LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006551.D
Acq On : 06 Aug 2021 22:12
Operator : CG/JU
Sample : M3297-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 123-24

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-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006551.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	380	386	396	rVB	1944311	2855878	22.23%	4.775%
2	6.928	647	653	667	rVB	1144856	1838476	14.31%	3.074%
3	7.752	786	793	800	rVB	859620	1323047	10.30%	2.212%
4	8.910	982	990	997	rBV	2815577	4520991	35.19%	7.559%
5	9.475	1070	1086	1097	rBV2	131616	510433	3.97%	0.853%
6	10.328	1225	1231	1239	rBV	311096	492447	3.83%	0.823%
7	10.534	1259	1266	1275	rVB	1109788	1857711	14.46%	3.106%
8	12.193	1540	1548	1560	rBV	356008	649697	5.06%	1.086%
9	13.010	1679	1687	1692	rBV	5997753	8876927	69.10%	14.842%
10	13.057	1692	1695	1700	rVB2	98549	138100	1.07%	0.231%
11	13.987	1848	1853	1858	rBV	106784	200017	1.56%	0.334%
12	14.381	1914	1920	1928	rBV	1582128	2338390	18.20%	3.910%
13	15.045	2029	2033	2037	rVB	352412	422637	3.29%	0.707%
14	15.328	2076	2081	2085	rBV	176882	266357	2.07%	0.445%
15	15.875	2168	2174	2184	rVB	4919417	6901253	53.72%	11.539%
16	16.133	2214	2218	2223	rVB5	90104	154469	1.20%	0.258%
17	16.533	2282	2286	2296	rBV4	87594	207422	1.61%	0.347%
18	16.651	2302	2306	2317	rVB	463220	722547	5.62%	1.208%
19	17.133	2383	2388	2394	rVB	1805915	2521305	19.63%	4.216%
20	17.628	2468	2472	2481	rBV2	121960	254750	1.98%	0.426%
21	17.816	2501	2504	2508	rVB4	125694	167042	1.30%	0.279%
22	18.045	2537	2543	2551	rBV	1167382	1658284	12.91%	2.773%
23	19.280	2749	2753	2761	rBV	692975	908232	7.07%	1.519%
24	19.710	2821	2826	2831	rBV	10798801	12846960	100.00%	21.480%
25	20.957	3034	3038	3044	rBV	403638	494813	3.85%	0.827%
26	21.227	3080	3084	3092	rVB2	2154194	2781757	21.65%	4.651%
27	22.892	3363	3367	3377	rVB2	563509	922950	7.18%	1.543%
28	23.557	3473	3480	3491	rVB	1566068	2975765	23.16%	4.975%

