LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
Data File : BF138621.D
Acq On : 23 Jul 2024 16:32
Operator : RC/JU
Sample : P3282-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDW-T1-01

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138621.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	4	13	19	rVB	3864379	6630592	100.00%	27.053%
2	2.969	142	149	158	rVB	252766	466841	7.04%	1.905%
3	5.075	503	507	514	rVB	71929	103004	1.55%	0.420%
4	5.481	566	576	587	rBV	1238465	1638148	24.71%	6.684%
5	6.487	741	747	758	rBV	852228	1153992	17.40%	4.708%
6	6.681	771	780	786	rBV	54055	80104	1.21%	0.327%
7	6.851	804	809	814	rBV	402522	489981	7.39%	1.999%
8	6.998	827	834	853	rVB	1051181	1562473	23.56%	6.375%
9	7.416	897	905	910	rBV	1340319	1910384	28.81%	7.794%
10	7.881	975	984	1000	rBV2	92339	202441	3.05%	0.826%
11	8.134	1021	1027	1039	rBV	530032	689537	10.40%	2.813%
12	8.445	1076	1080	1090	rVB	113802	174703	2.63%	0.713%
13	9.210	1203	1210	1215	rVB	2358428	3123880	47.11%	12.746%
14	9.886	1316	1325	1330	rBV	591850	744552	11.23%	3.038%
15	9.981	1333	1341	1347	rBV	70400	125568	1.89%	0.512%
16	10.675	1453	1459	1474	rBV	1338599	1797431	27.11%	7.334%
17	11.369	1572	1577	1585	rBV	513870	657197	9.91%	2.681%
18	11.892	1661	1666	1675	rBV2	117200	194244	2.93%	0.793%
19	12.463	1758	1763	1775	rVB3	36483	85279	1.29%	0.348%
20	12.704	1801	1804	1811	rVB2	50292	75057	1.13%	0.306%
21	12.957	1841	1847	1852	rVB	1334305	1755164	26.47%	7.161%
22	13.869	1998	2002	2012	rVB	52201	114844	1.73%	0.469%
23	14.004	2021	2025	2031	rVB	270022	355930	5.37%	1.452%
24	15.468	2268	2274	2284	rVB	245077	378288	5.71%	1.543%

