LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139105.D
Acq On : 21 Aug 2024 16:50
Operator : RC/JU
Sample : P3660-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-901-J-0.5-1-081624

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-BF082024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	15	26	rVV	801411	1216851	87.06%	9.572%
2	2.293	29	34	43	rVB2	8490	15749	1.13%	0.124%
3	3.381	213	219	234	rBV	29577	65607	4.69%	0.516%
4	5.104	503	512	524	rVB	64134	96868	6.93%	0.762%
5	5.504	574	580	586	rBV	1005978	1331307	95.25%	10.472%
6	6.510	745	751	756	rBV	1051827	1397716	100.00%	10.994%
7	6.716	779	786	791	rBV	11172	14981	1.07%	0.118%
8	6.892	811	816	821	rBV	427938	540904	38.70%	4.255%
9	7.051	839	843	847	rVB	25627	29120	2.08%	0.229%
10	7.451	905	911	916	rBV	654627	832710	59.58%	6.550%
11	7.710	951	955	959	rVB	12703	14875	1.06%	0.117%
12	8.175	1029	1034	1039	rBV	540974	659588	47.19%	5.188%
13	8.486	1082	1087	1091	rBV	55231	68485	4.90%	0.539%
14	9.251	1212	1217	1222	rBV	1131108	1355353	96.97%	10.661%
15	9.928	1327	1332	1337	rBV	530652	654095	46.80%	5.145%
16	10.028	1343	1349	1356	rBV	30455	46079	3.30%	0.362%
17	10.716	1460	1466	1479	rVB	530332	677376	48.46%	5.328%
18	11.416	1580	1585	1592	rVB	418487	520568	37.24%	4.095%
19	11.939	1664	1674	1685	rBV3	37529	65898	4.71%	0.518%
20	12.627	1786	1791	1797	rBV	28097	38437	2.75%	0.302%
21	12.727	1804	1808	1815	rBV3	11713	18344	1.31%	0.144%
