LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130381.D
Acq On : 22 Sep 2022 18:08
Operator : CG\JU
Sample : N4609-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DSN003

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_F\Methods\8270-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.834	463	467	473	rBV	66440	78193	2.28%	0.431%
2	5.257	535	539	552	rBV	1477921	1307978	38.07%	7.208%
3	6.292	711	715	732	rVB	837087	833952	24.27%	4.595%
4	6.657	773	777	780	rBV	705534	640751	18.65%	3.531%
5	7.222	867	873	876	rBV	1898769	1952752	56.84%	10.760%
6	7.416	901	906	910	rVB2	34072	39795	1.16%	0.219%
7	7.516	920	923	929	rVB	41974	41548	1.21%	0.229%
8	7.857	979	981	983	rBV	237428	270974	7.89%	1.493%
9	7.939	991	995	998	rVB	861183	791816	23.05%	4.363%
10	8.310	1052	1058	1061	rBV	45221	62326	1.81%	0.343%
11	8.822	1138	1145	1149	rBV	66221	62265	1.81%	0.343%
12	8.928	1160	1163	1167	rVB	65415	53108	1.55%	0.293%
13	9.016	1172	1178	1181	rBV	4151624	3435562	100.00%	18.931%
14	9.145	1195	1200	1210	rVB	132198	205087	5.97%	1.130%
15	9.375	1231	1239	1243	rBV6	23902	46387	1.35%	0.256%
16	9.686	1286	1292	1295	rBV	999877	800785	23.31%	4.413%
17	9.845	1316	1319	1324	rBV	84392	89362	2.60%	0.492%
18	10.475	1422	1426	1429	rBV	2023823	1703066	49.57%	9.385%
19	10.598	1443	1447	1454	rVB2	31130	52479	1.53%	0.289%
20	10.933	1501	1504	1509	rVB	235613	181402	5.28%	1.000%
21	11.045	1519	1523	1525	rBV2	48185	45887	1.34%	0.253%
22	11.169	1540	1544	1547	rBV	759029	646710	18.82%	3.564%
23	11.575	1608	1613	1616	rBV	192521	185121	5.39%	1.020%
24	11.710	1632	1636	1643	rBV2	304053	327346	9.53%	1.804%
25	12.274	1729	1732	1740	rVB	260077	221954	6.46%	1.223%
26	12.363	1744	1747	1750	rVB	56266	47381	1.38%	0.261%
27	12.492	1766	1769	1774	rBV3	42219	60645	1.77%	0.334%
28	12.680	1797	1801	1804	rBV	99568	85787	2.50%	0.473%
29	12.757	1809	1814	1817	rBV	2765551	2333068	67.91%	12.856%
30	13.798	1987	1991	1997	rBV	681692	603594	17.57%	3.326%
31	13.904	2003	2009	2013	rBV	261307	315669	9.19%	1.739%
32	14.645	2131	2135	2140	rVB	77142	78614	2.29%	0.433%
33	15.192	2223	2228	2232	rBV	486485	546073	15.89%	3.009%

