.11 ng	2883490	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	98
2	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	90
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	87
4	Palmitoleic acid	254	C16H30O2	000373-49-9	87
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	87





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Data File : BP007103.D
Acq On : 22 Sep 2021 18:02
Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

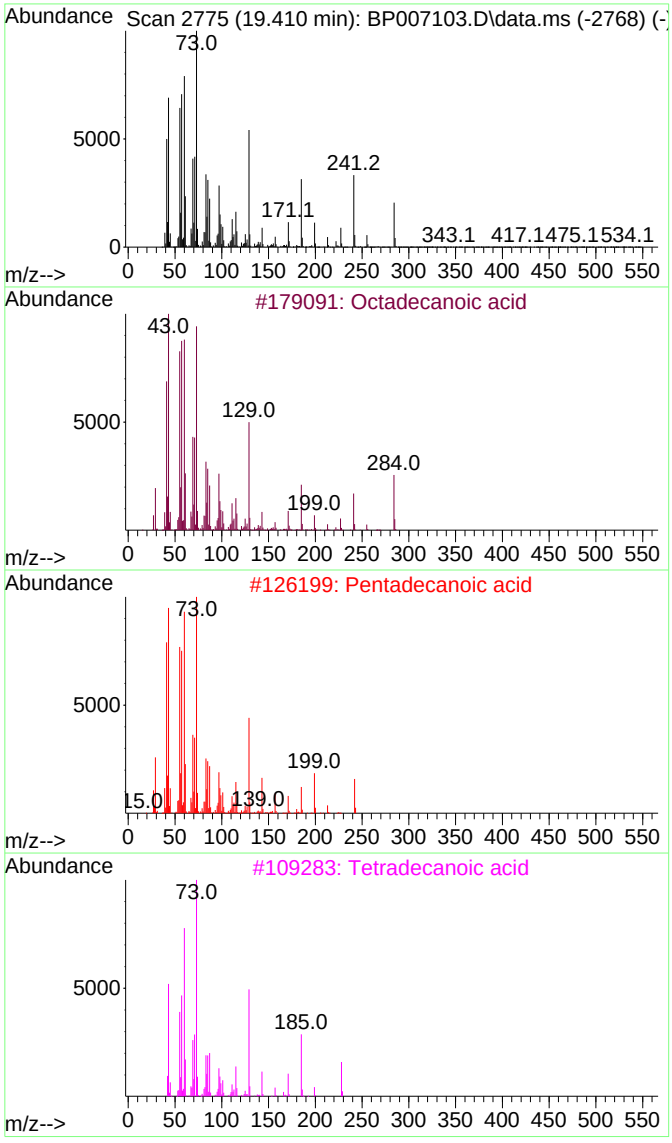
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

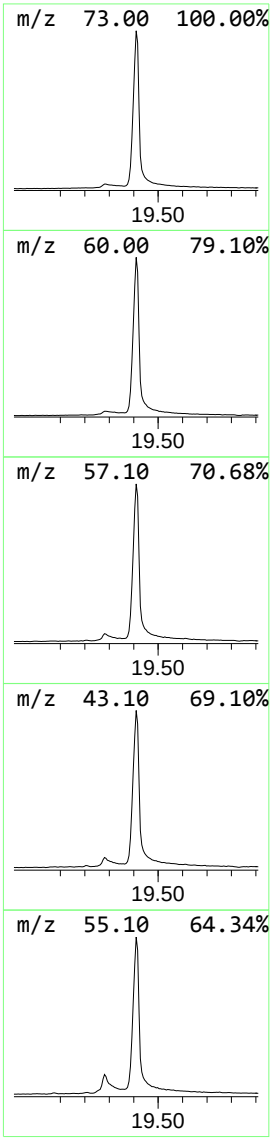
****

Peak Number 17 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.410	117.25 ng	20726300	Chrysene-d12	21.357

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





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Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