22	12.869	1820	1832	1847	rVV2	111043	265263	18.98%	2.087%
23	12.998	1849	1854	1860	rVB	765679	985834	70.53%	7.754%
24	13.904	2003	2008	2016	rBV	68562	102493	7.33%	0.806%
25	14.051	2027	2033	2042	rBV	395574	532563	38.10%	4.189%
26	14.539	2111	2116	2129	rVB	43114	78527	5.62%	0.618%
27	14.798	2147	2160	2177	rBV7	122524	496480	35.52%	3.905%
28	15.051	2199	2203	2206	rBV	14796	18003	1.29%	0.142%
29	15.098	2206	2211	2221	rVB	18124	44058	3.15%	0.347%
30	15.198	2223	2228	2237	rBV3	18062	44804	3.21%	0.352%
31	15.462	2269	2273	2278	rVB	11711	17242	1.23%	0.136%
32	15.527	2278	2284	2291	rBV	279450	427310	30.57%	3.361%
33	16.033	2366	2370	2374	rBV2	10733	16729	1.20%	0.132%
34	16.086	2374	2379	2381	rBV5	13495	22927	1.64%	0.180%

Sum of corrected areas: 12713144

Instrument :
BNA_F
ClientSampleId :
S-901-J-0.5-1-081624

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
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Misc :
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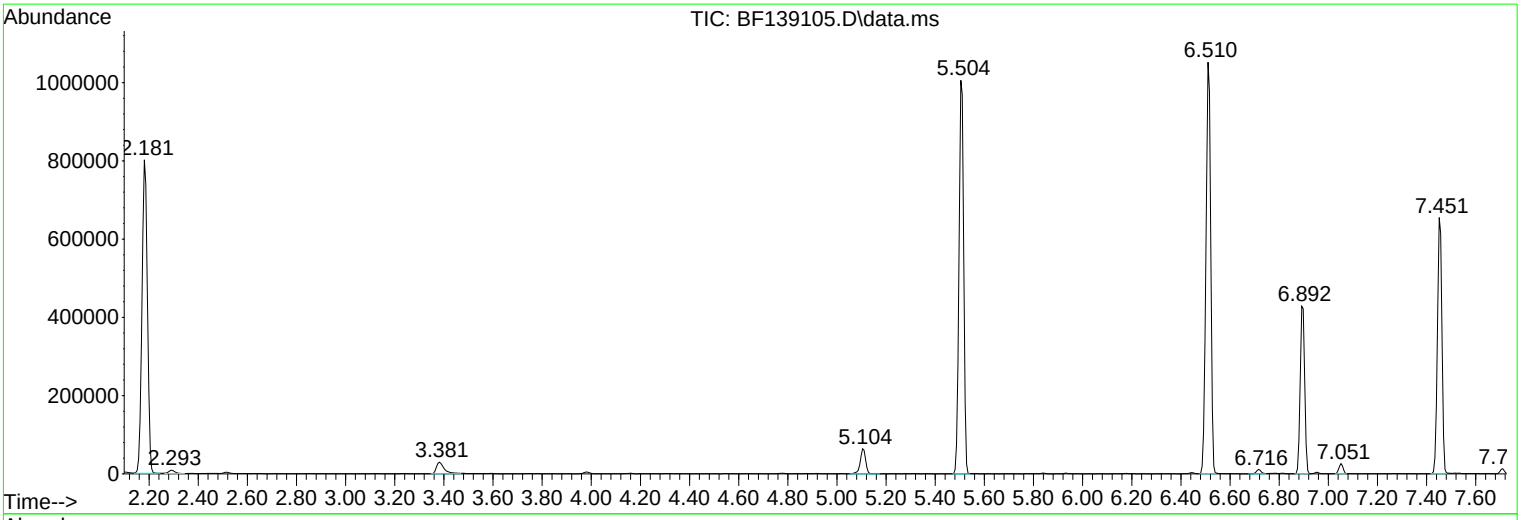
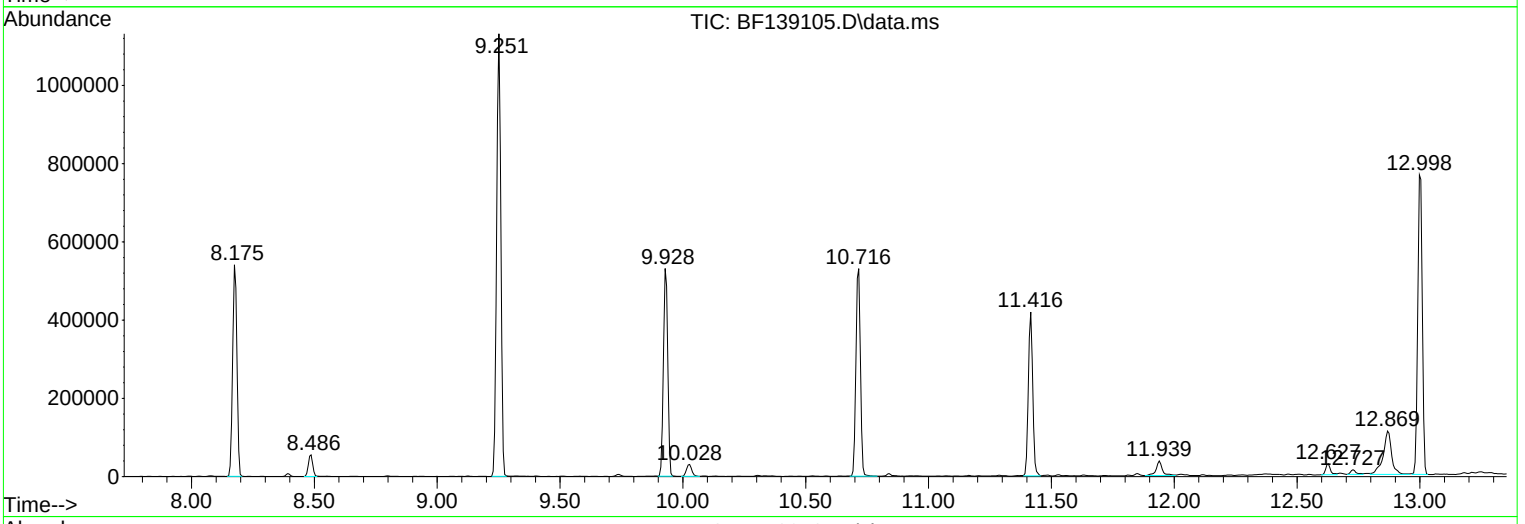
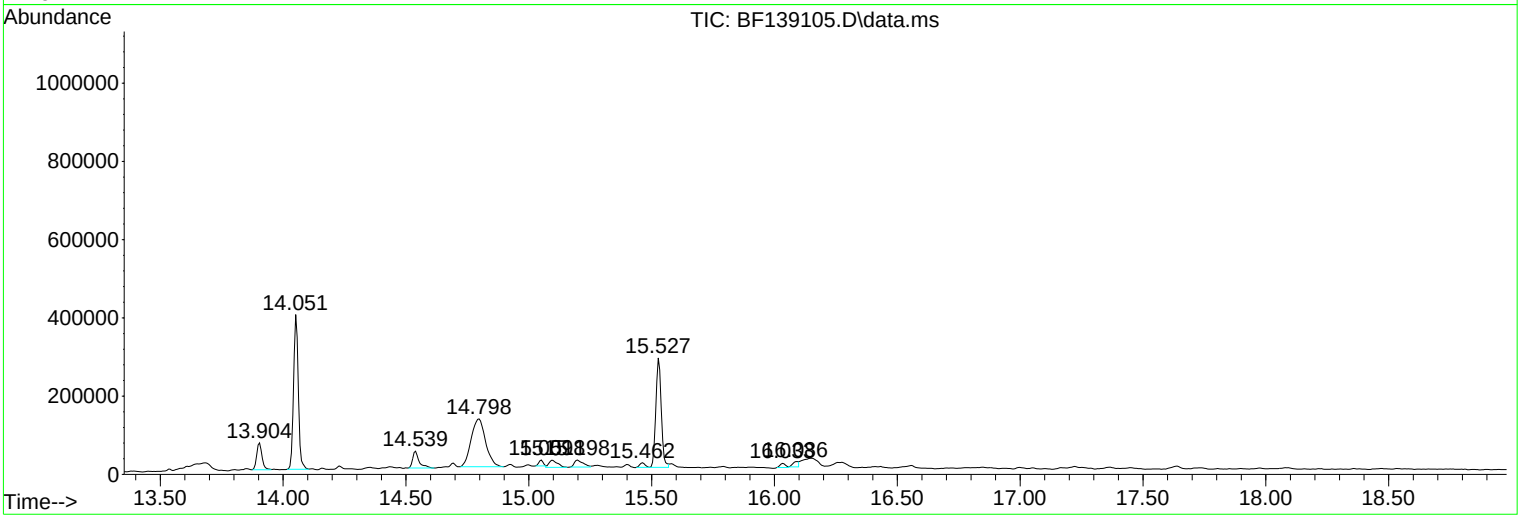
ClientSampleId :
S-901-J-0.5-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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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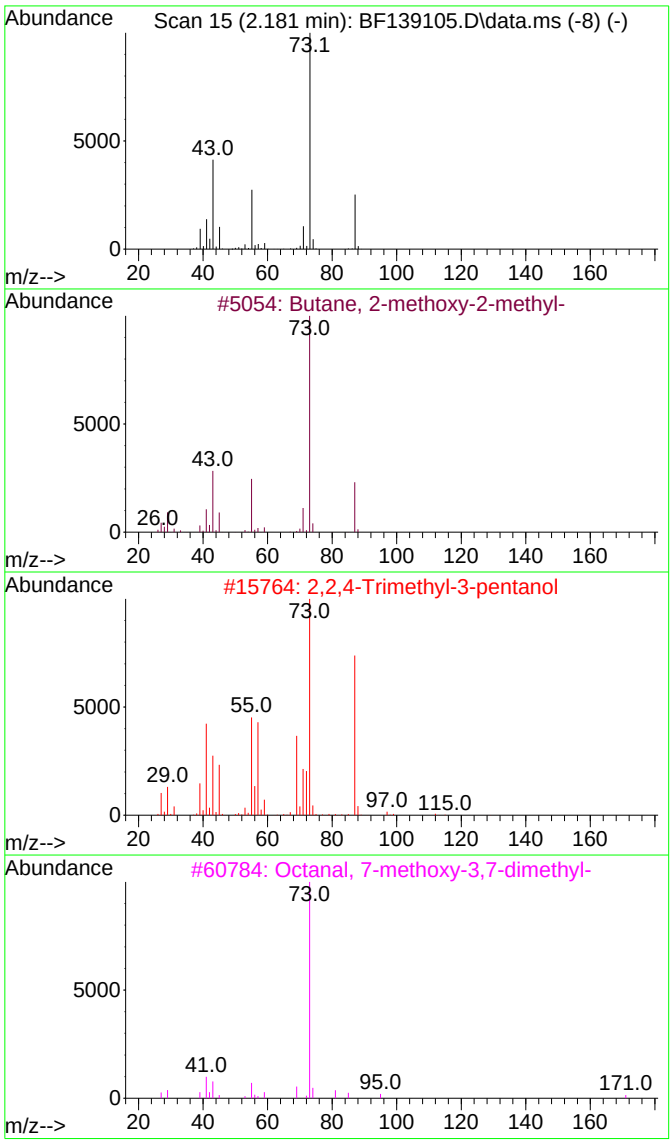
TIC Integration Parameters: LSCINT.P