Sum of corrected areas: 18147437

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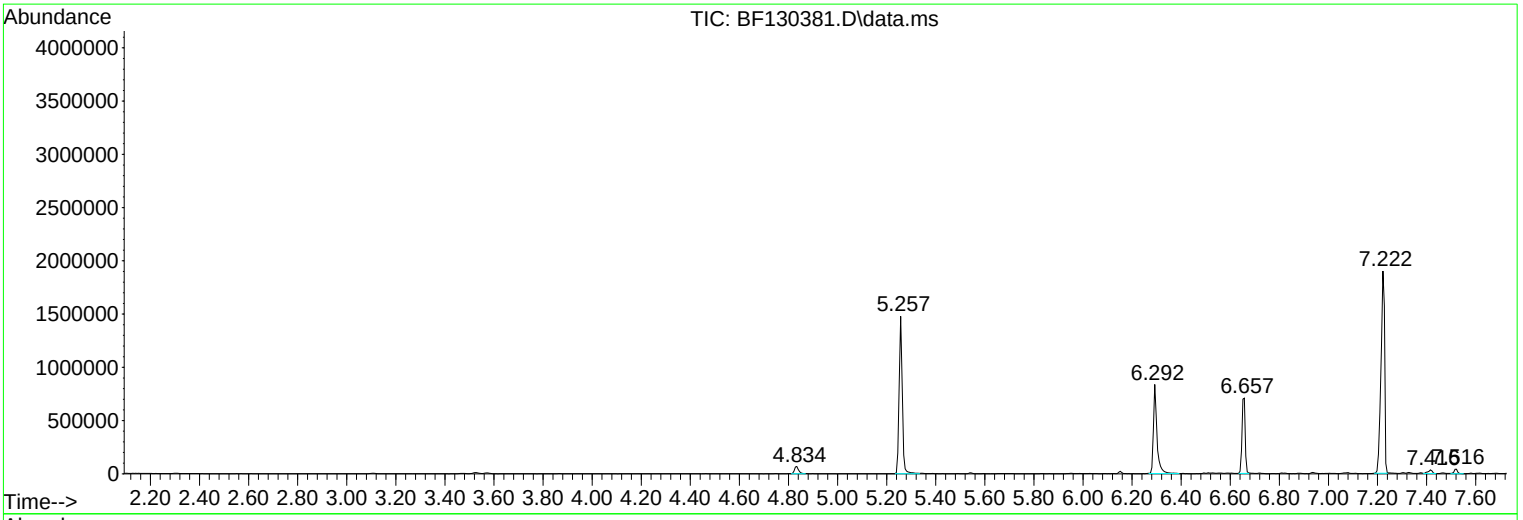
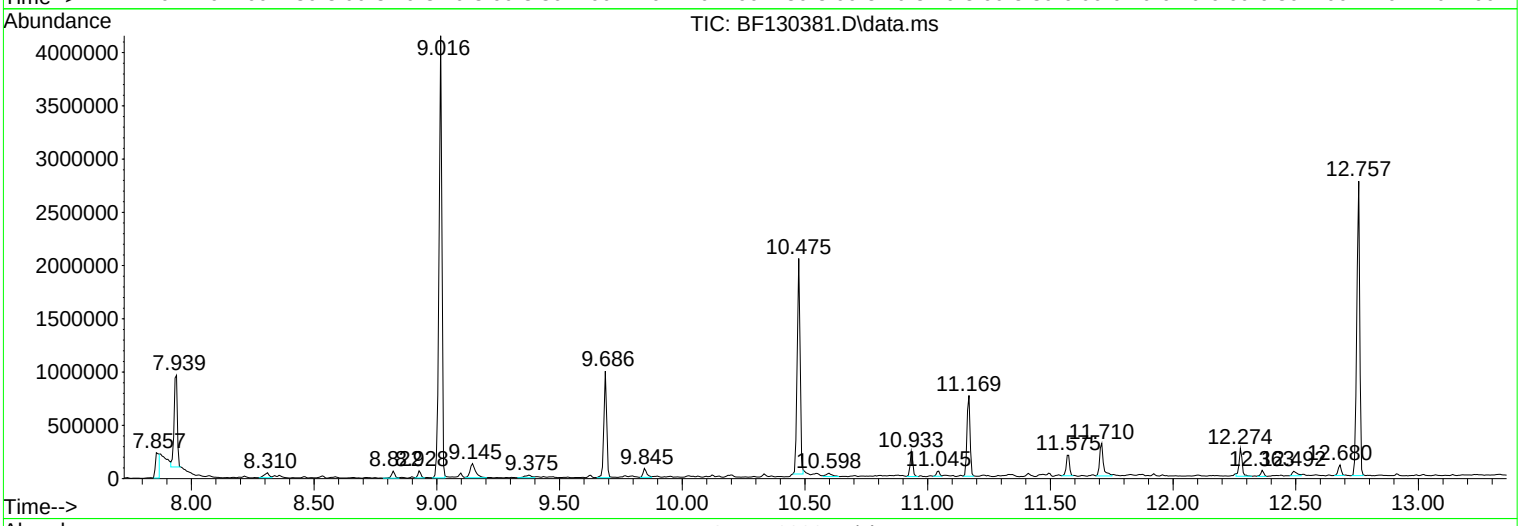
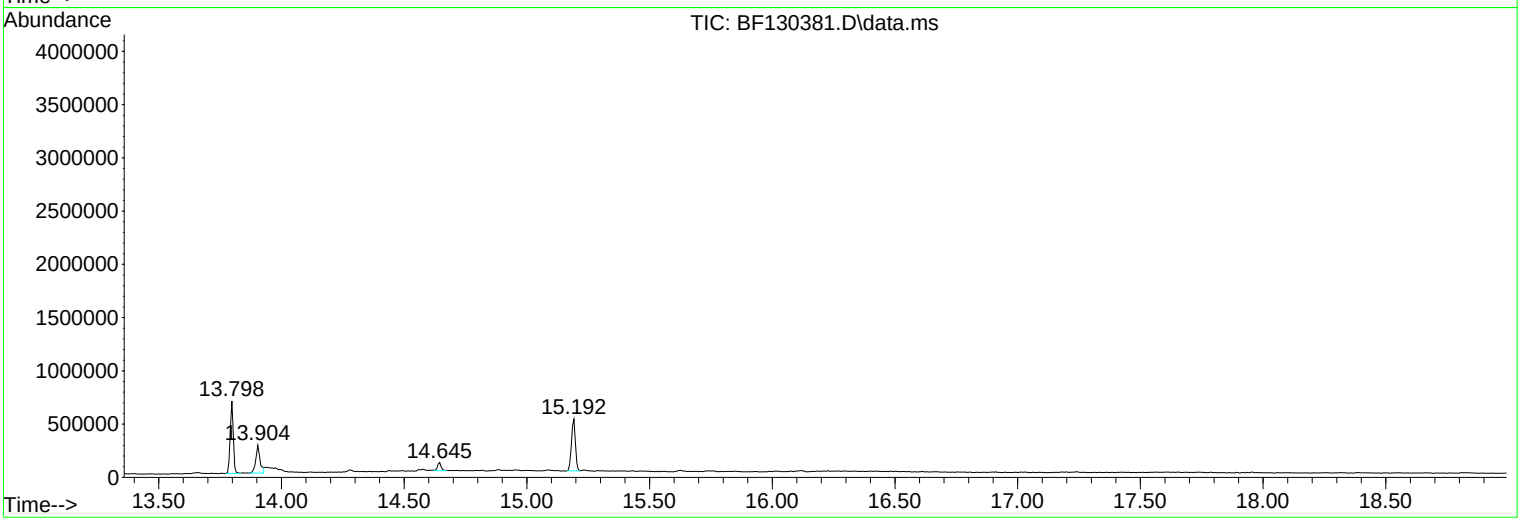
Instrument :
BNA_F
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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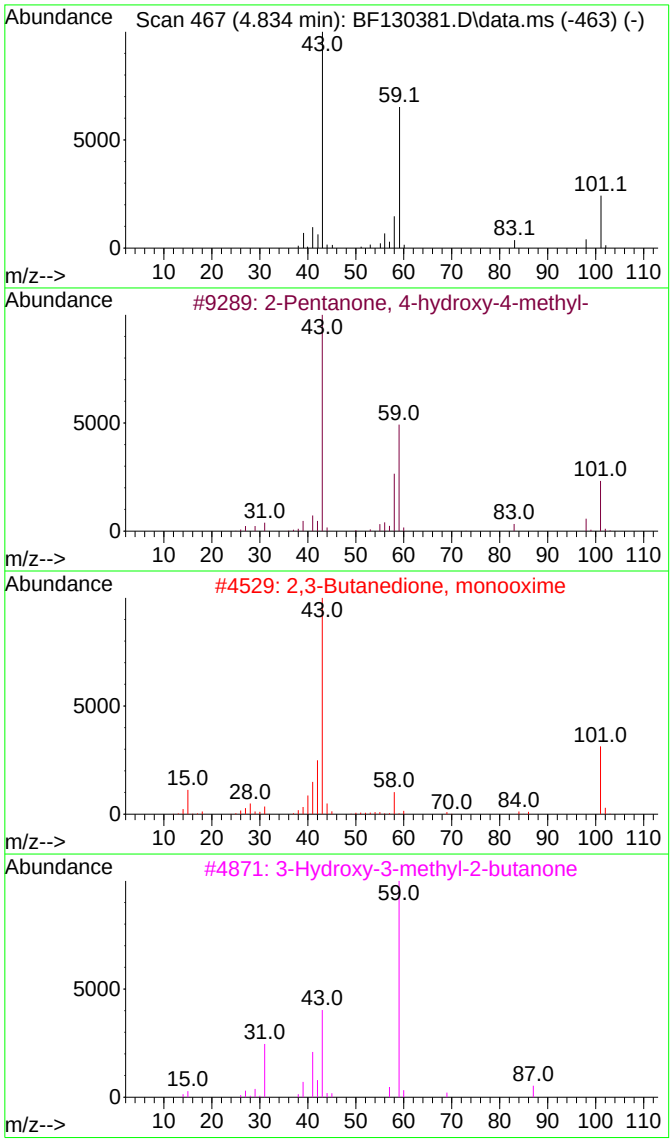
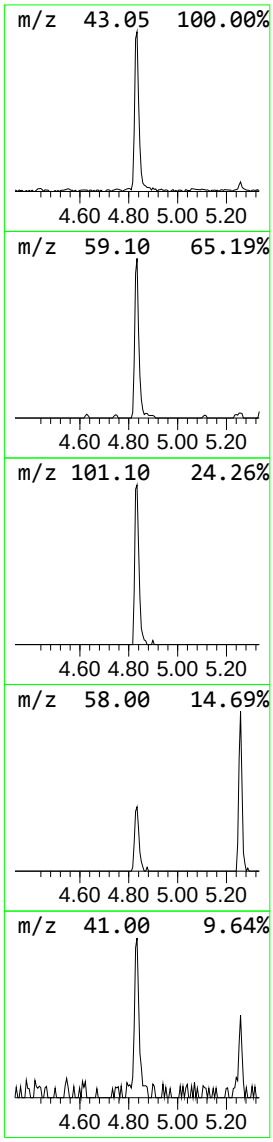
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.834	2.44 ng	78193	1,4-Dichlorobenzene-d4	6.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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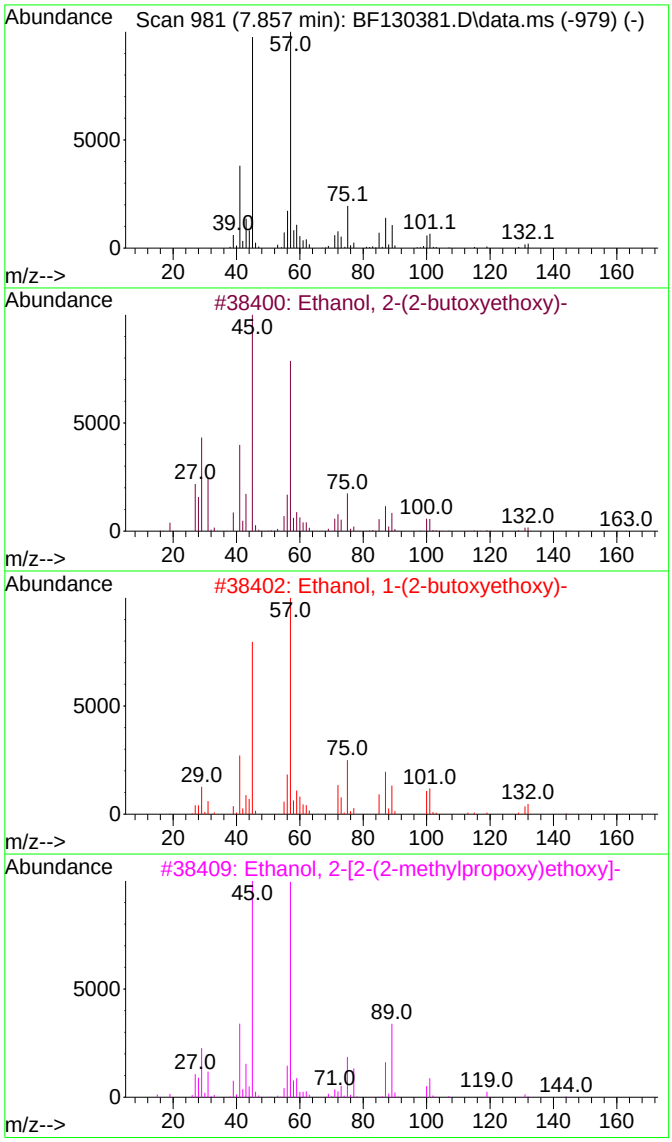
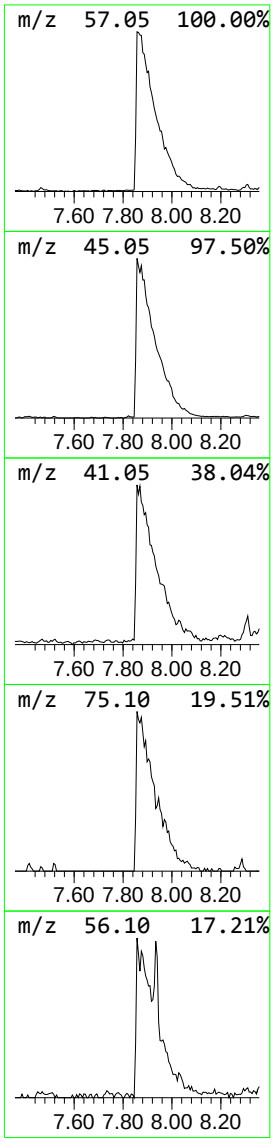
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.857	6.84 ng	270974	Naphthalene-d8	7.939