Sum of corrected areas: 24509634

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
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Misc :
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Instrument :
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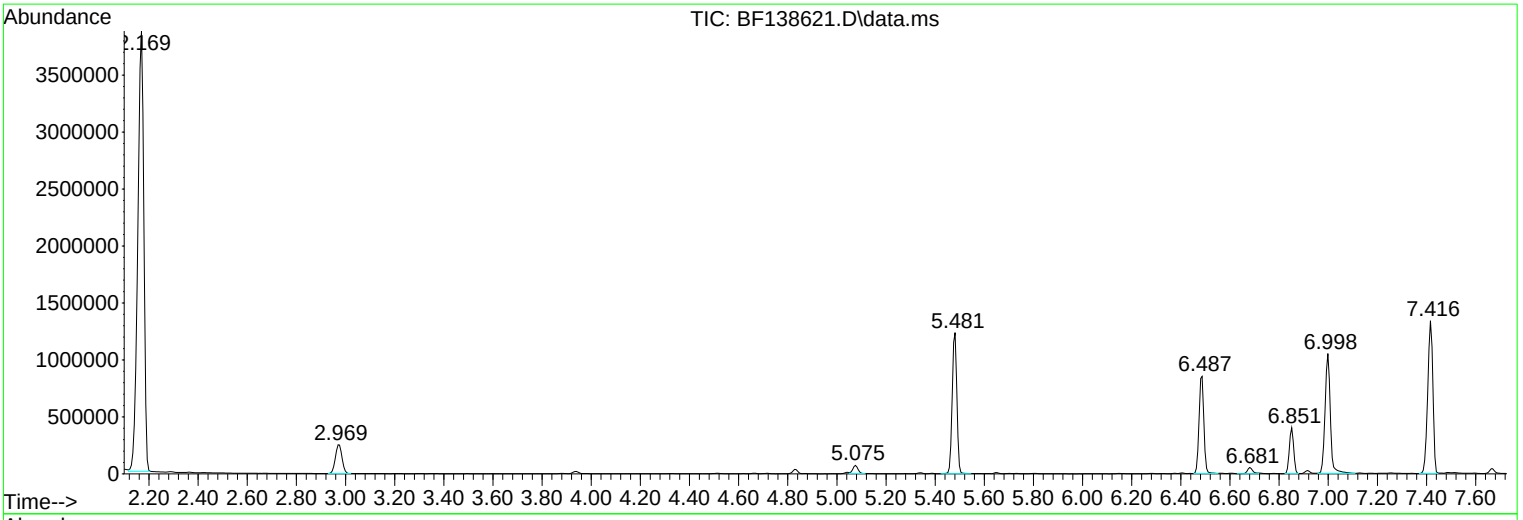
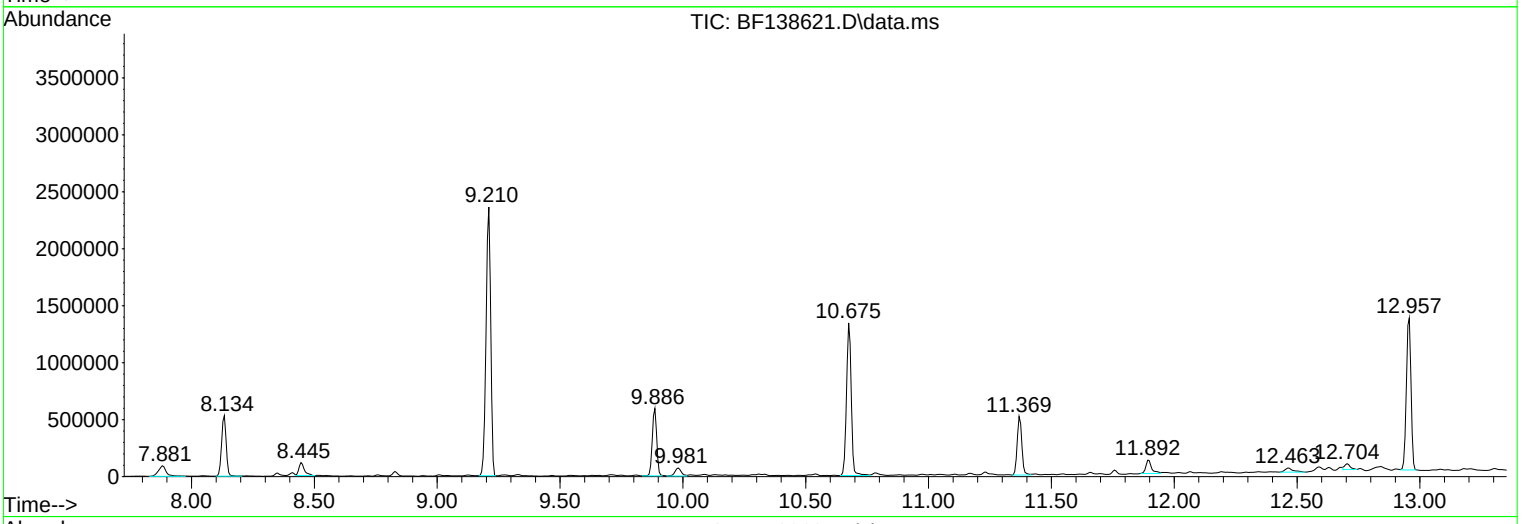
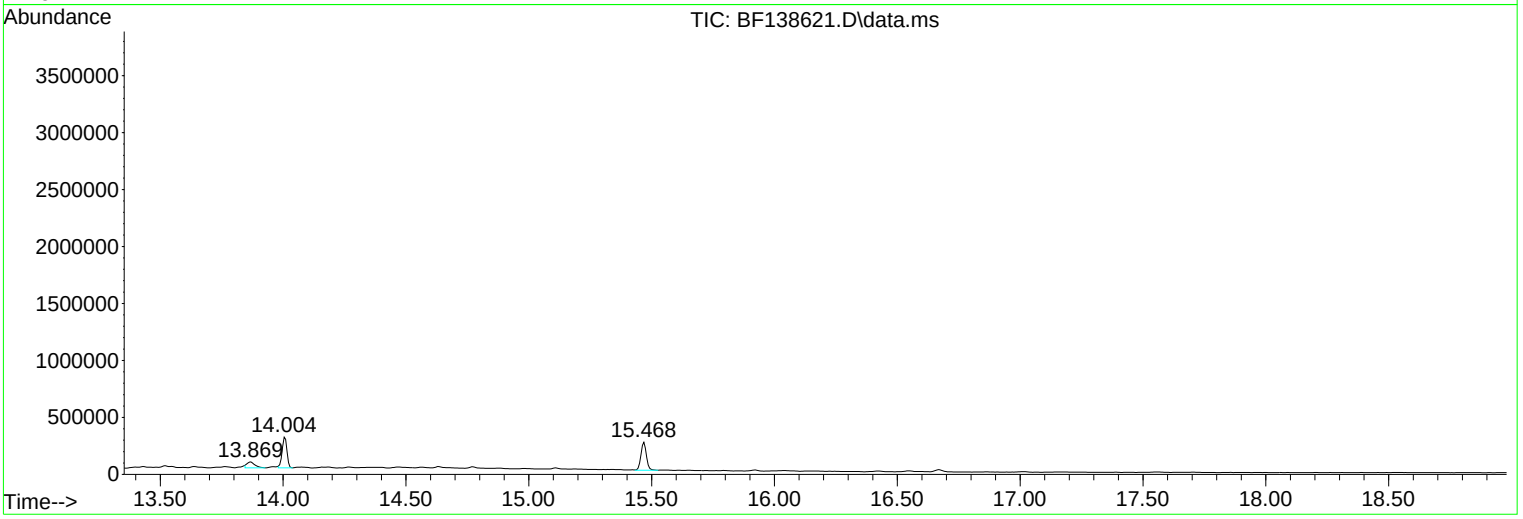
ClientSampleId :
IDW-T1-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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TIC Library : C:\Database\NIST20.L
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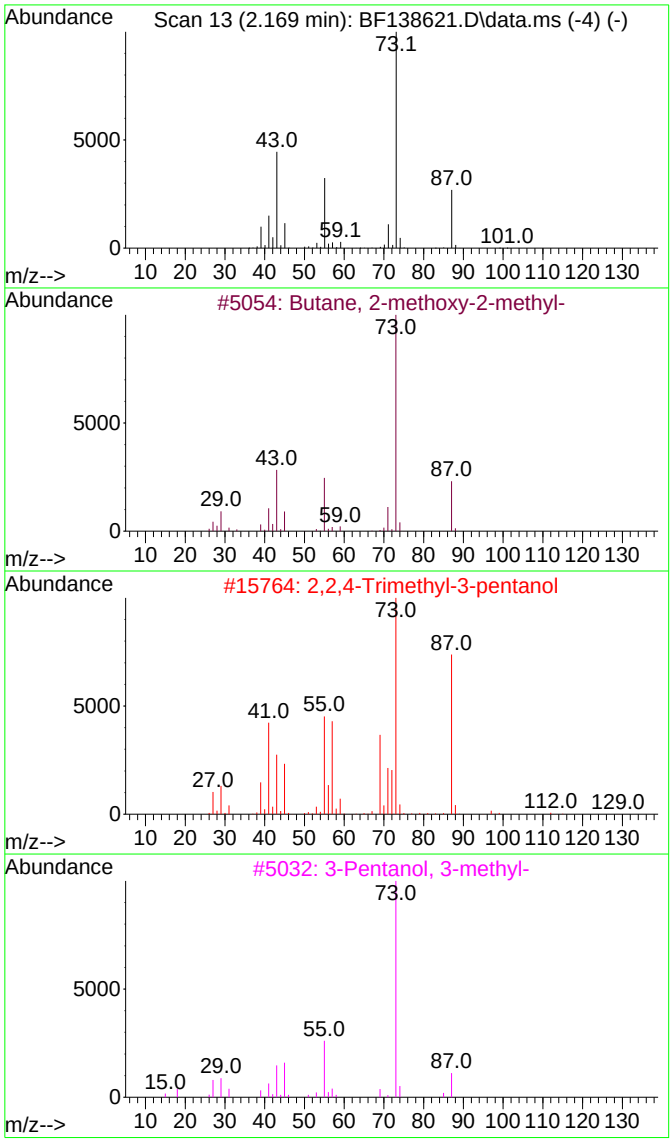
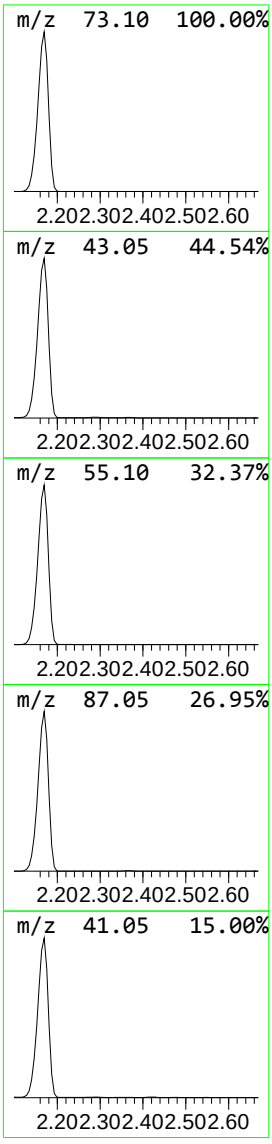
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	270.65 ng	6630590	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF138621.D
Acq On : 23 Jul 2024 16:32
Operator : RC/JU
Sample : P3282-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDW-T1-01