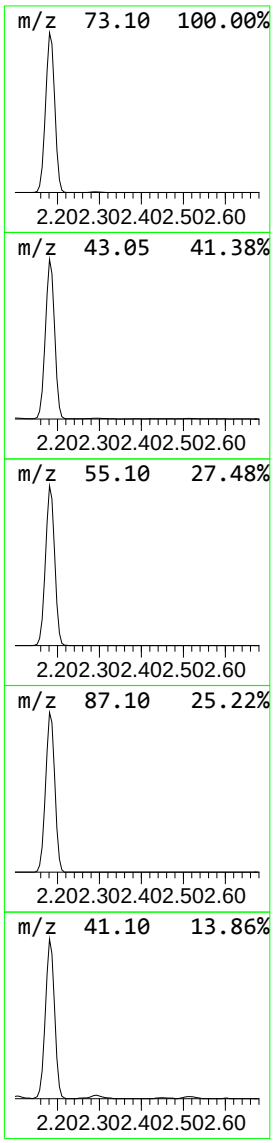
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	44.99 ng	1216850	1,4-Dichlorobenzene-d4	6.898

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	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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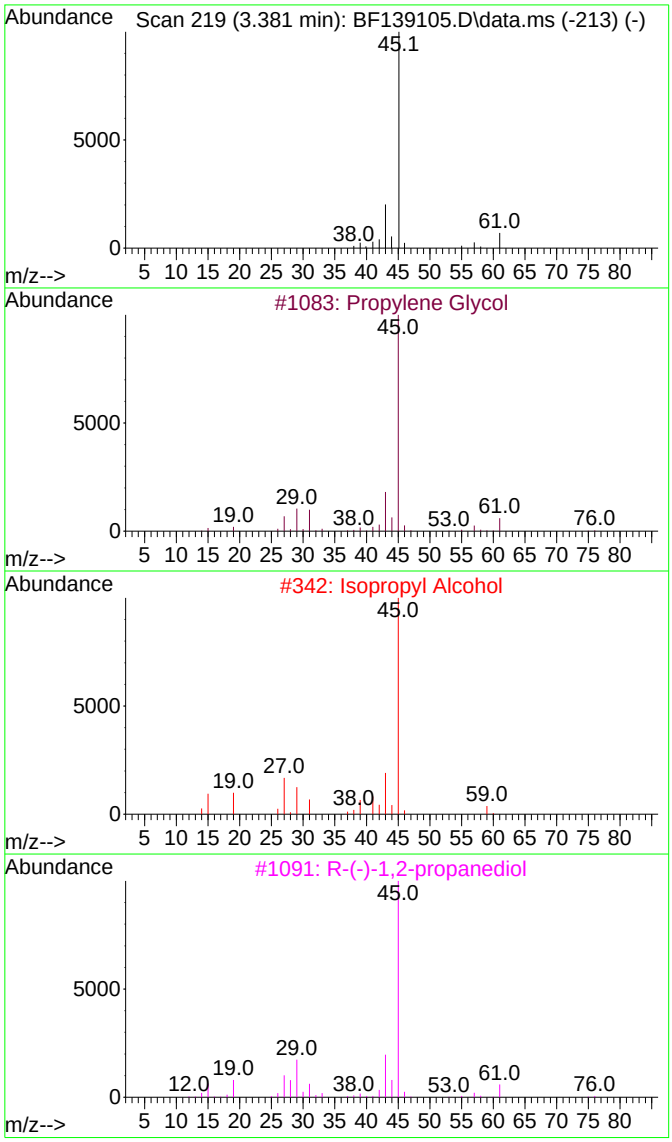
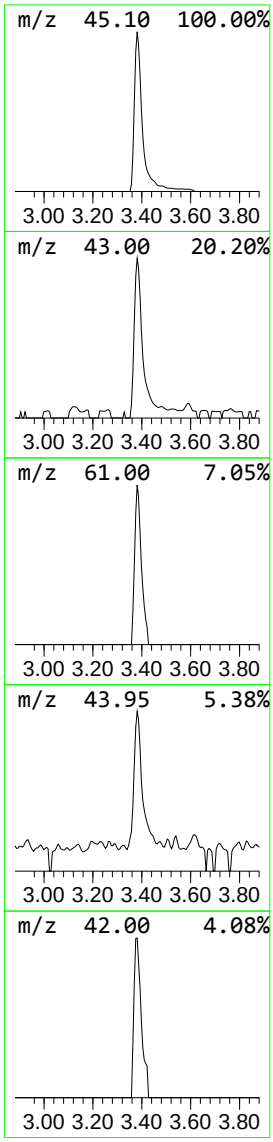
****

Peak Number 2 unknown3.381 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.381	2.43 ng	65607	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	Formamide	45	CH3NO	000075-12-7	5
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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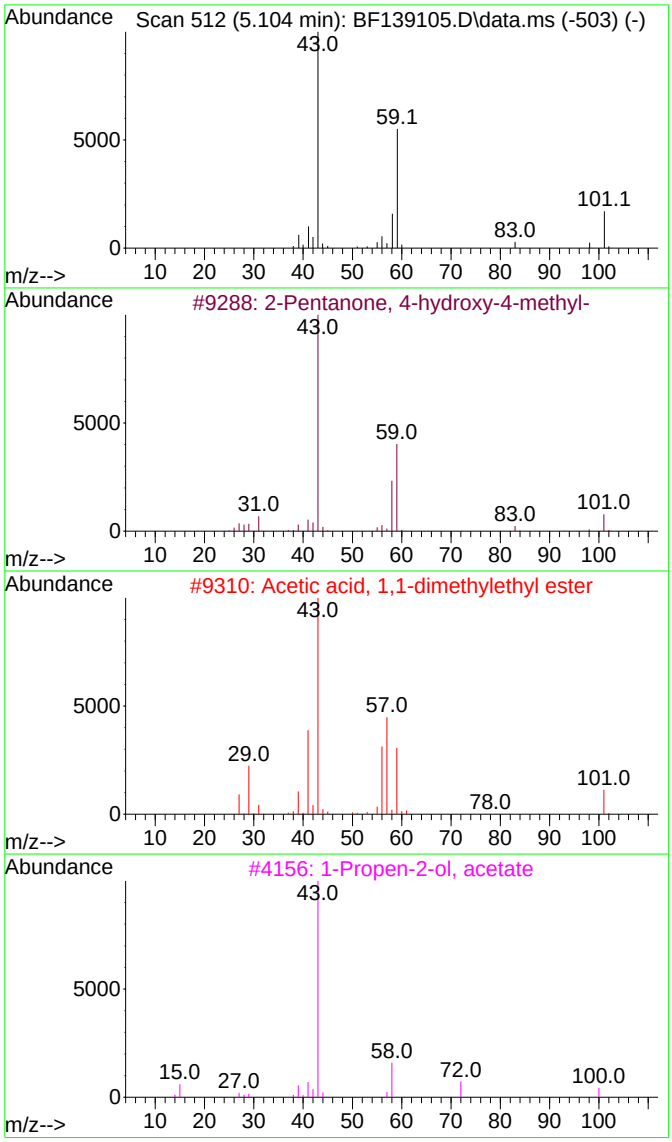