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	78
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





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Instrument :
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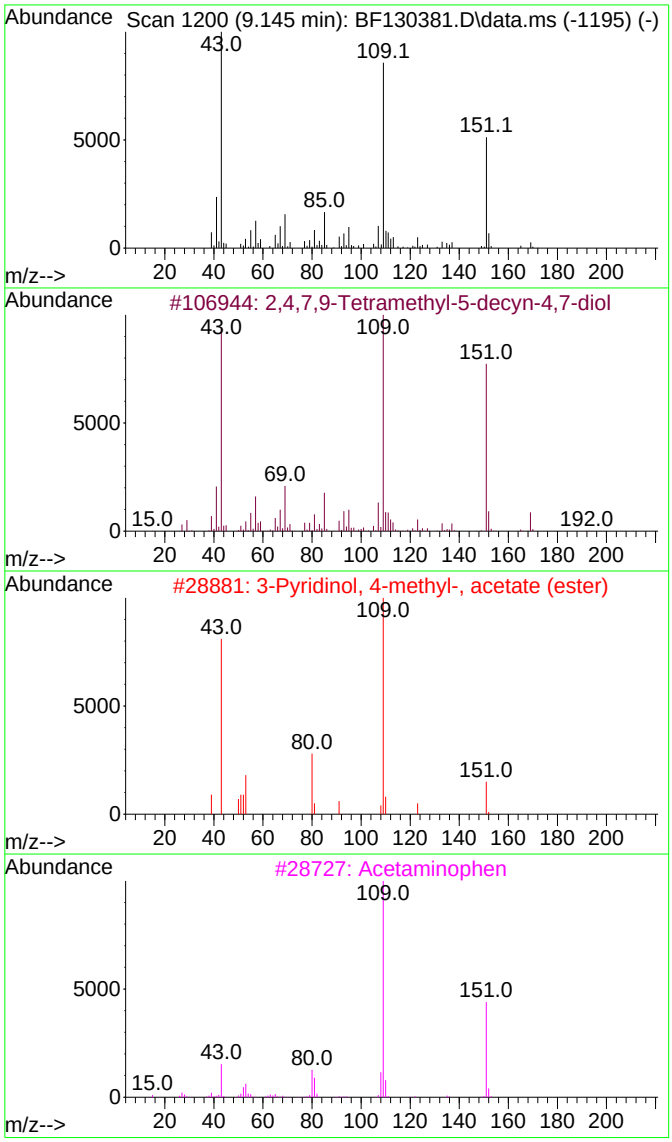
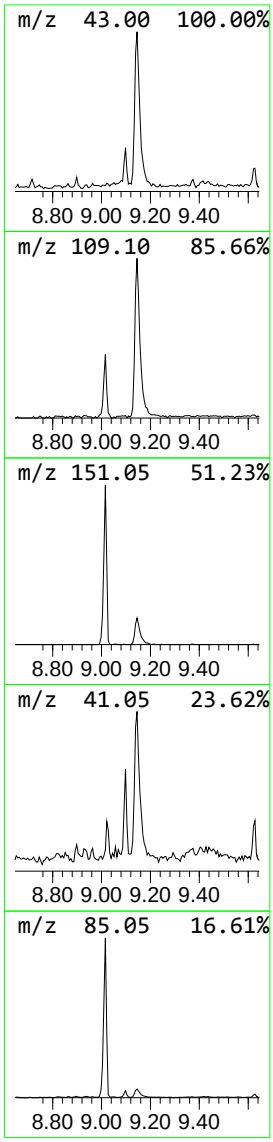
****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.145	5.12 ng	205087	Acenaphthene-d10	9.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
3	Acetaminophen	151	C8H9NO2	000103-90-2	53
4	Metacetamol	151	C8H9NO2	000621-42-1	53
5	N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN	1000250-88-9	47