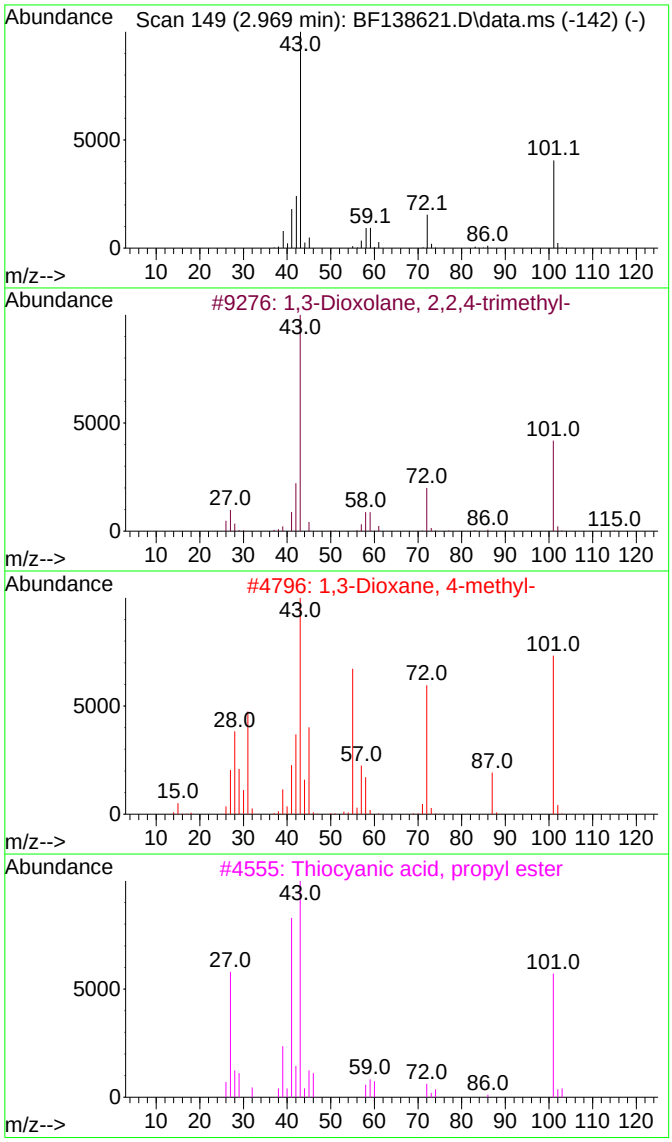
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

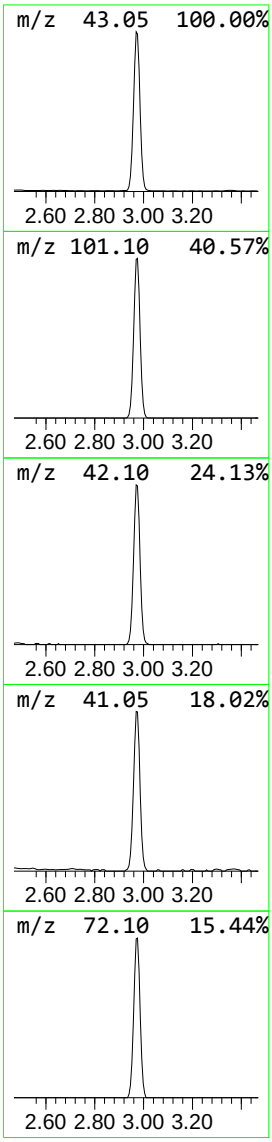
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.969	19.06 ng	466841	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	86
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	42
3	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	33
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	33
5	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9





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Acq On : 23 Jul 2024 16:32
Operator : RC/JU
Sample : P3282-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDW-T1-01