Sum of corrected areas: 59808657

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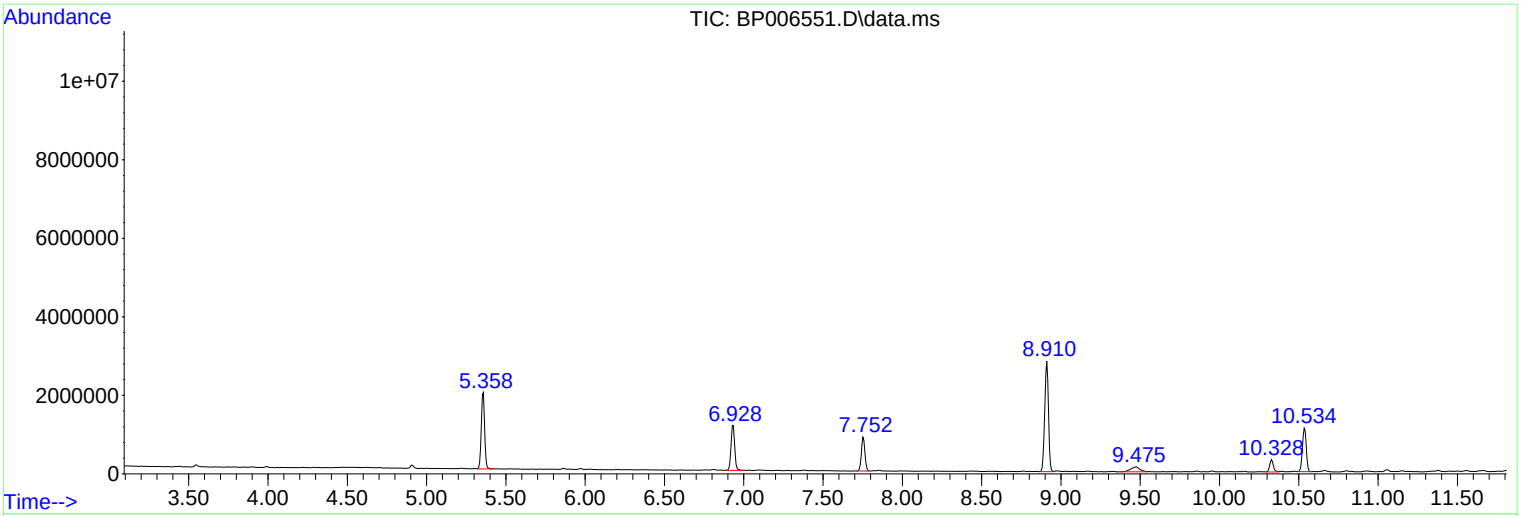
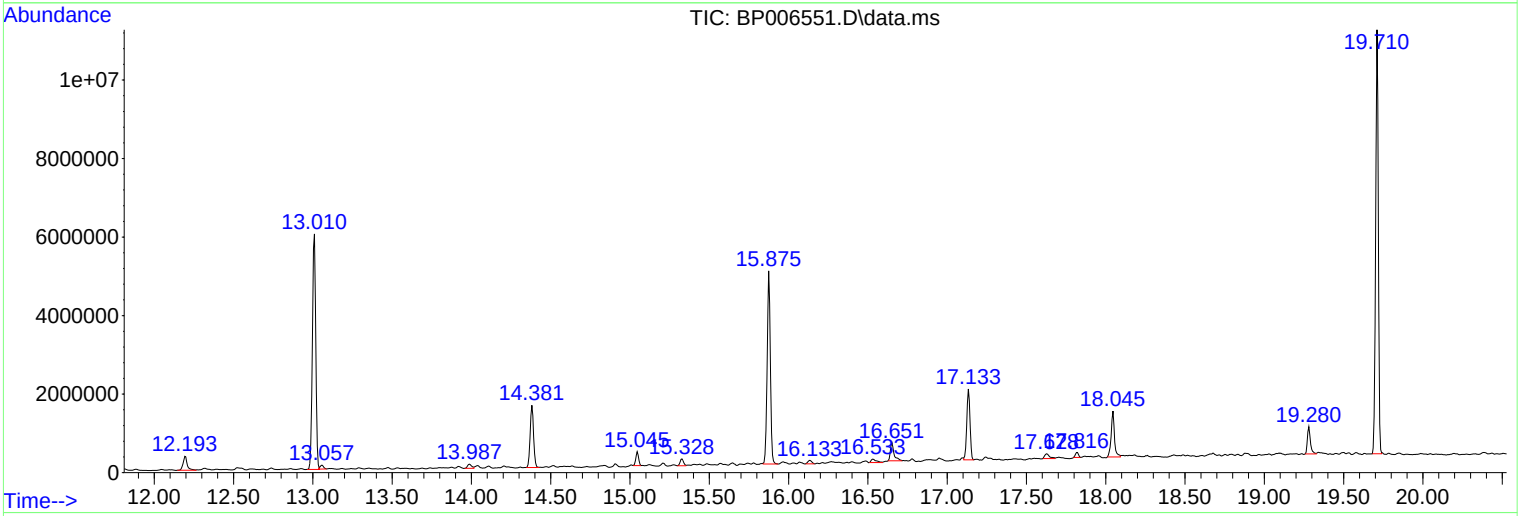
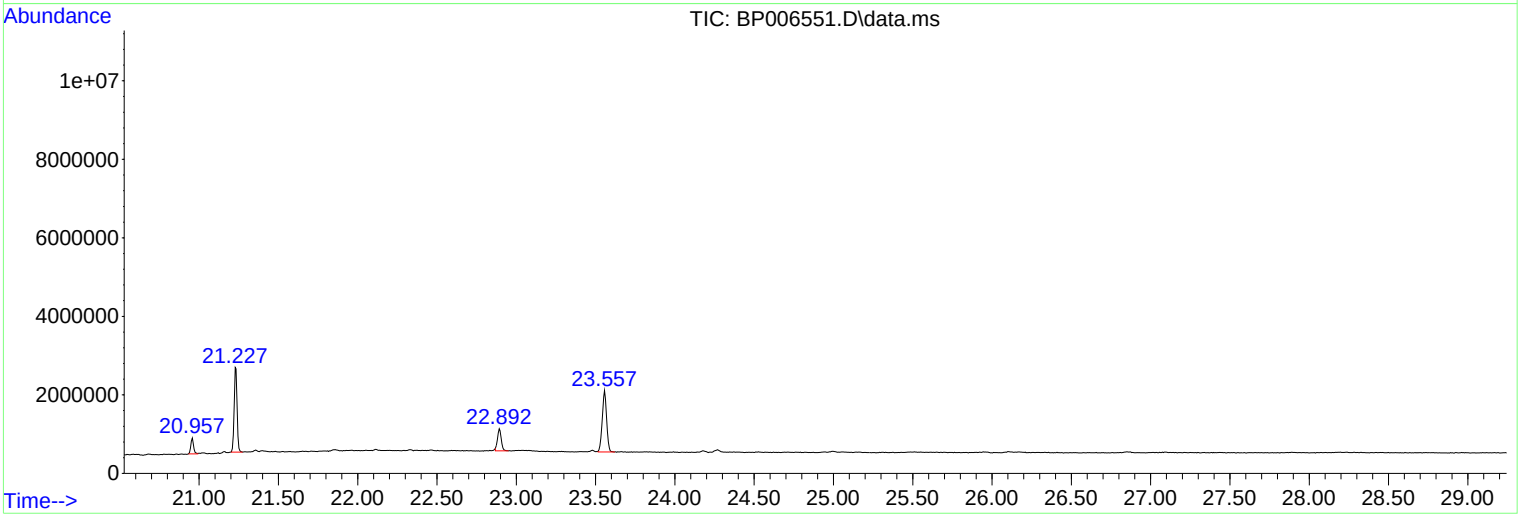
Instrument :
BNA_P
ClientSampleId :
123-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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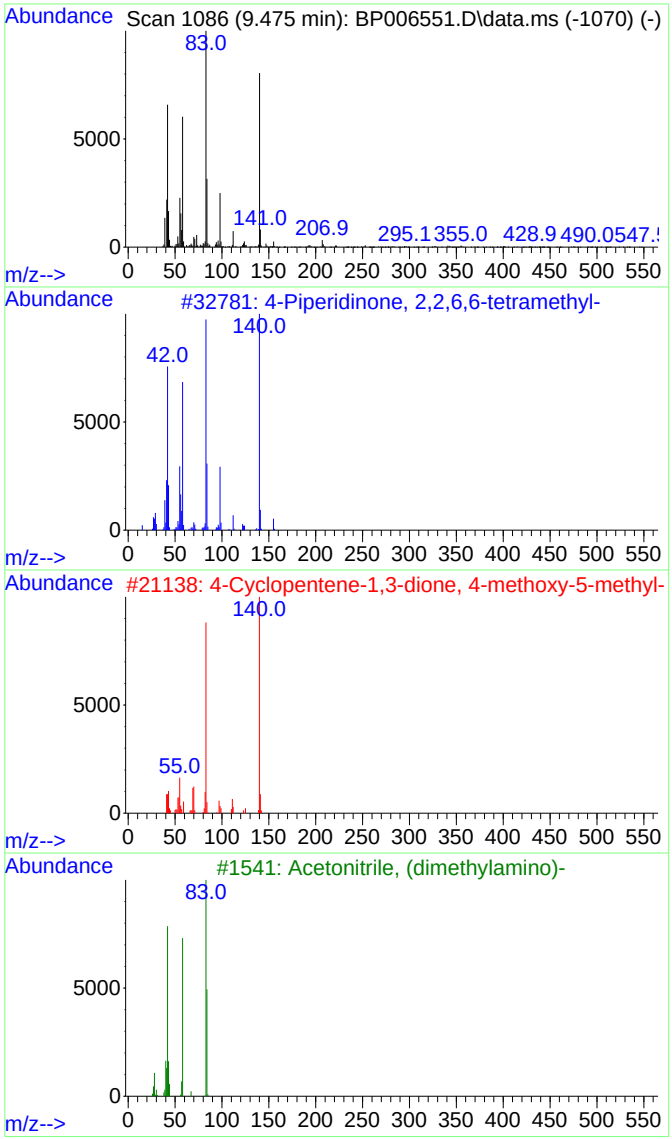
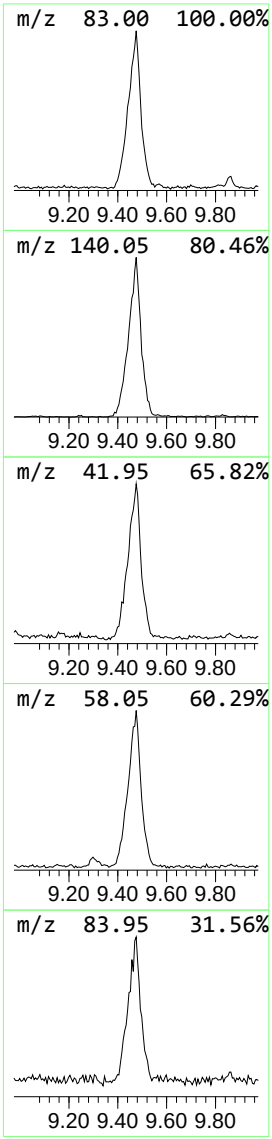
****
Peak Number 1 4-Piperidinone, 2,2,6,6-tet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.475	5.50 ng	510433	Naphthalene-d8	10.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Piperidinone, 2,2,6,6-tetramet...	155	C9H17NO	000826-36-8	95
2	4-Cyclopentene-1,3-dione, 4-meth...	140	C7H8O3	007180-62-3	43
3	Acetonitrile, (dimethylamino)-	84	C4H8N2	000926-64-7	38
4	2,4(1H,3H)-Pyrimidinedione, 1,3-...	140	C6H8N2O2	000874-14-6	35
5	1H-Pyrazole, 4,5-dihydro-1,5-dim...	98	C5H10N2	005775-96-2	32