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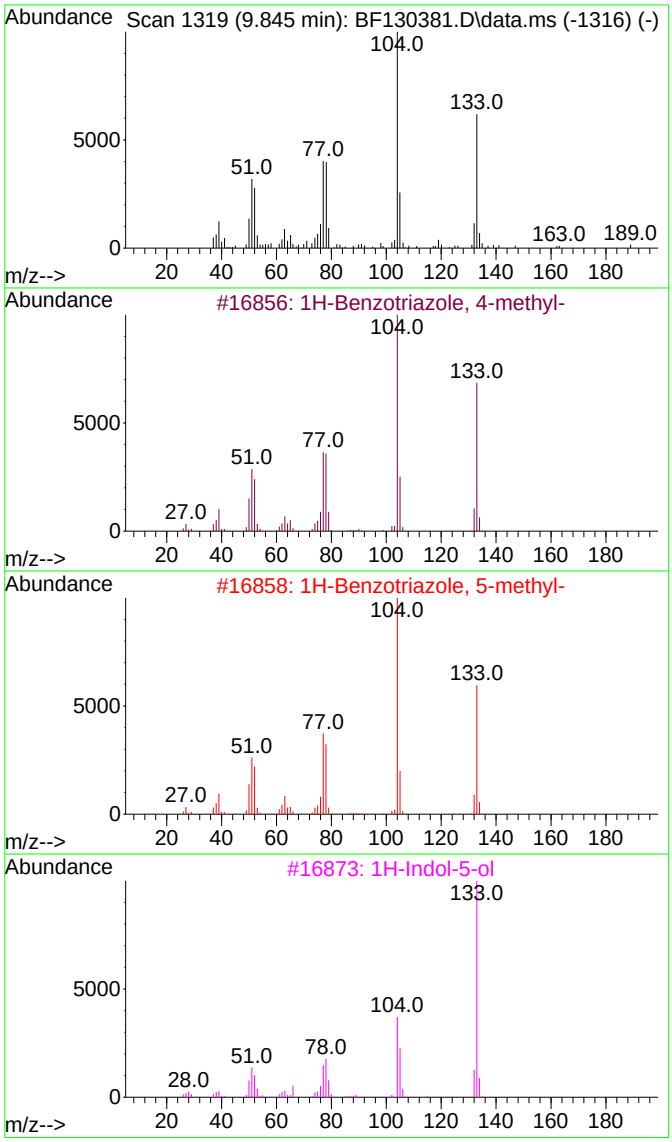
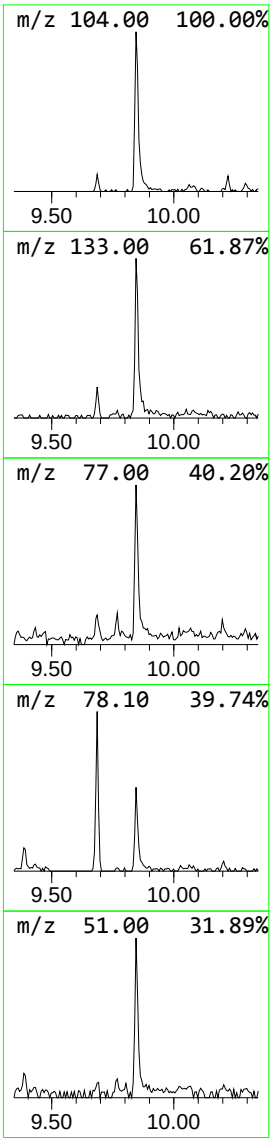
****

Peak Number 4 1H-Benzotriazole, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.845	2.23 ng	89362	Acenaphthene-d10	9.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	98
2	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	97
3	1H-Indol-5-ol	133	C8H7NO	001953-54-4	64
4	1H-Indol-4-ol	133	C8H7NO	002380-94-1	62
5	Benzene, 1-isocyanato-3-methyl-	133	C8H7NO	000621-29-4	47





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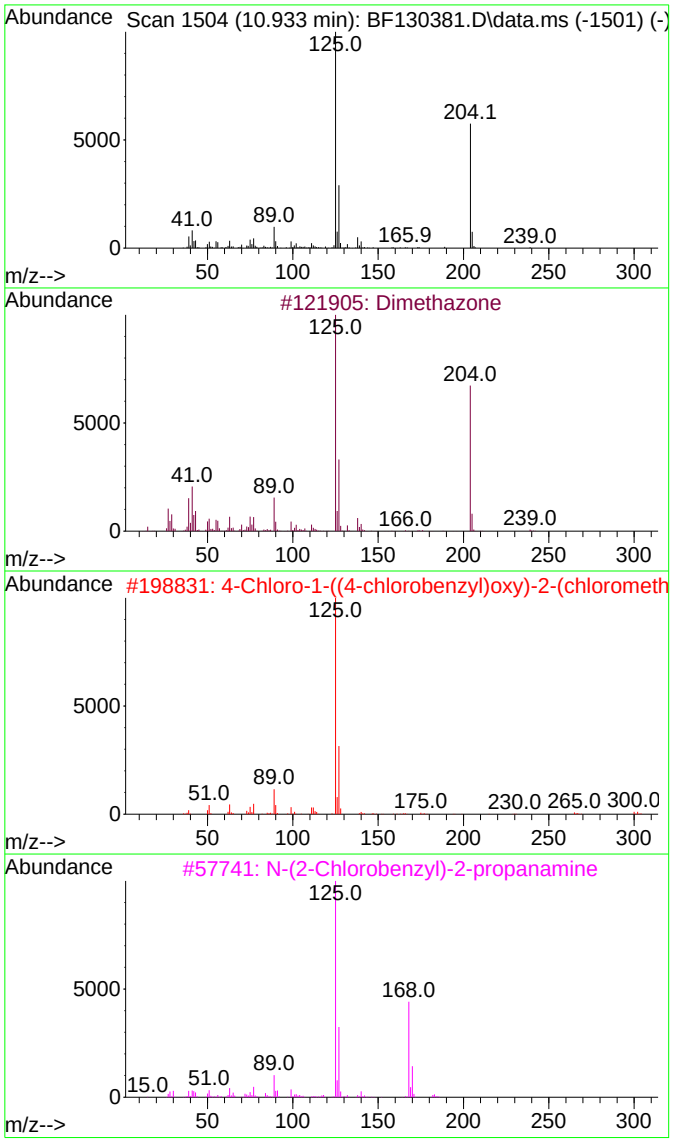
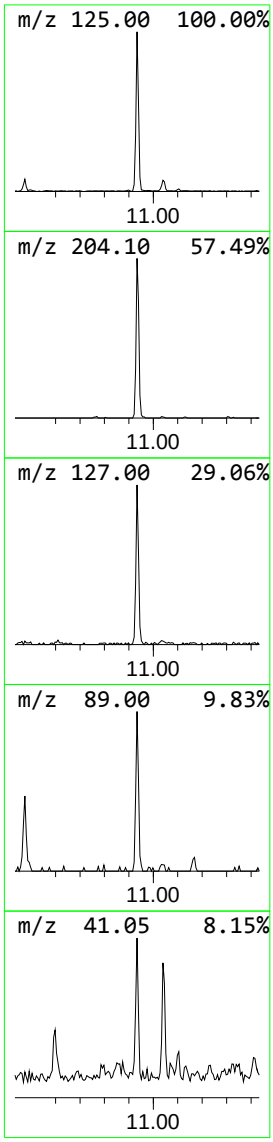
****