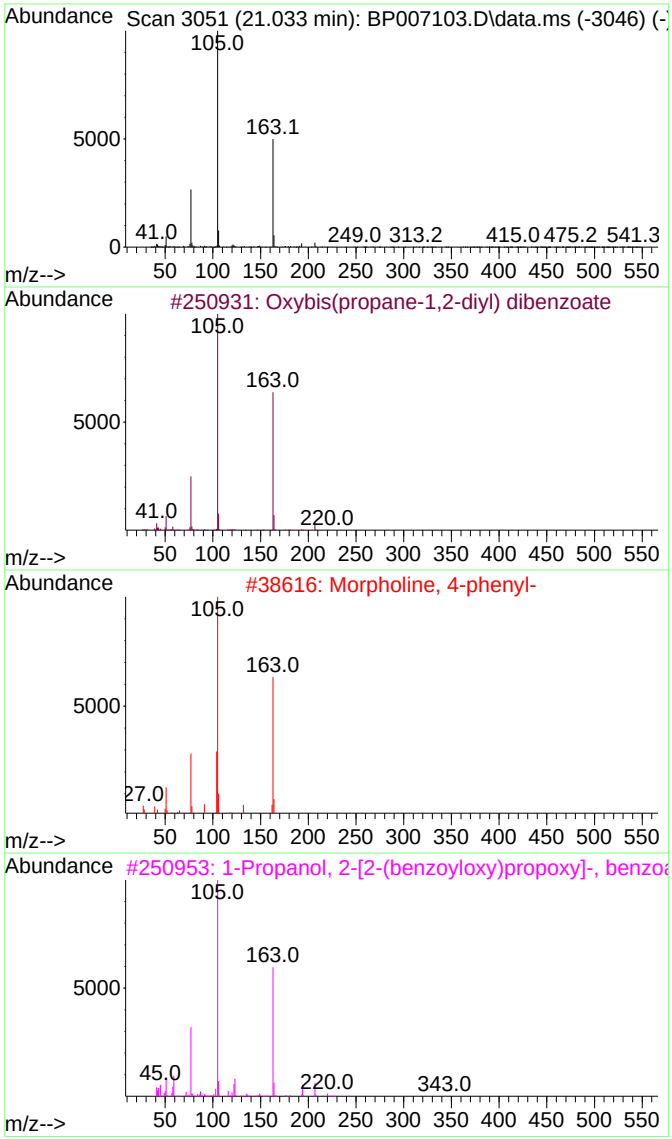
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

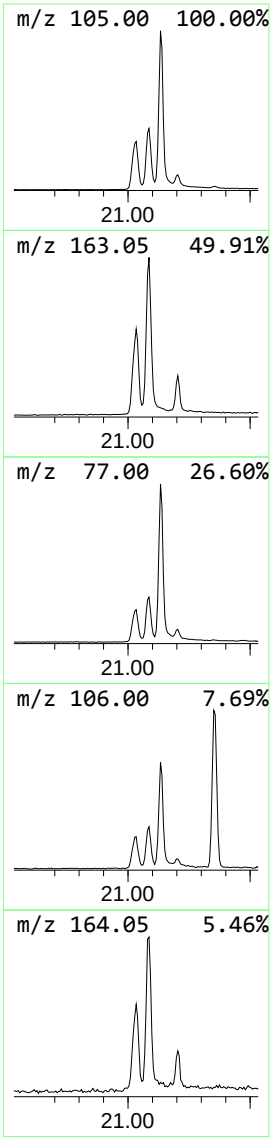
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Oxybis(propane-1,2-diyl) di... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	3.96 ng	700838	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	80
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	43
4	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	9
5	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	9





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Acq On : 22 Sep 2021 18:02
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Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