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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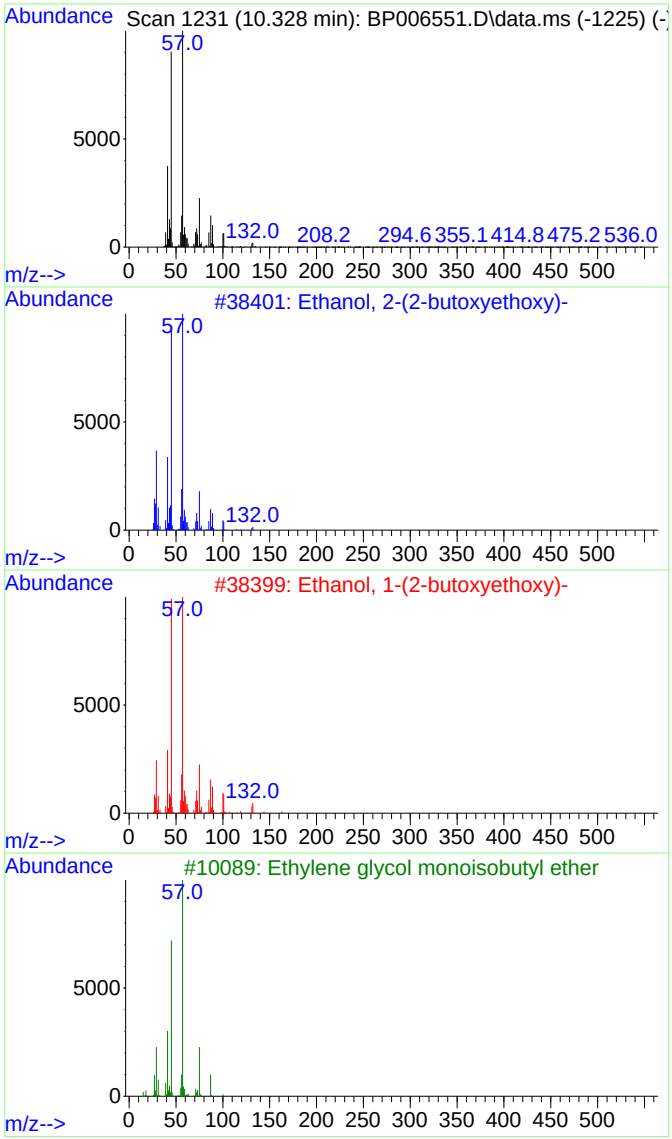
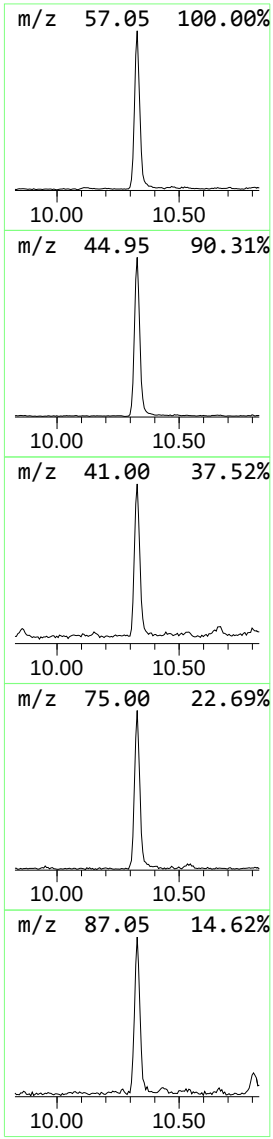
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	5.30 ng	492447	Naphthalene-d8	10.534

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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Carbonic acid, bis(1-methylpropy...	174	C9H18O3	000623-63-2	50





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Instrument : BNA_P
ClientSampleId : 123-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

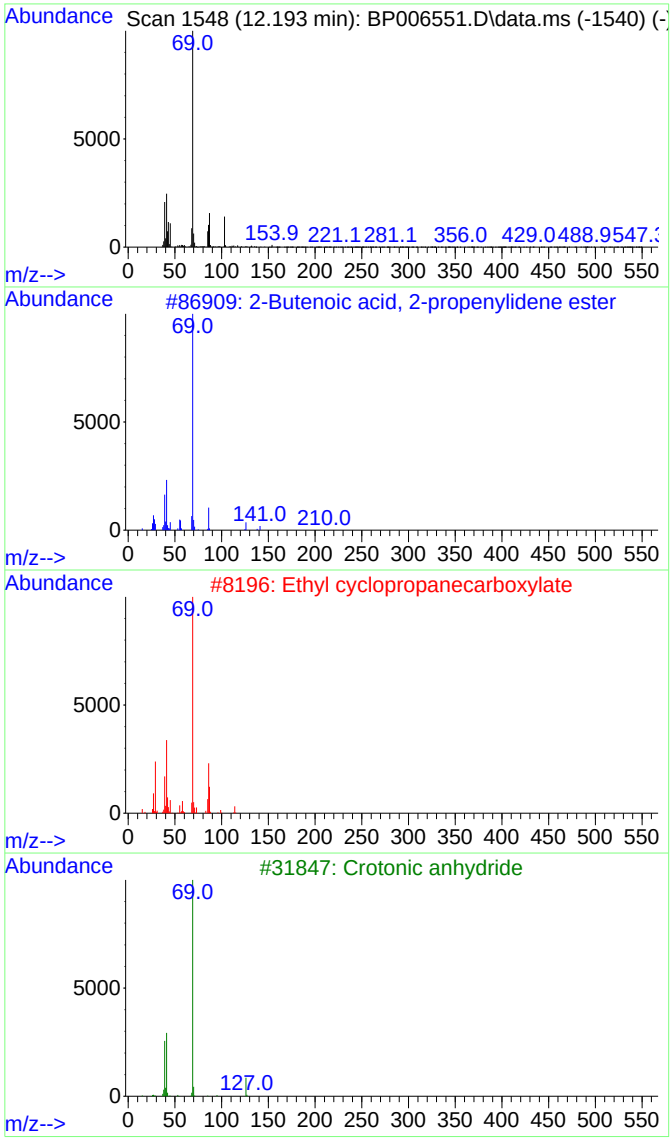
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