Peak Number 5 Dimethazone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.933	5.61 ng	181402	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethazone	239	C12H14ClNO2	081777-89-1	93
2	4-Chloro-1-((4-chlorobenzyl)oxy)...	300	C14H11Cl3O	1094411-25-2	52
3	N-(2-Chlorobenzyl)-2-propanamine	183	C10H14ClN	046054-87-9	50
4	2-[(4-Chlorobenzyl)oxy]benzaldehyde	246	C14H11ClO2	1000484-43-2	50
5	Benzeneacetic acid, 4-chloro-, m...	184	C9H9ClO2	052449-43-1	50





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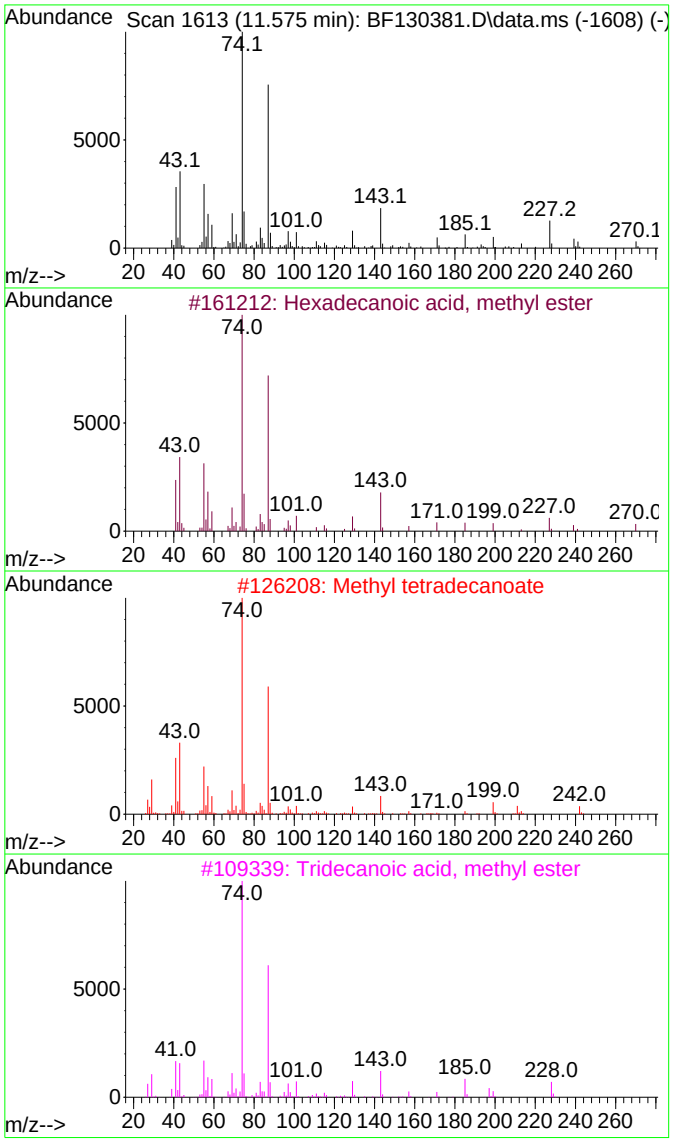
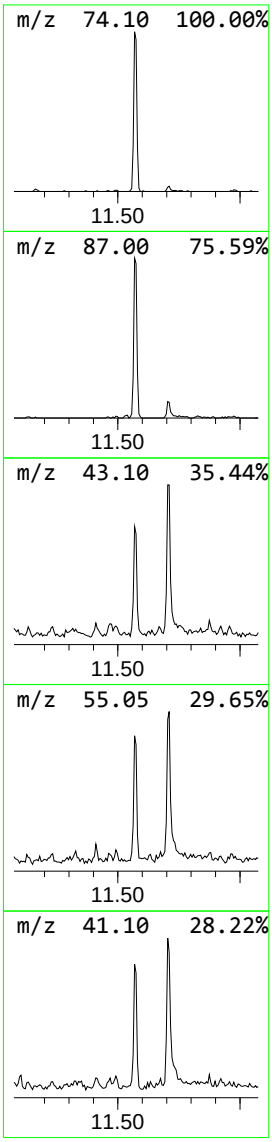
****
Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.575	5.73 ng	185121	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	86
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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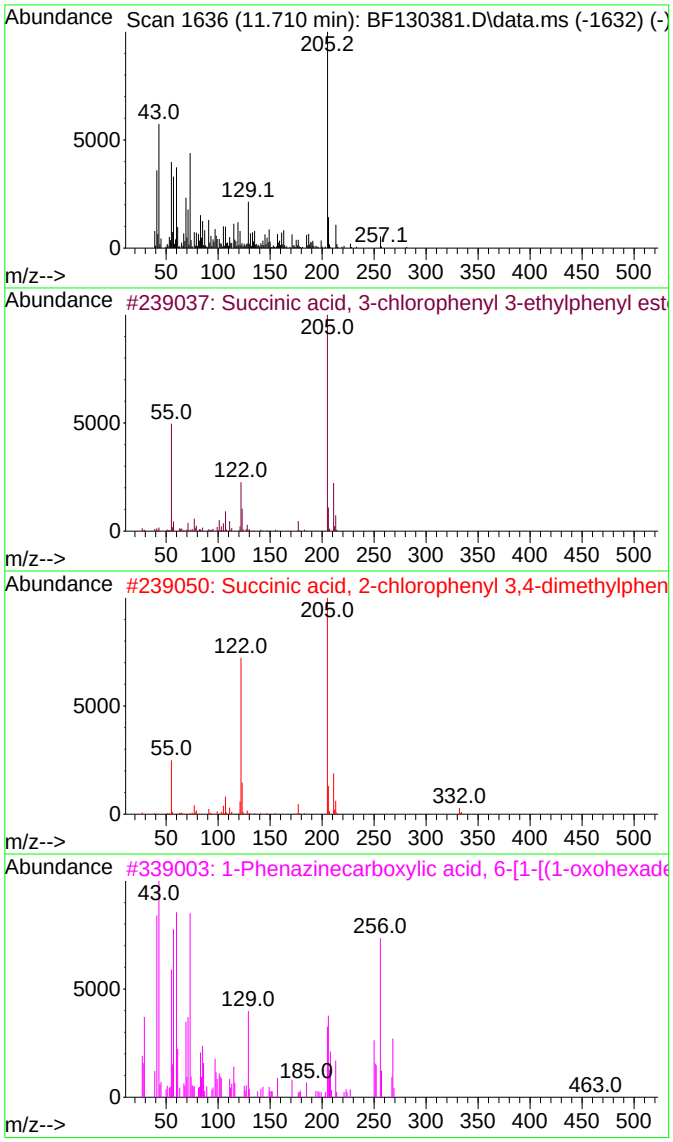
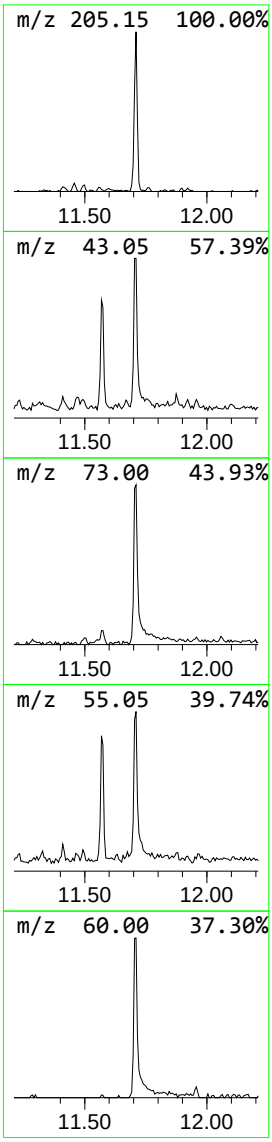
Peak Number 7 unknown11.710 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.710	10.12 ng	327346	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 3-chlorophenyl 3-...	332	C18H17ClO4	1000390-10-7	47
2	Succinic acid, 2-chlorophenyl 3,...	332	C18H17ClO4	1000357-55-3	43
3	1-Phenazinecarboxylic acid, 6-[1...	506	C31H42N2O4	120464-92-8	43
4	Pyridine, 3,5-dichloro-4-methoxy...	205	C8H9Cl2NO	051050-42-1	38
5	Succinic acid, di(2-ethylphenyl)...	326	C20H22O4	1000389-95-7	38