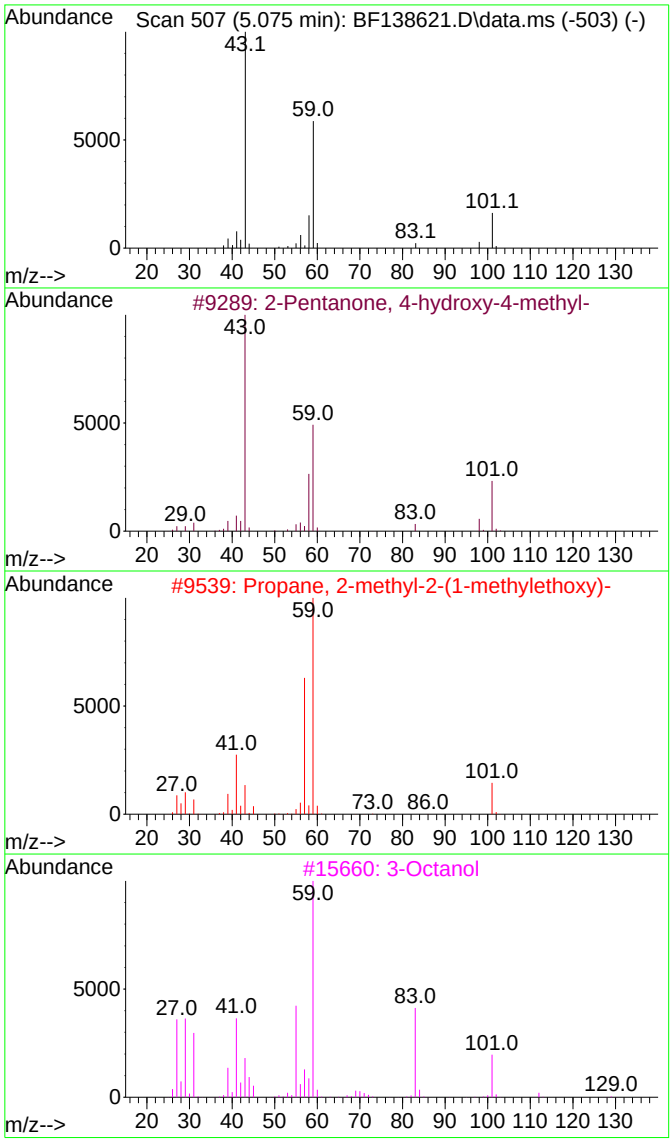
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

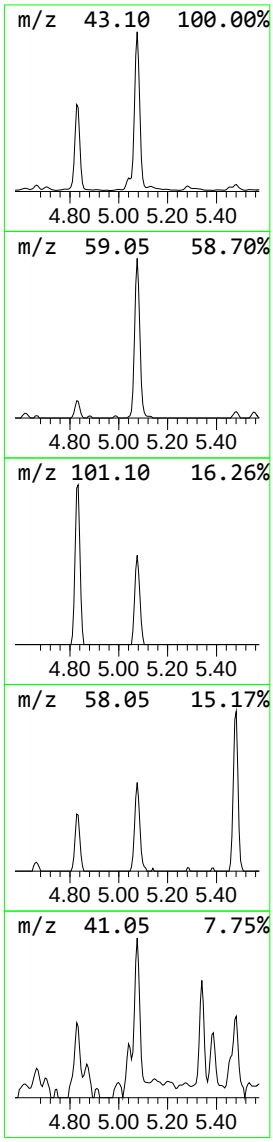
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	4.20 ng	103004	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Octanol	130	C8H18O	000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





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Operator : RC/JU
Sample : P3282-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDW-T1-01

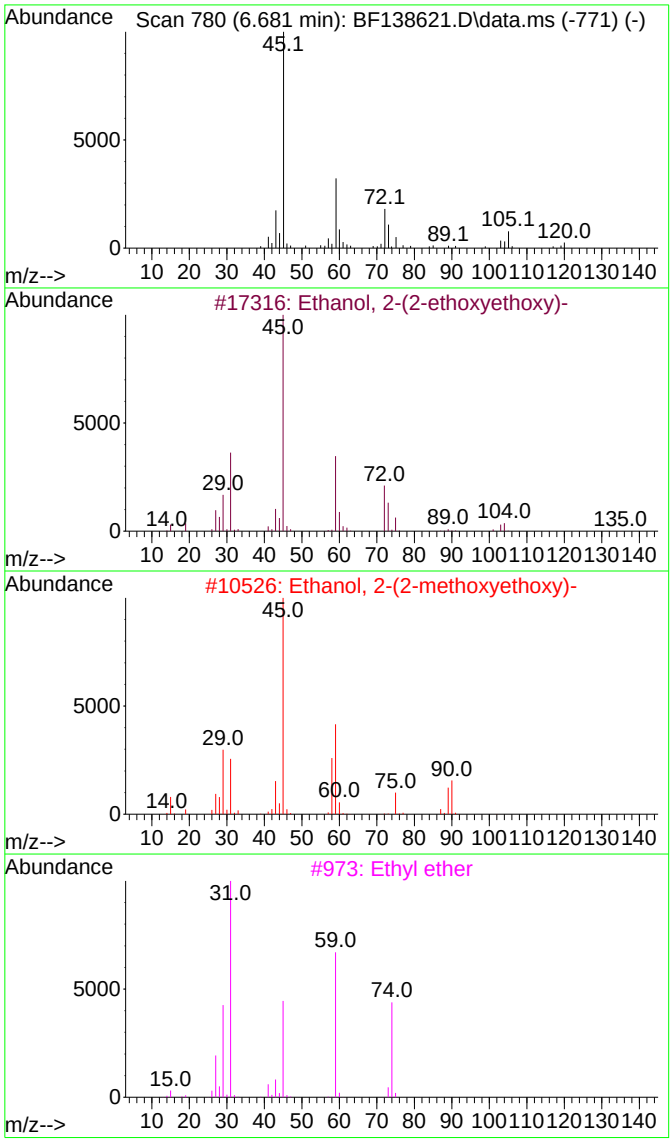
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