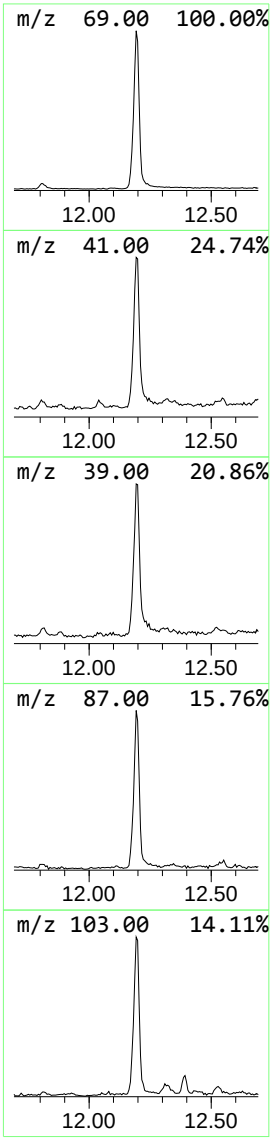
****

Peak Number 3 2-Butenoic acid, 2-propenyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.193	6.99 ng	649697	Naphthalene-d8	10.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	53
2	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	40
3	Crotonic anhydride	154	C8H10O3	000623-68-7	38
4	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	33
5	Oxazole	69	C3H3NO	000288-42-6	9





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Instrument :
BNA_P
ClientSampleId :
123-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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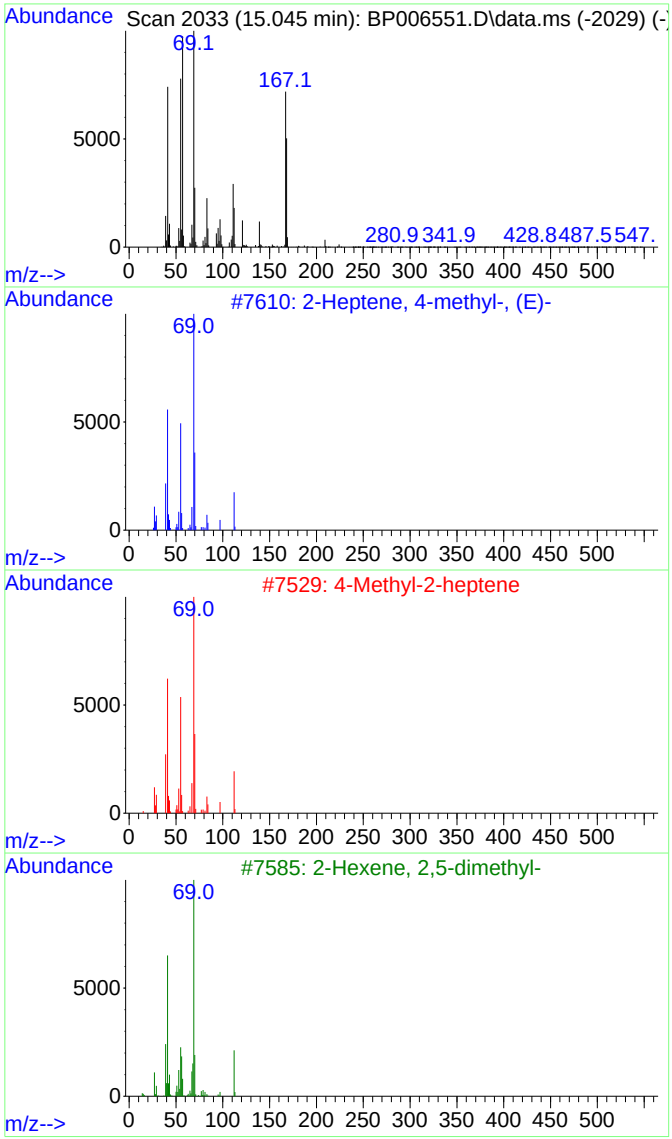
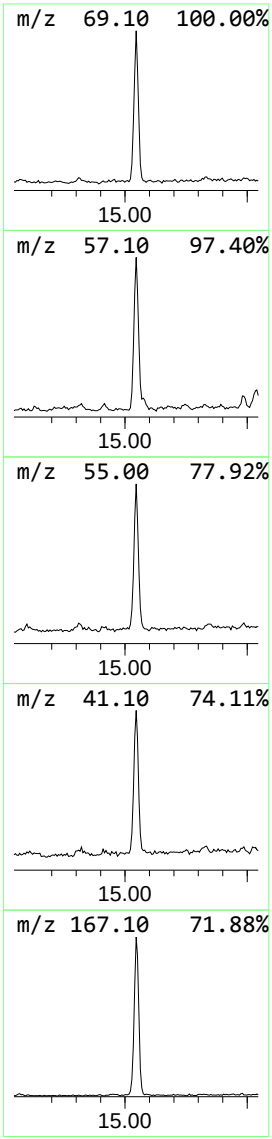
****

Peak Number 4 unknown15.045 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.045	3.61 ng	422637	Acenaphthene-d10	14.381

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptene, 4-methyl-, (E)-	112	C8H16	066225-17-0	38
2	4-Methyl-2-heptene	112	C8H16	003404-56-6	38
3	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	27
4	3-Hexene, 2,5-dimethyl-	112	C8H16	015910-22-2	27
5	1-Octene, 3,3-dimethyl-	140	C10H20	074511-51-6	27