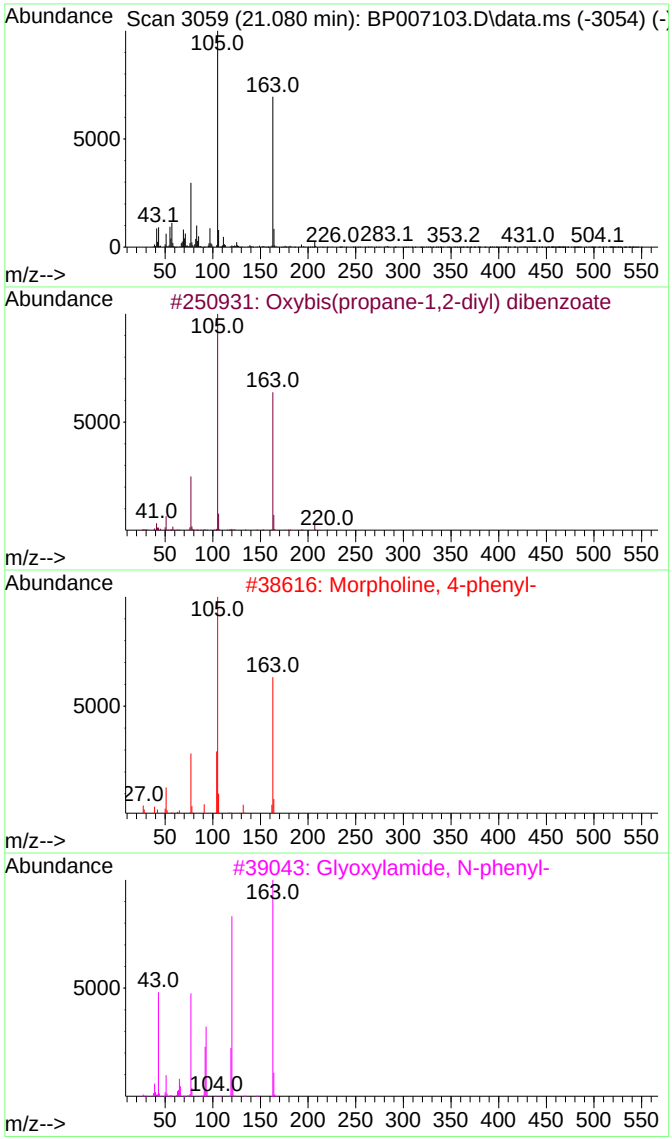
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

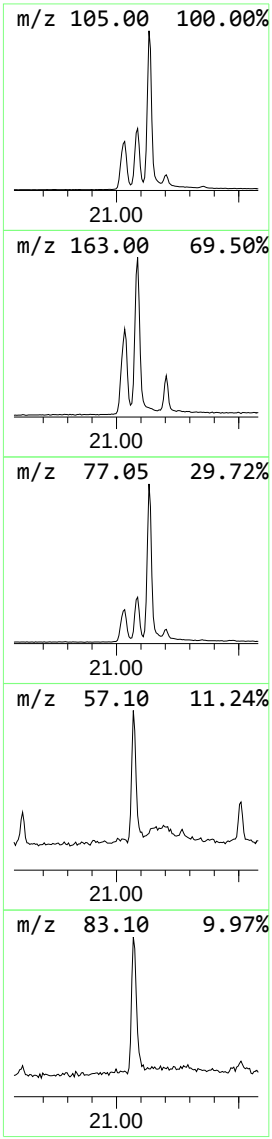
****

Peak Number 19 Morpholine, 4-phenyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	8.37 ng	1479140	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	62
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	38
4	Ethanone, 1-[2-(dimethylamino)ph...	163	C10H13NO	010336-55-7	38
5	Hexadecyl methyl phthalate	404	C25H40O4	101762-77-0	38





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Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

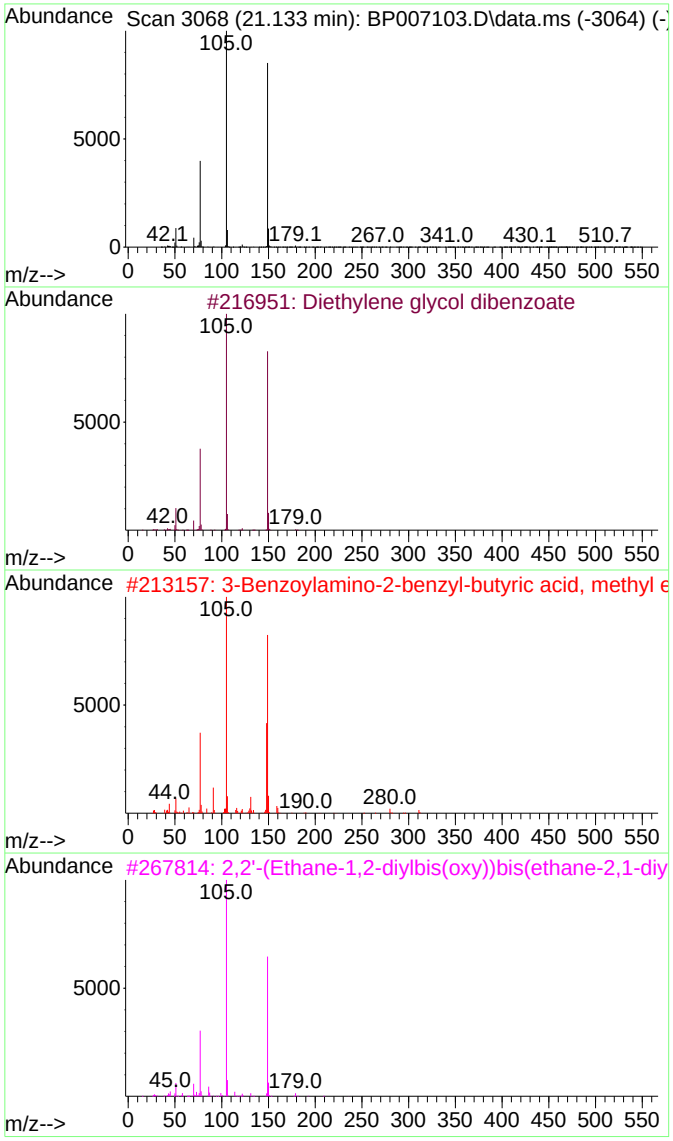
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