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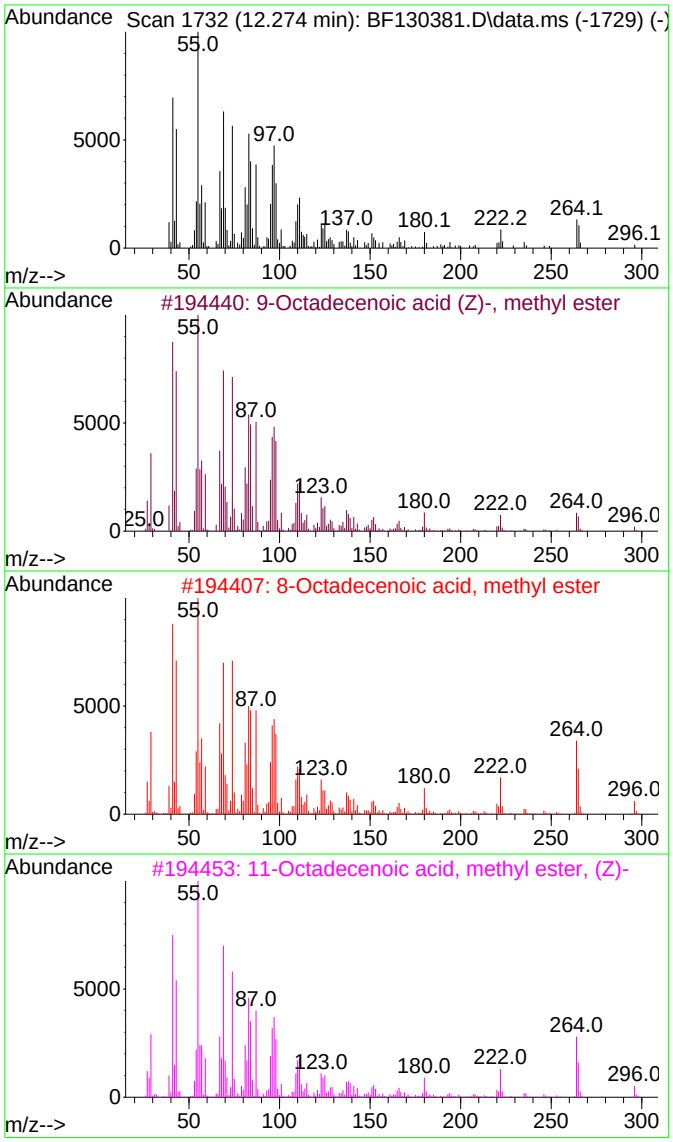
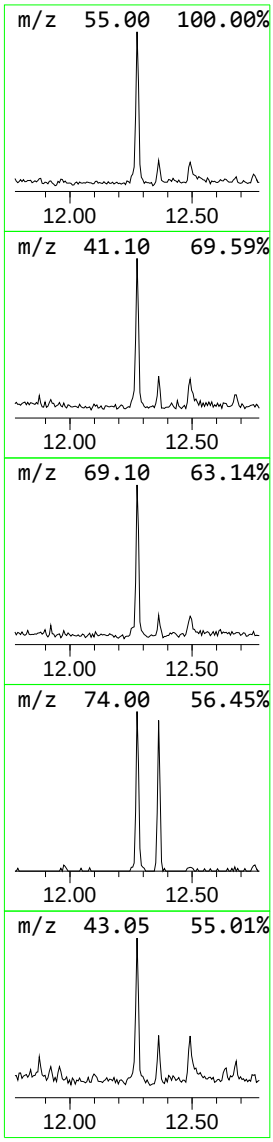
****
Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.275	6.86 ng	221954	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99





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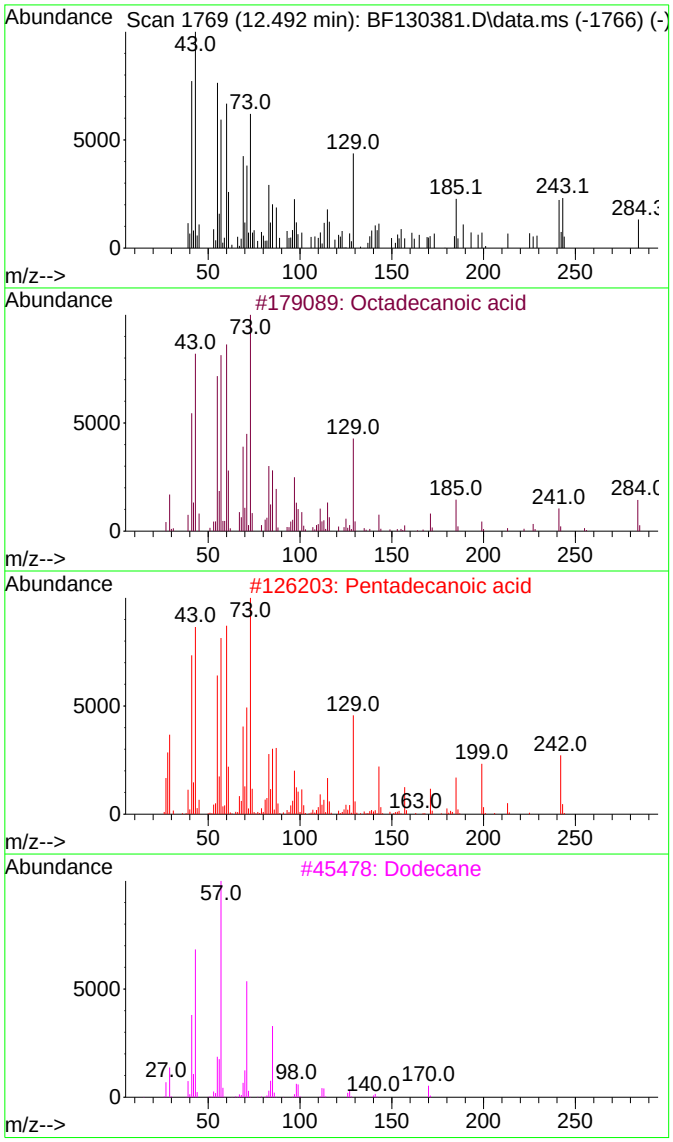
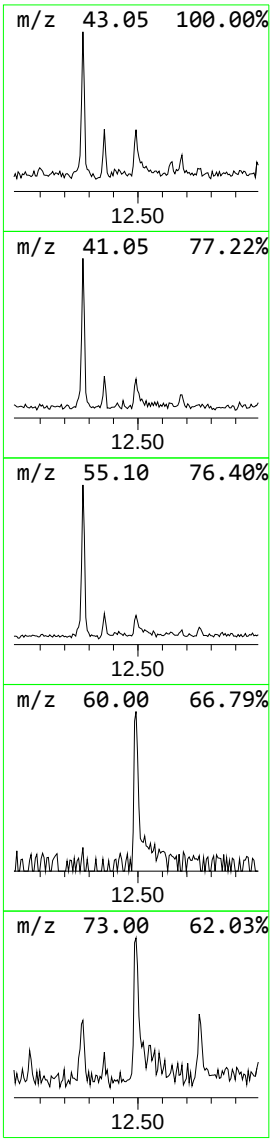
Peak Number 9 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	2.01 ng	60645	Chrysene-d12	13.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Dodecane	170	C12H26	000112-40-3	15
4	Octane, 2-methyl-	128	C9H20	003221-61-2	15
5	Tridecane	184	C13H28	000629-50-5	15