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Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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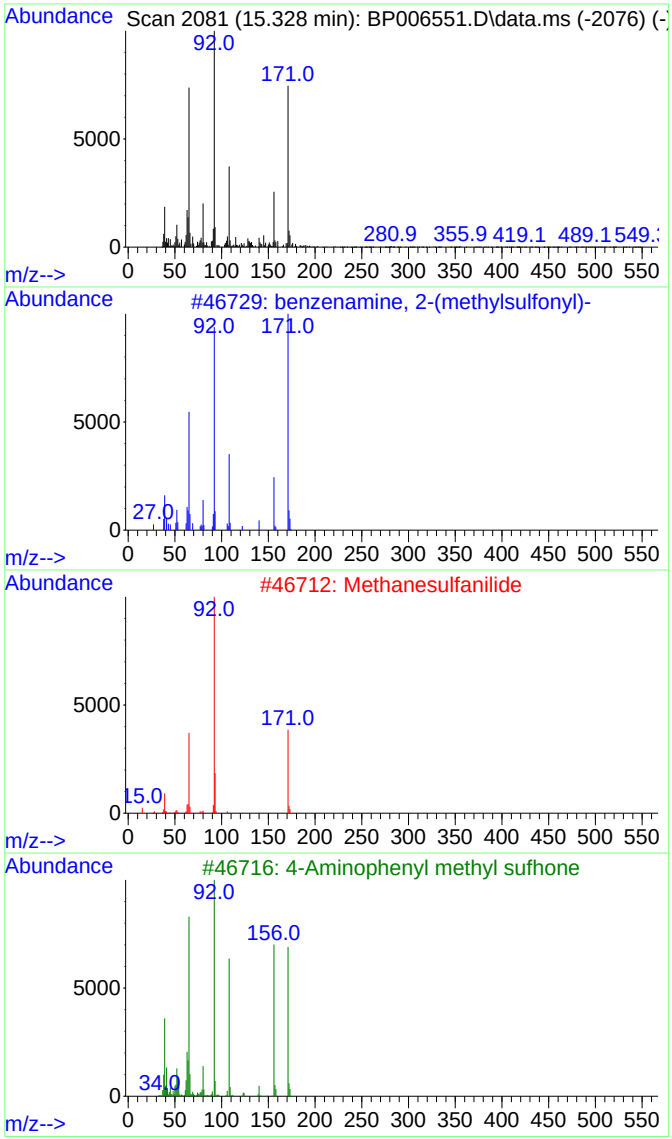
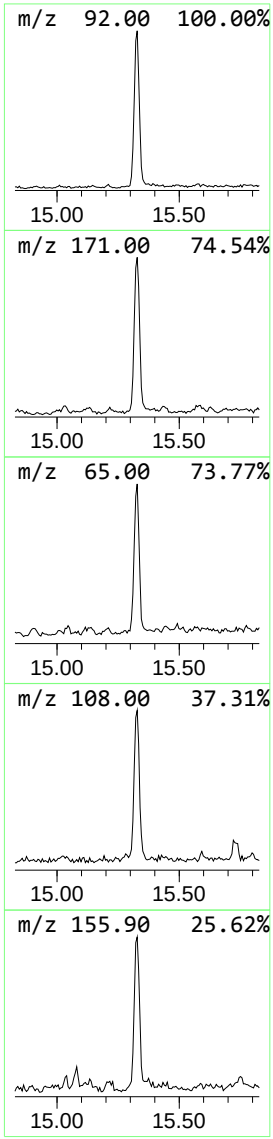
****
Peak Number 5 benzenamine, 2-(methylsulfo... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.328	2.28 ng	266357	Acenaphthene-d10	14.381

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	benzenamine, 2-(methylsulfonyl)-	171	C7H9NO2S	1000404-60-9	94
2	Methanesulfanilide	171	C7H9NO2S	001197-22-4	86
3	4-Aminophenyl methyl sufhone	171	C7H9NO2S	005470-49-5	78
4	2-(Difluoromethylsulfonyl)aniline	207	C7H7F2NO2S	024906-75-0	72
5	Carbamic acid, (methylsulfonyl)p...	243	C10H13NO4S	1000327-62-9	64





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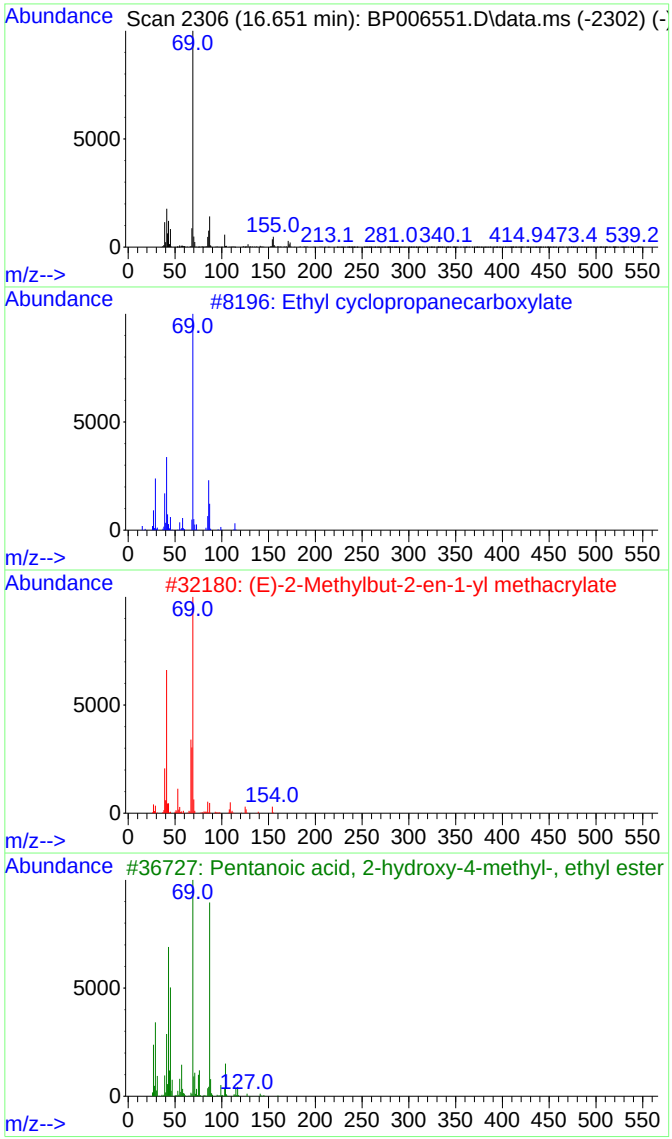
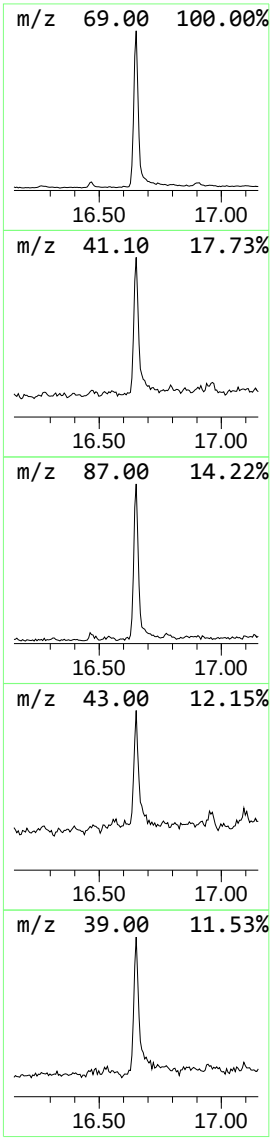
****

Peak Number 6 unknown16.651 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.651	5.73 ng	722547	Phenanthrene-d10	17.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	45
2	(E)-2-Methylbut-2-en-1-yl methac...	154	C9H14O2	088142-95-4	45
3	Pentanoic acid, 2-hydroxy-4-meth...	160	C8H16O3	010348-47-7	38
4	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	36
5	2,3'-Bifuran, 2,2',3',5-tetrahydro-	138	C8H10O2	098869-93-3	33