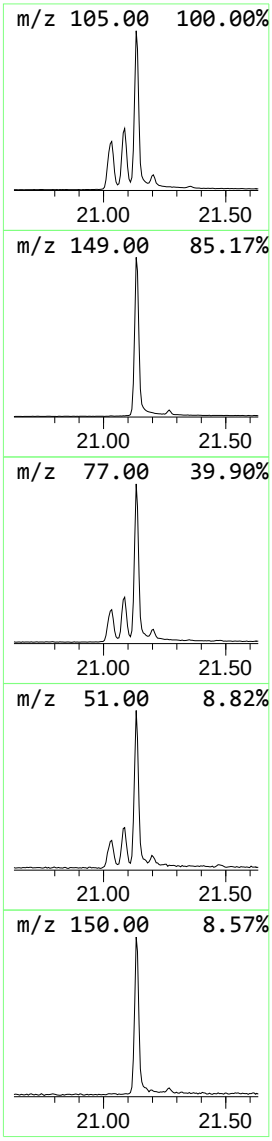
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Diethylene glycol dibenzoate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	12.53 ng	2214570	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	91
2	3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	78
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	74





Tentatively Identified Compound (LSC) summary

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Data File : BP007103.D
Acq On : 22 Sep 2021 18:02
Operator : CG/JU
Sample : M3835-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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
Butanoic acid, ...	4.828	27.4	ng	2074730	1	7.899	1512810	20.0
Pentanoic acid,...	6.322	3.4	ng	259549	1	7.899	1512810	20.0
Cyclohexanecarb...	9.440	47.6	ng	5080530	2	10.698	2133140	20.0
Phenol, 3-ethyl-	10.146	94.4	ng	10070200	2	10.698	2133140	20.0
Ethanol, 2-(2-b...	10.481	13.1	ng	1398330	2	10.698	2133140	20.0
Benzeneacetic acid	11.251	7.7	ng	816515	2	10.698	2133140	20.0
Benzeneacetic a...	11.934	2.1	ng	228990	2	10.698	2133140	20.0
Hydrocinnamic acid	12.540	42.1	ng	4486090	2	10.698	2133140	20.0
2-(Methylmercap...	15.733	3.1	ng	491583	3	14.528	3198070	20.0
2(3H)-Benzothia...	16.204	11.7	ng	1978330	4	17.275	3369760	20.0
unknown16.281	16.281	2.6	ng	441200	4	17.275	3369760	20.0
2-Octanol, 2-me...	16.363	3.6	ng	601906	4	17.275	3369760	20.0
n-Hexadecanoic ...	18.174	62.0	ng	10450100	4	17.275	3369760	20.0
Oleic Acid	19.280	17.1	ng	2883490	4	17.275	3369760	20.0
Octadecanoic acid	19.410	117.3	ng	20726300	5	21.357	3535560	20.0
Oxybis(propane-...	21.033	4.0	ng	700838	5	21.357	3535560	20.0
Morpholine, 4-p...	21.080	8.4	ng	1479140	5	21.357	3535560	20.0
Diethylene glyc...	21.133	12.5	ng	2214570	5	21.357	3535560	20.0