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Data File : BF130381.D
Acq On : 22 Sep 2022 18:08
Operator : CG\JU
Sample : N4609-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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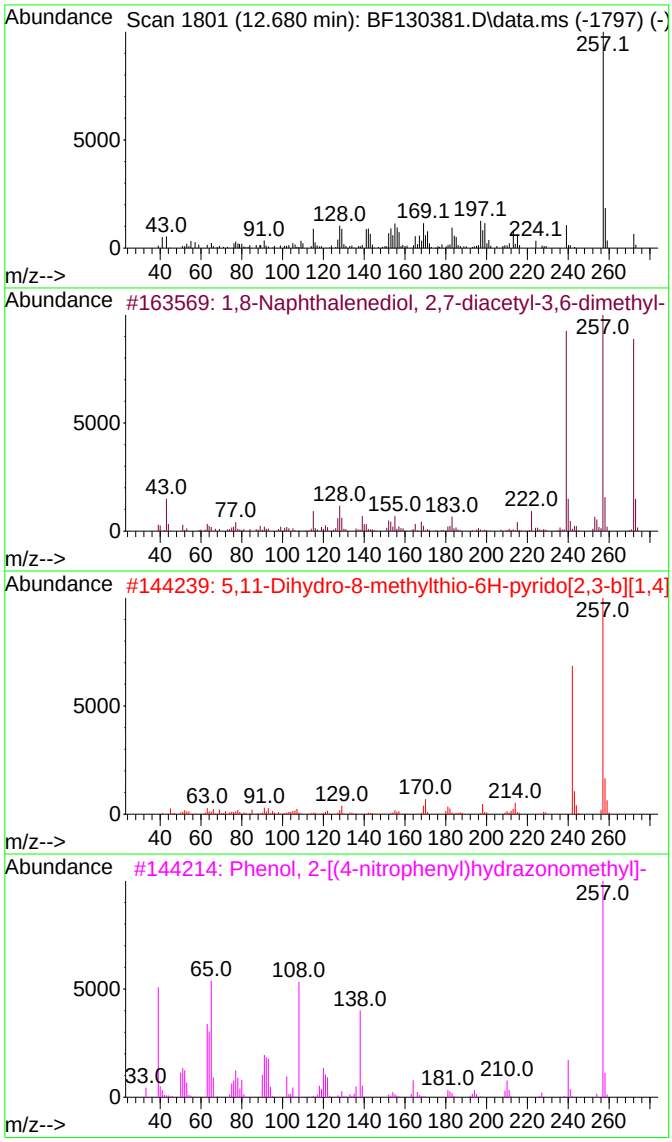
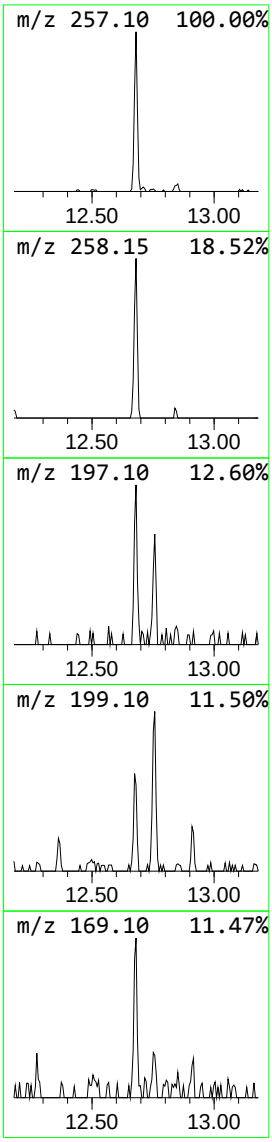
Peak Number 10 1,8-Naphthalenediol, 2,7-di... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	2.84 ng	85787	Chrysene-d12	13.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,8-Naphthalenediol, 2,7-diacety...	272	C16H16O4	100198-05-8	50
2	5,11-Dihydro-8-methylthio-6H-pyr...	257	C13H11N3OS	133727-45-4	47
3	Phenol, 2-[(4-nitrophenyl)hydraz...	257	C13H11N3O3	003155-24-6	46
4	3-Methyl-1-phenyl-4-azafluorene	257	C19H15N	062578-43-2	43
5	Benz[a]acridine, 1,5-dimethyl-	257	C19H15N	055030-47-2	43