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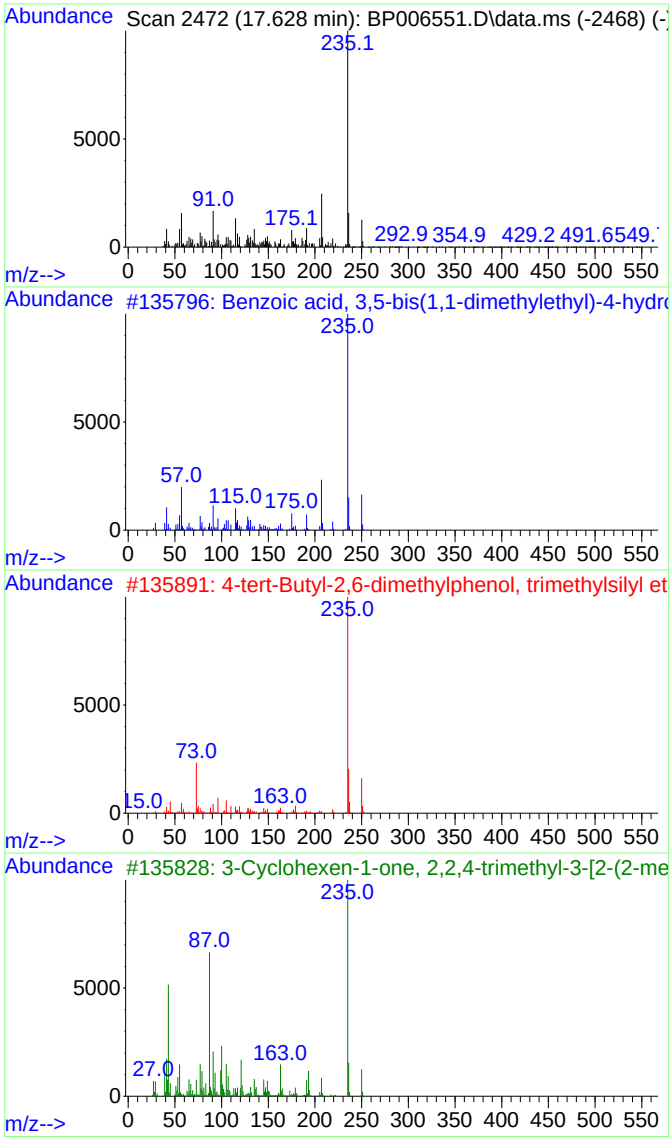
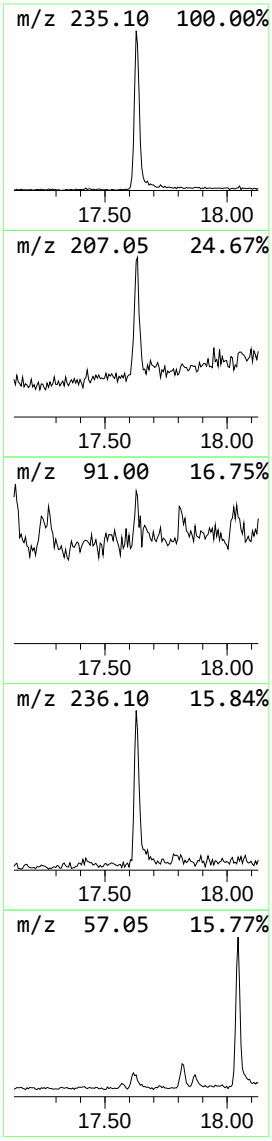
****
Peak Number 7 Benzoic acid, 3,5-bis(1,1-d... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.628	2.02 ng	254750	Phenanthrene-d10	17.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 3,5-bis(1,1-dimeth...	250	C15H22O3	001421-49-4	98
2	4-tert-Butyl-2,6-dimethylphenol,...	250	C15H26OSi	1000495-37-2	70
3	3-Cyclohexen-1-one, 2,2,4-trimet...	250	C15H22O3	1000197-90-2	68
4	2,4,6(1H,3H,5H)-Pyrimidinetrione...	250	C13H18N2O3	000726-79-4	59
5	3-tert-Butylbenzoic acid, TMS	250	C14H22O2Si	1000507-56-6	59