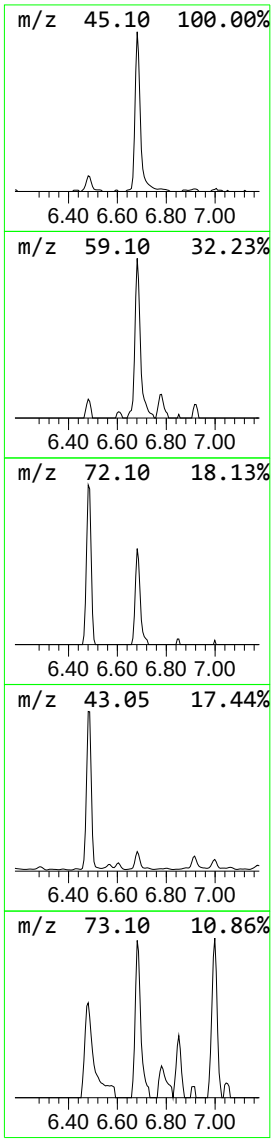
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.681	3.27 ng	80104	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
3	Ethyl ether	74	C4H10O	000060-29-7	42
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
5	Butane, 1,2,4-trimethoxy-	148	C7H16O3	020637-48-3	38





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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TIC Library : C:\Database\NIST20.L
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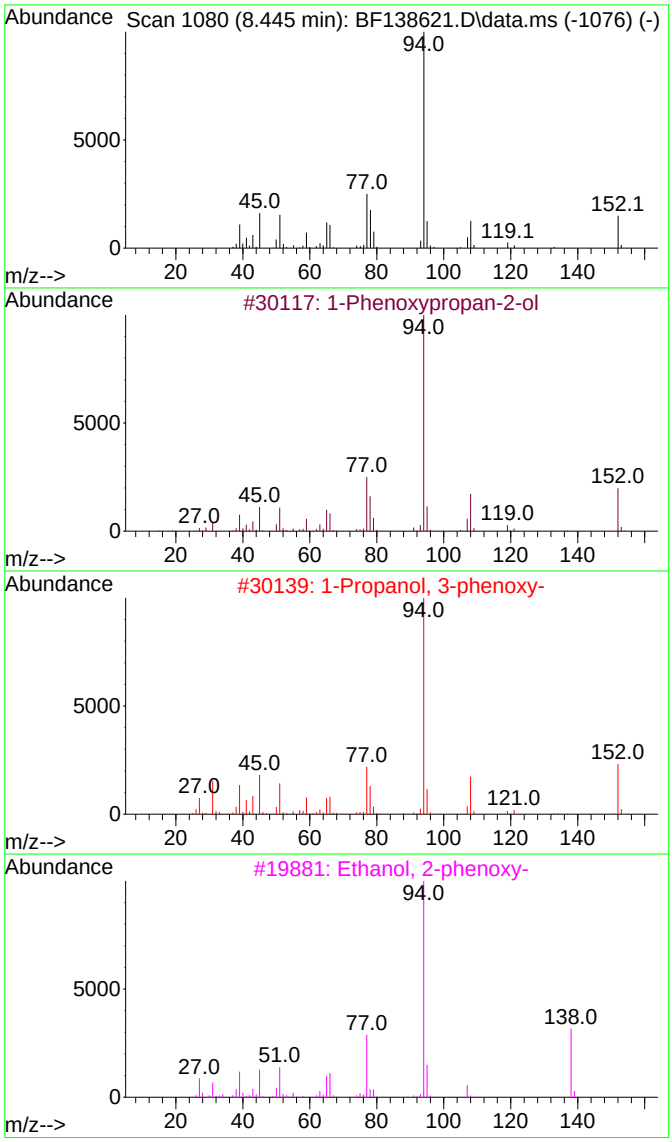
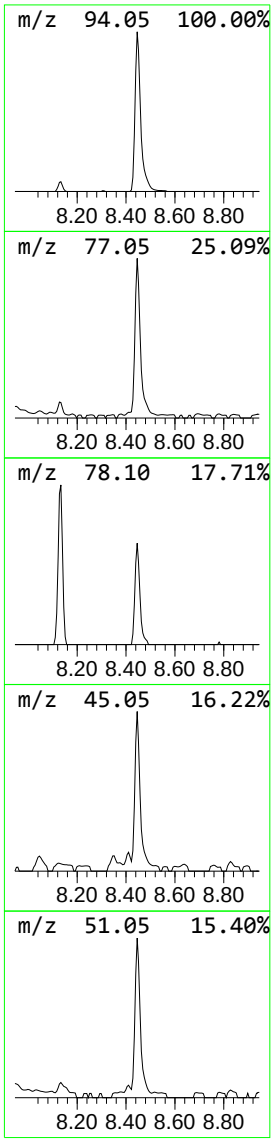
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	5.07 ng	174703	Naphthalene-d8	8.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5	2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	53