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Operator : CG\JU
Sample : N4609-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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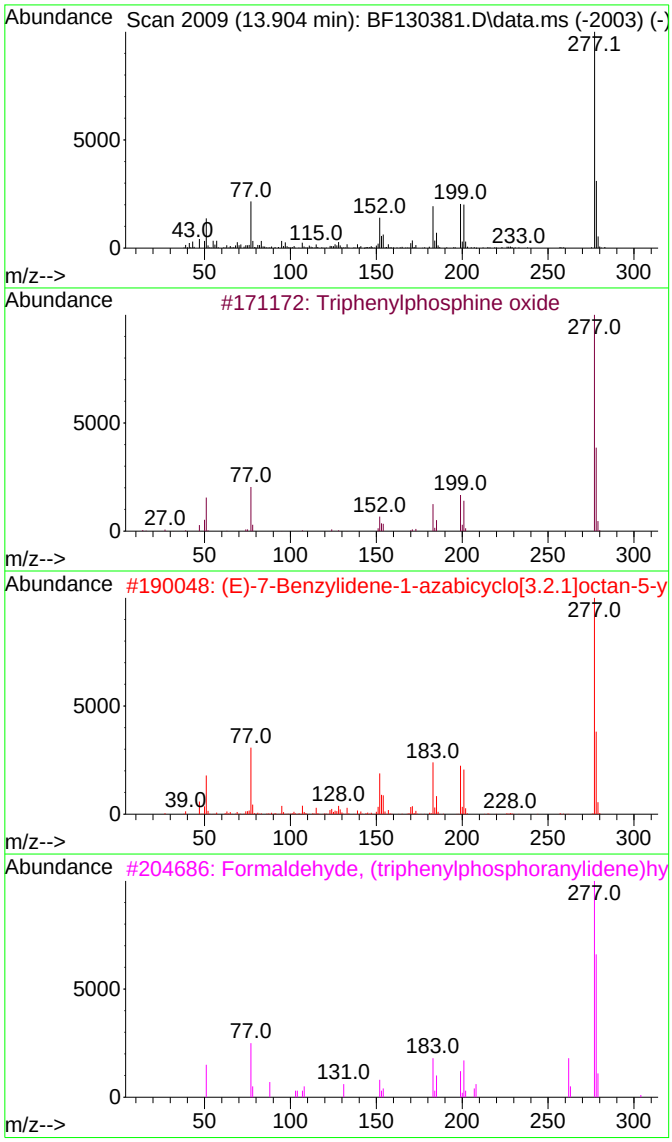
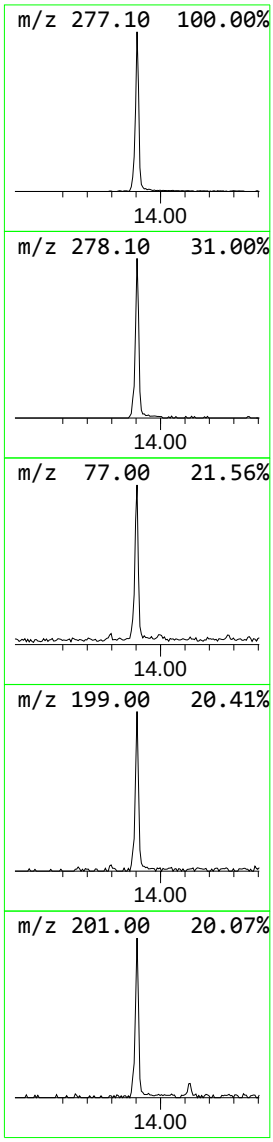
Peak Number 11 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	10.46 ng	315669	Chrysene-d12	13.798

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	76
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38





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Data File : BF130381.D
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Operator : CG\JU
Sample : N4609-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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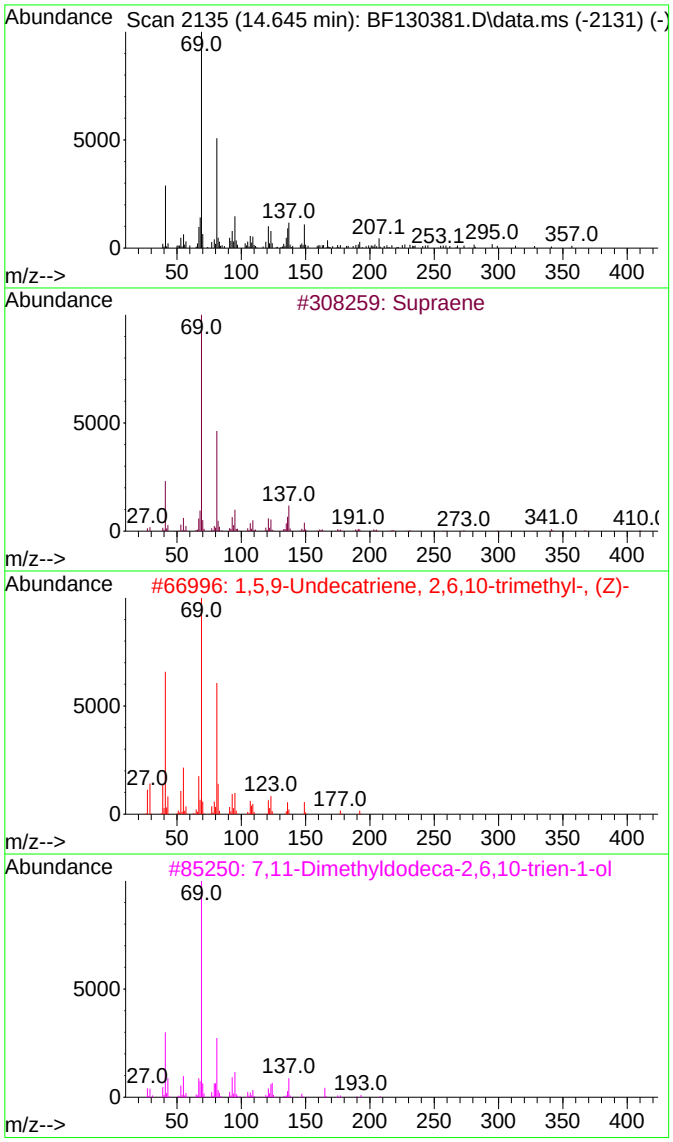
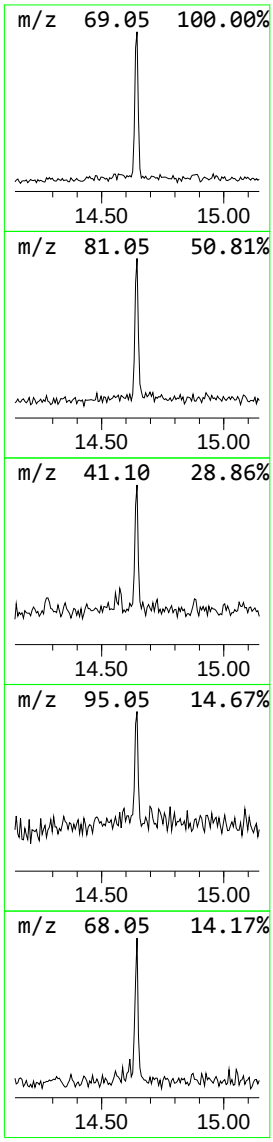
Peak Number 12 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.645	2.88 ng	78614	Perylene-d12	15.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	68
4	Farnesol isomer a	222	C15H26O	1000108-92-4	64
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59





Tentatively Identified Compound (LSC) summary

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Data File : BF130381.D
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Misc :
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Instrument :
BNA_F
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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.834	2.4	ng	78193	1	6.657	640751	20.0
Ethanol, 2-(2-b...	7.857	6.8	ng	270974	2	7.939	791816	20.0
2,4,7,9-Tetrame...	9.145	5.1	ng	205087	3	9.686	800785	20.0
1H-Benzotriazol...	9.845	2.2	ng	89362	3	9.686	800785	20.0
Dimethazone	10.933	5.6	ng	181402	4	11.169	646710	20.0
Hexadecanoic ac...	11.575	5.7	ng	185121	4	11.169	646710	20.0
unknown11.710	11.710	10.1	ng	327346	4	11.169	646710	20.0
9-Octadecenoic ...	12.275	6.9	ng	221954	4	11.169	646710	20.0
Octadecanoic acid	12.492	2.0	ng	60645	5	13.798	603594	20.0
1,8-Naphthalene...	12.680	2.8	ng	85787	5	13.798	603594	20.0
Triphenylphosph...	13.904	10.5	ng	315669	5	13.798	603594	20.0
Supraene	14.645	2.9	ng	78614	6	15.192	546073	20.0