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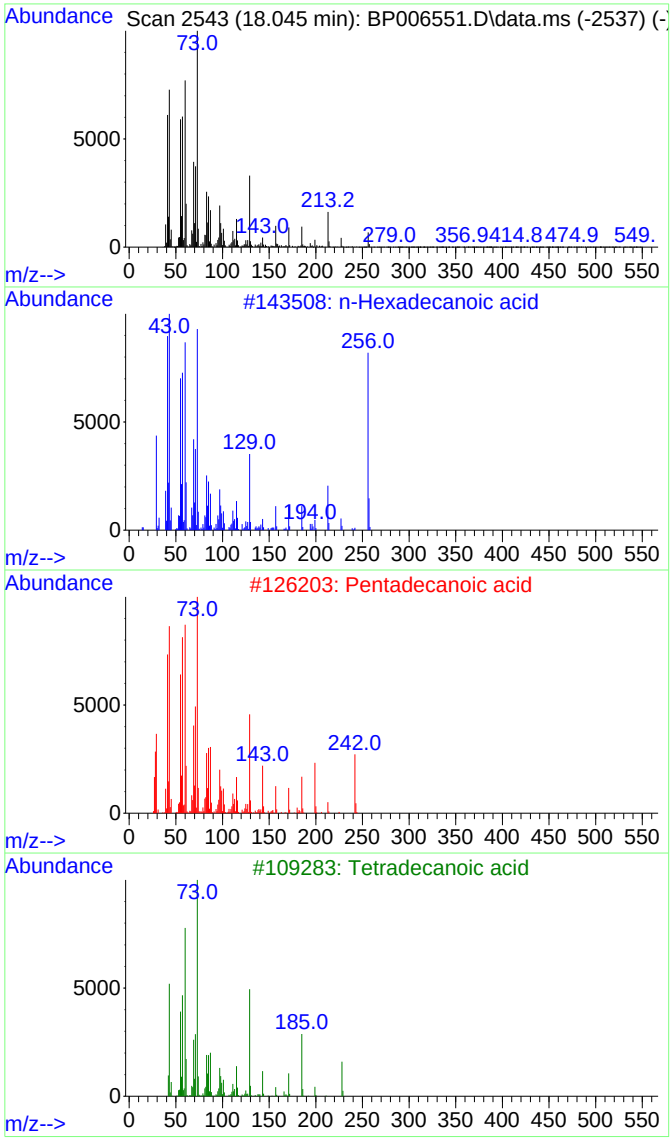
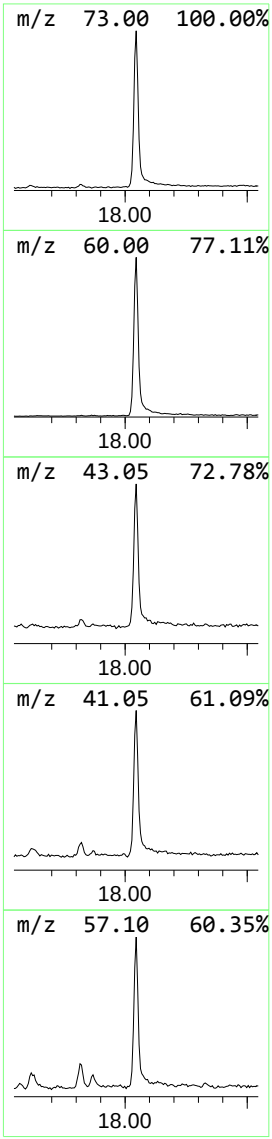
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	13.15 ng	1658280	Phenanthrene-d10	17.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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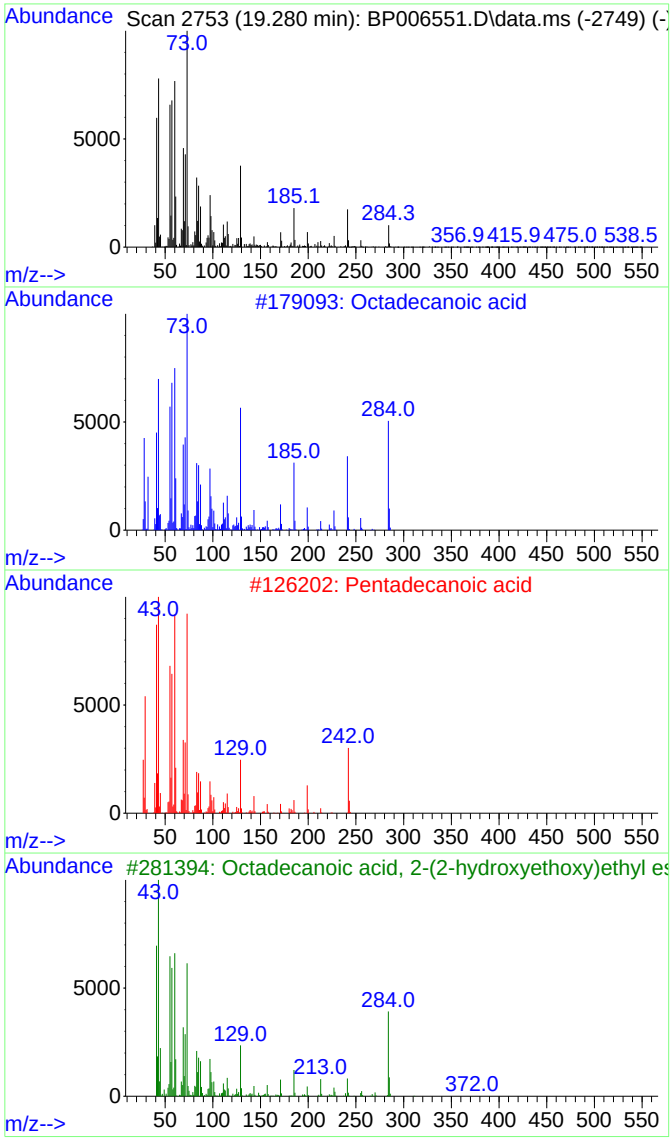
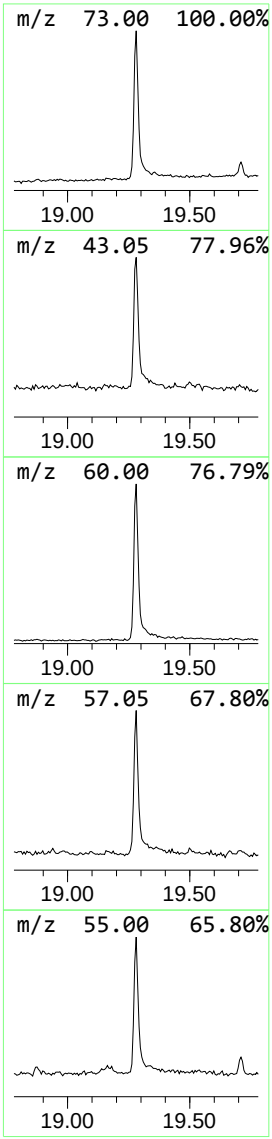
****

Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.280	6.53 ng	908232	Chrysene-d12	21.233

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	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