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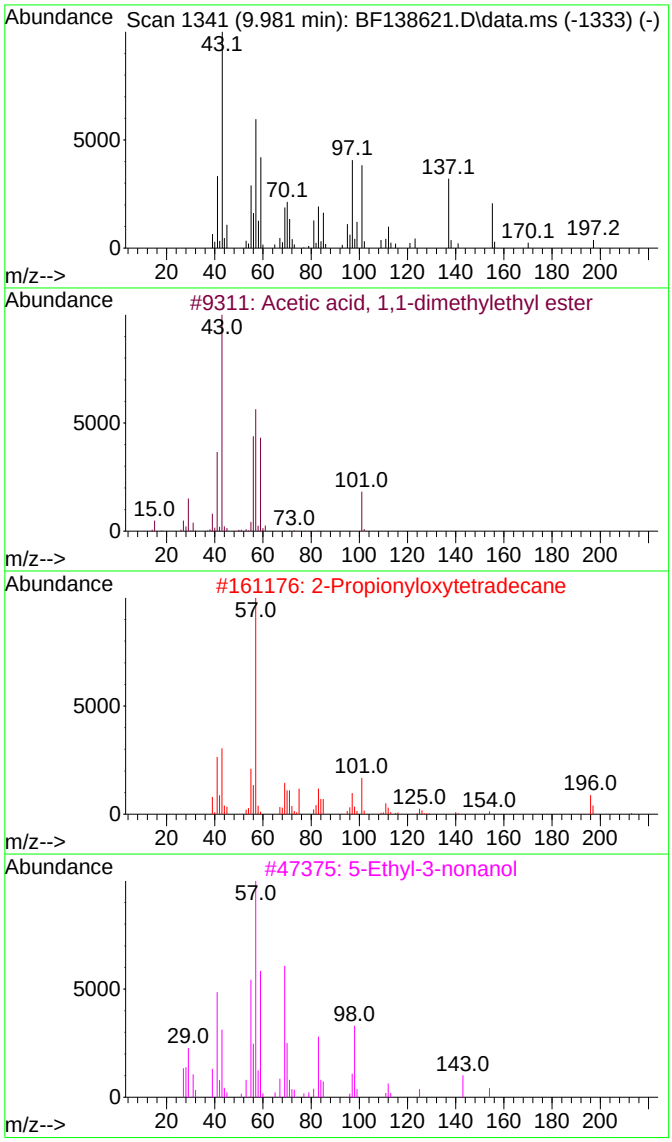
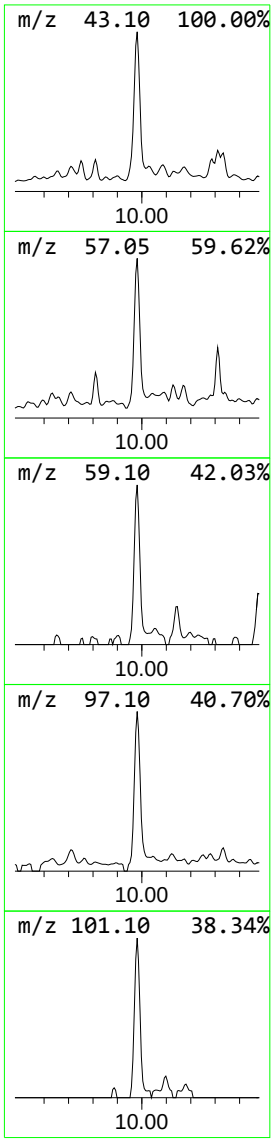
****

Peak Number 6 unknown9.981 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.981	3.37 ng	125568	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22
2	2-Propionyloxytetradecane	270	C17H34O2	1000245-62-7	16
3	5-Ethyl-3-nonanol	172	C11H24O	019780-71-3	12
4	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	12
5	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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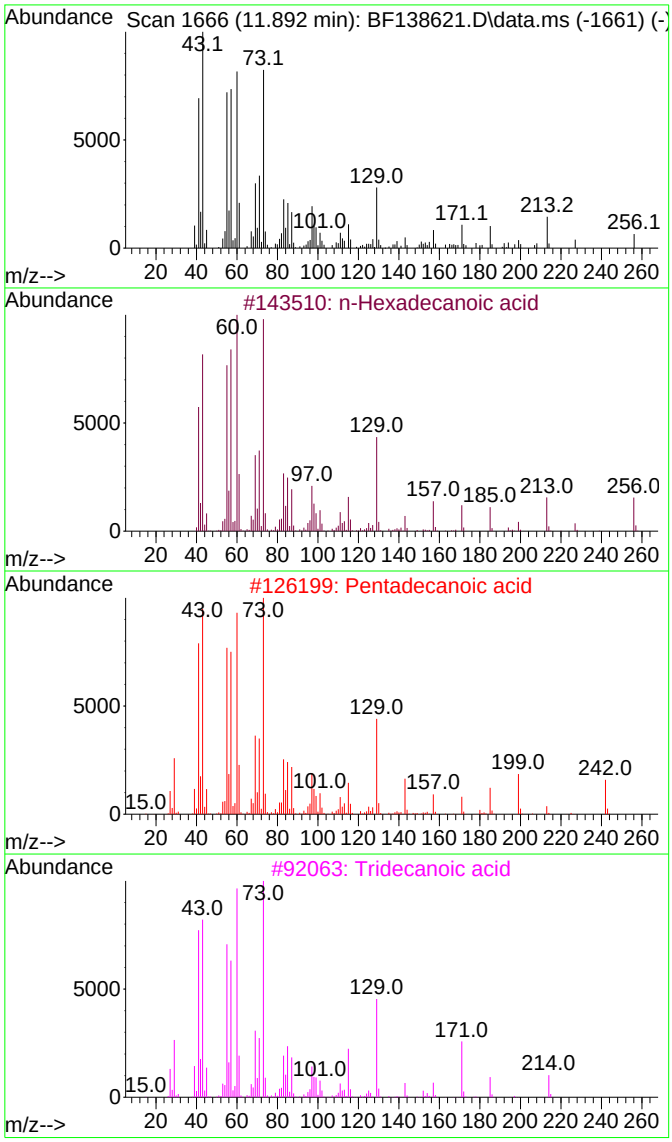
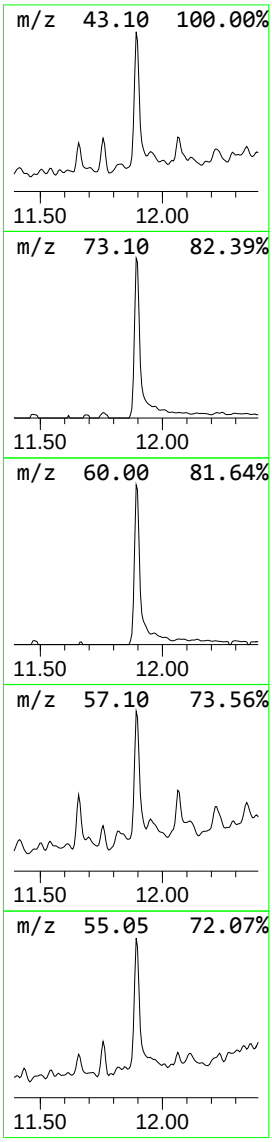
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	5.91 ng	194244	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	60





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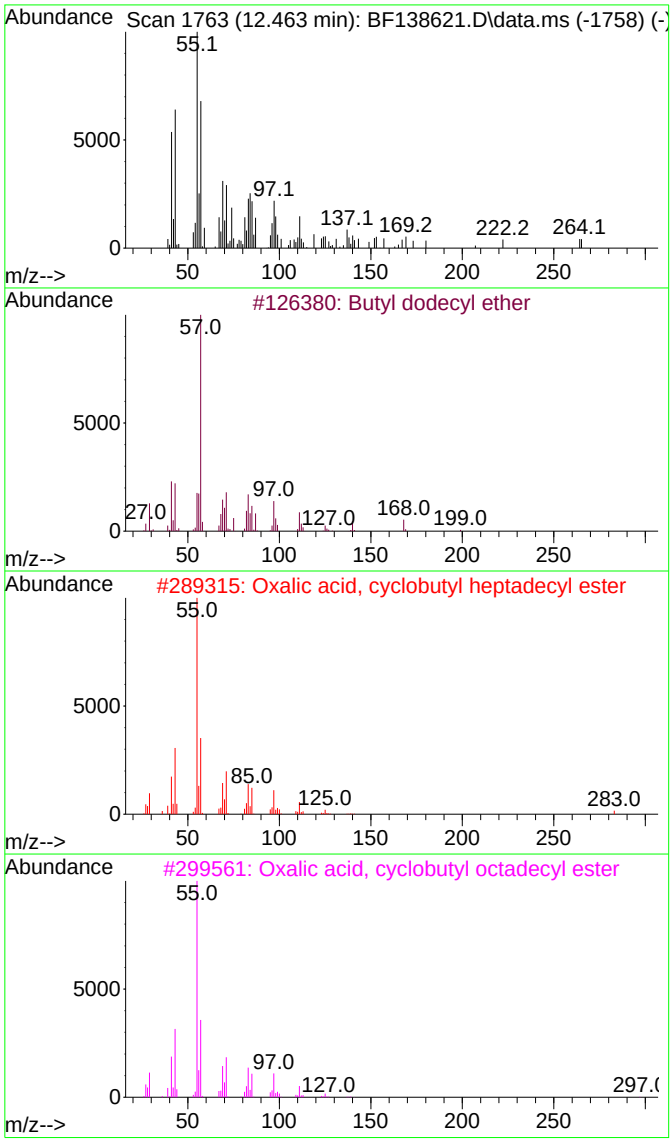
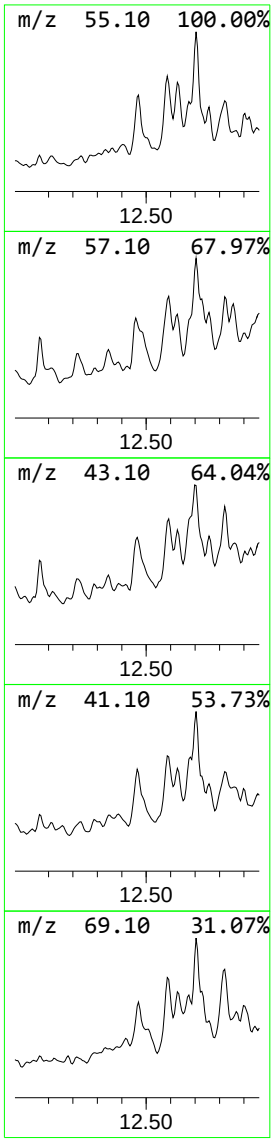
Peak Number 8 unknown12.463 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	2.60 ng	85279	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl dodecyl ether	242	C16H34O	1000406-40-3	49
2	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	46
3	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	46
4	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	46
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	43





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Operator : RC/JU
Sample : P3282-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDW-T1-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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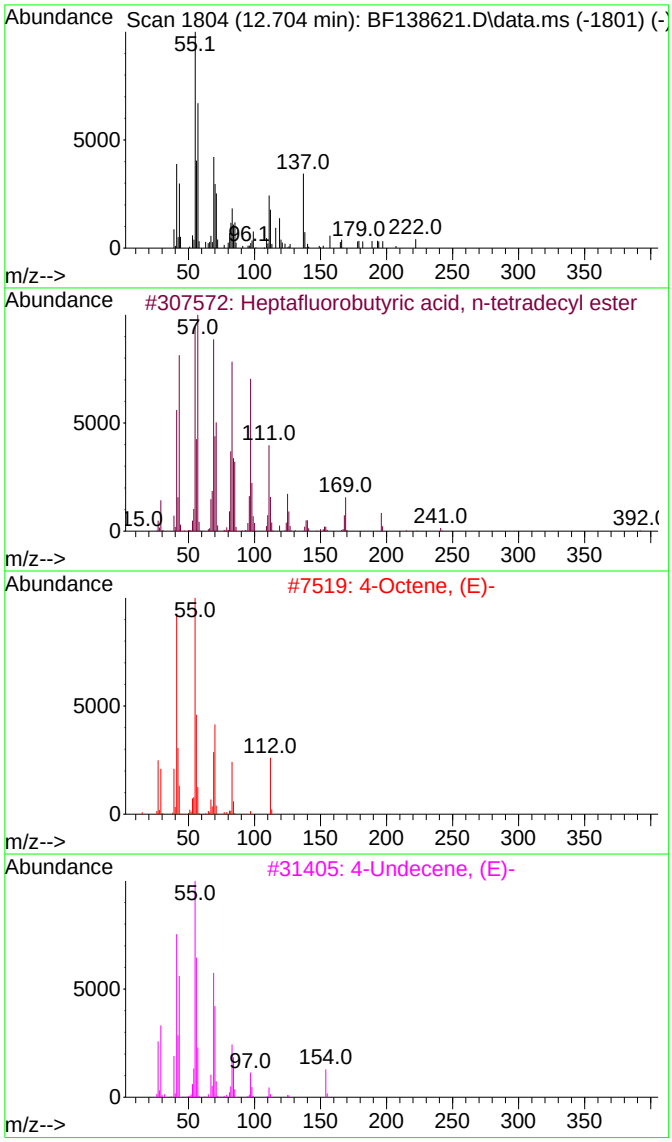
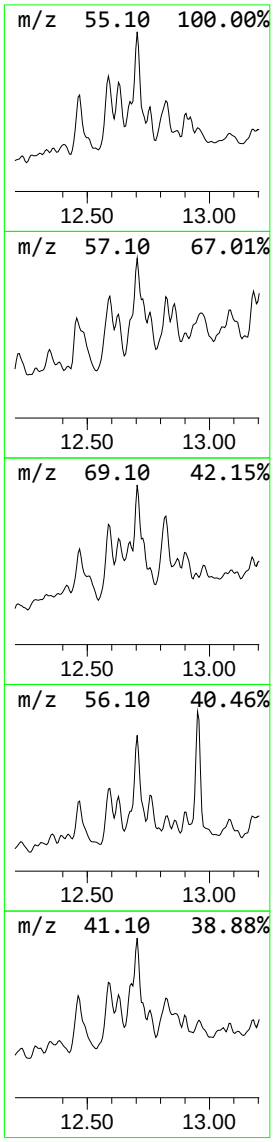
****