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Acq On : 06 Aug 2021 22:12
Operator : CG/JU
Sample : M3297-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
123-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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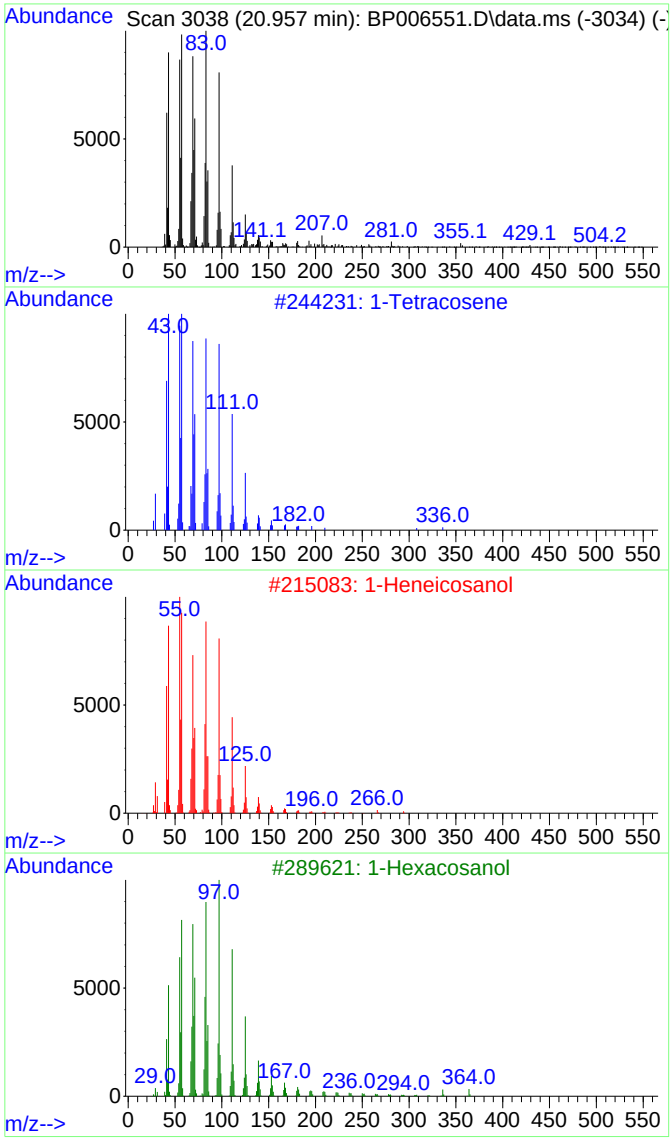
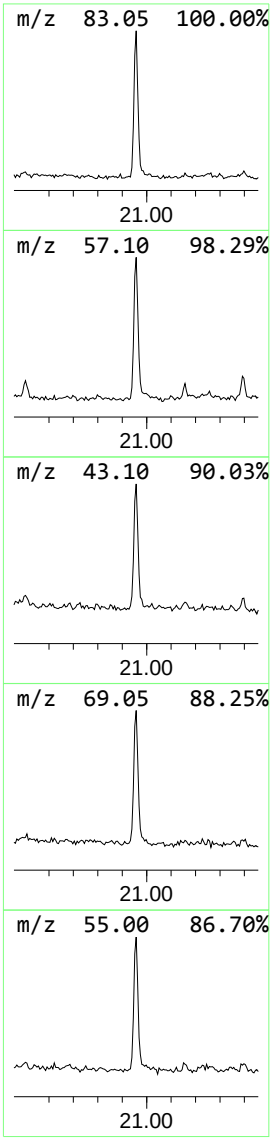
Peak Number 10 1-Tetracosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	3.56 ng	494813	Chrysene-d12	21.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	1-Hexacosanol	382	C26H54O	000506-52-5	91
4	Octacosanol	410	C28H58O	000557-61-9	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006551.D
Acq On : 06 Aug 2021 22:12
Operator : CG/JU
Sample : M3297-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
123-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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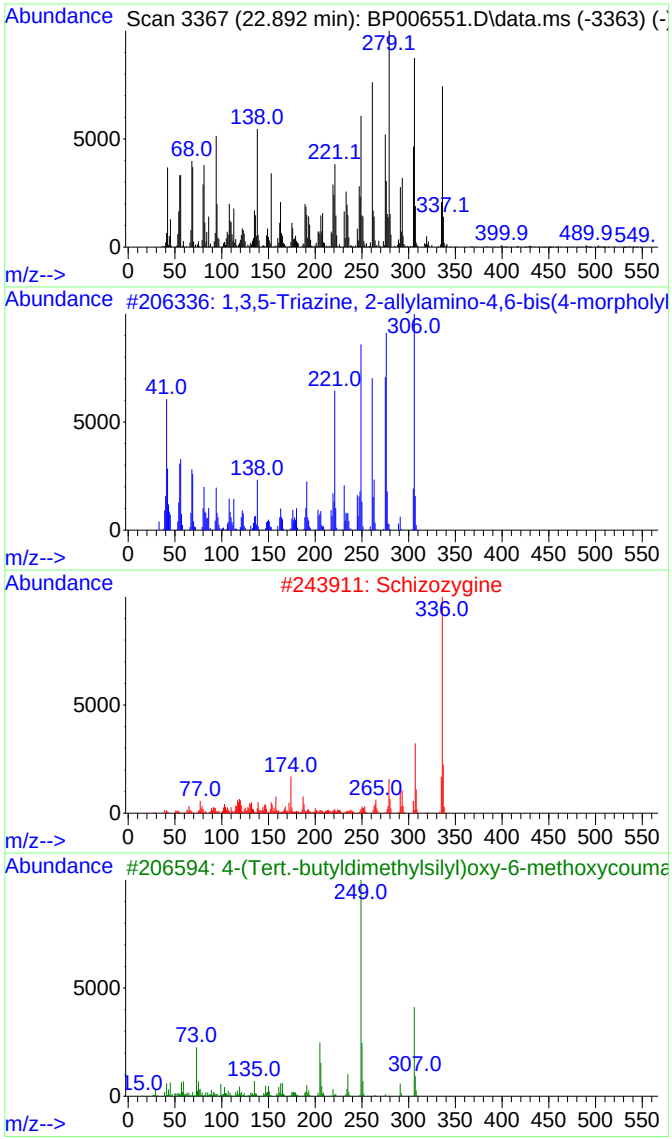
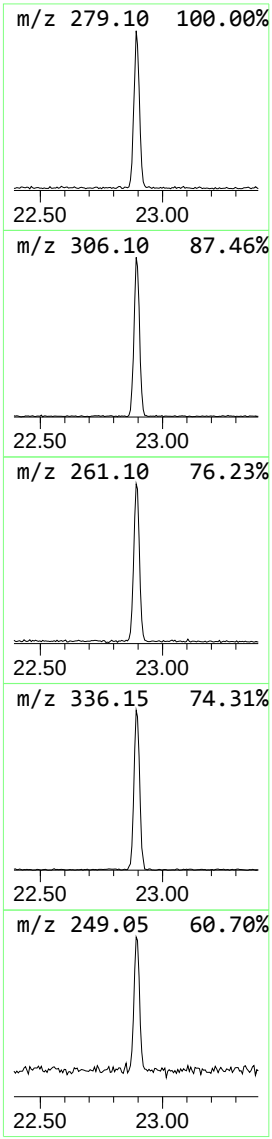
Peak Number 11 unknown22.892 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.892	6.20 ng	922950	Perylene-d12	23.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine, 2-allylamino-4,6...	306	C14H22N6O2	332409-13-9	42
2	Schizozygine	336	C20H20N2O3	002047-63-4	25
3	4-(Tert.-butyldimethylsilyl)oxy-...	306	C16H22O4Si	1000454-70-3	25
4	Benzene, 1,4-bis(3-methylindol-2...	336	C24H20N2	164936-89-4	25
5	5H-1,5,7,9a-Tetraazafluorene-6,8...	306	C17H14N4O2	1000310-72-9	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006551.D
Acq On : 06 Aug 2021 22:12
Operator : CG/JU
Sample : M3297-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 123-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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
4-Piperidinone,...	9.475	5.5	ng	510433	2	10.534	1857710	20.0
Ethanol, 2-(2-b...	10.328	5.3	ng	492447	2	10.534	1857710	20.0
2-Butenoic acid...	12.193	7.0	ng	649697	2	10.534	1857710	20.0
unknown15.045	15.045	3.6	ng	422637	3	14.381	2338390	20.0
benzenamine, 2-...	15.328	2.3	ng	266357	3	14.381	2338390	20.0
unknown16.651	16.651	5.7	ng	722547	4	17.133	2521310	20.0
Benzoic acid, 3...	17.628	2.0	ng	254750	4	17.133	2521310	20.0
n-Hexadecanoic ...	18.045	13.2	ng	1658280	4	17.133	2521310	20.0
Octadecanoic acid	19.280	6.5	ng	908232	5	21.233	2781760	20.0
1-Tetracosene	20.957	3.6	ng	494813	5	21.233	2781760	20.0
unknown22.892	22.892	6.2	ng	922950	6	23.557	2975770	20.0