Peak Number 9 unknown12.704 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	4.22 ng	75057	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	27
2	4-Octene, (E)-	112	C8H16	014850-23-8	25
3	4-Undecene, (E)-	154	C11H22	000693-62-9	22
4	Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	22
5	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
Data File : BF138621.D
Acq On : 23 Jul 2024 16:32
Operator : RC/JU
Sample : P3282-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDW-T1-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

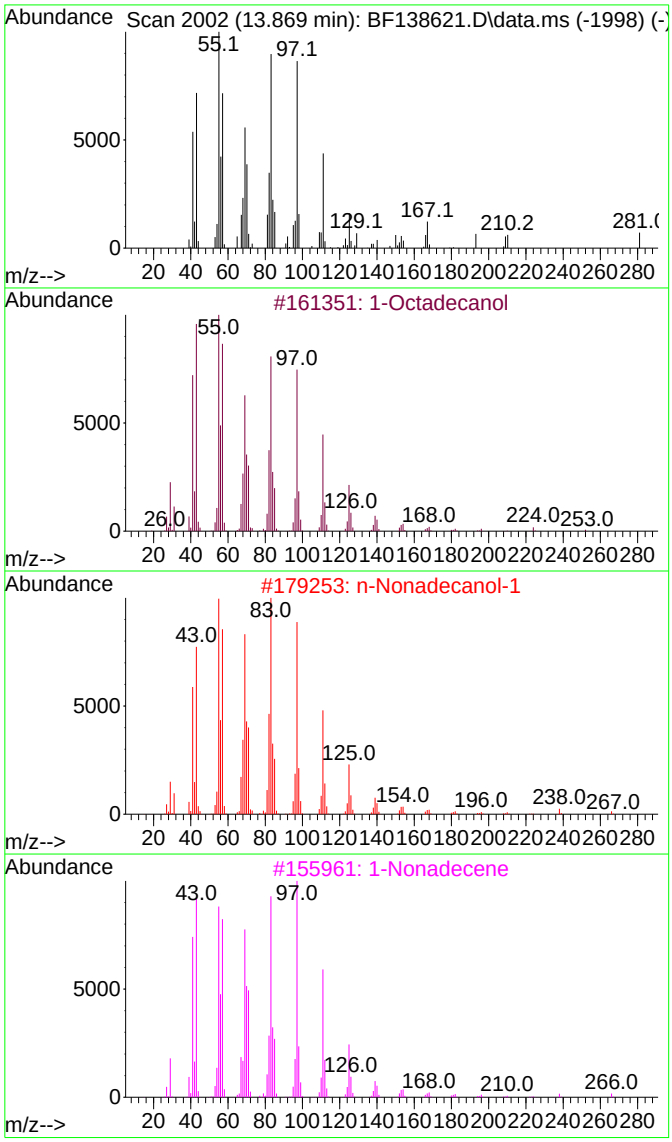
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

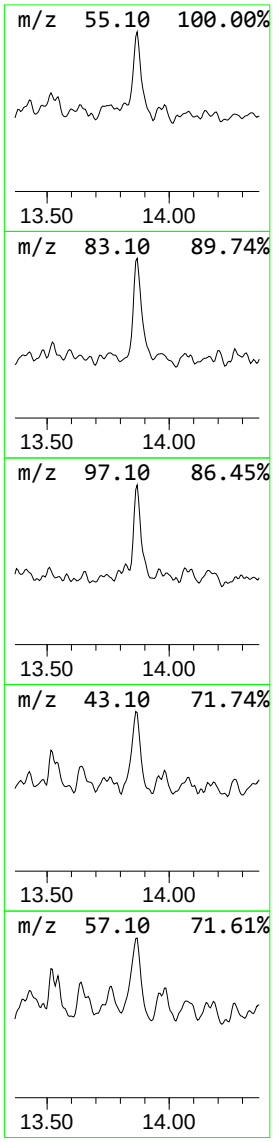
****

Peak Number 10 1-Octadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.869	6.45 ng	114844	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	87
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3	1-Nonadecene	266	C19H38	018435-45-5	74
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	68
5	Cyclopentadecane	210	C15H30	000295-48-7	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
Data File : BF138621.D
Acq On : 23 Jul 2024 16:32
Operator : RC/JU
Sample : P3282-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDW-T1-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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
Butane, 2-metho...	2.169	270.6	ng	6630590	1	6.851	489981	20.0
1,3-Dioxolane, ...	2.969	19.1	ng	466841	1	6.851	489981	20.0
2-Pentanone, 4-...	5.075	4.2	ng	103004	1	6.851	489981	20.0
Ethanol, 2-(2-e...	6.681	3.3	ng	80104	1	6.851	489981	20.0
1-Phenoxypropan...	8.445	5.1	ng	174703	2	8.134	689537	20.0
unknown9.981	9.981	3.4	ng	125568	3	9.886	744552	20.0
n-Hexadecanoic ...	11.892	5.9	ng	194244	4	11.369	657197	20.0
unknown12.463	12.463	2.6	ng	85279	4	11.369	657197	20.0
unknown12.704	12.704	4.2	ng	75057	5	14.004	355930	20.0
1-Octadecanol	13.869	6.5	ng	114844	5	14.004	355930	20.0