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

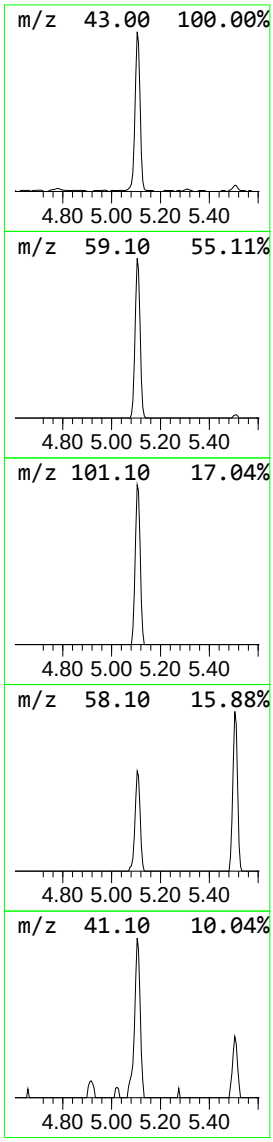
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	3.58 ng	96868	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetone	58	C3H6O	000067-64-1	9





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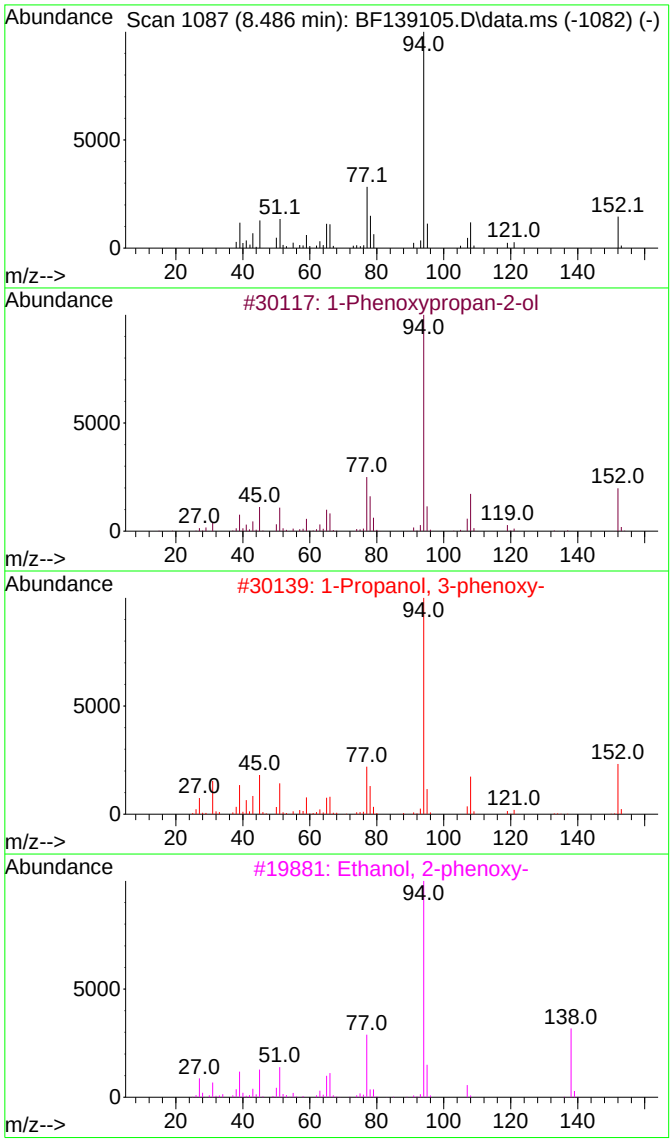
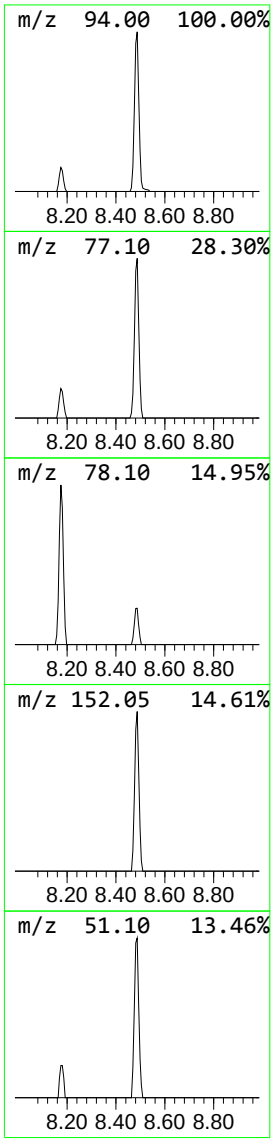
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.486	2.08 ng	68485	Naphthalene-d8	8.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
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	Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	53





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

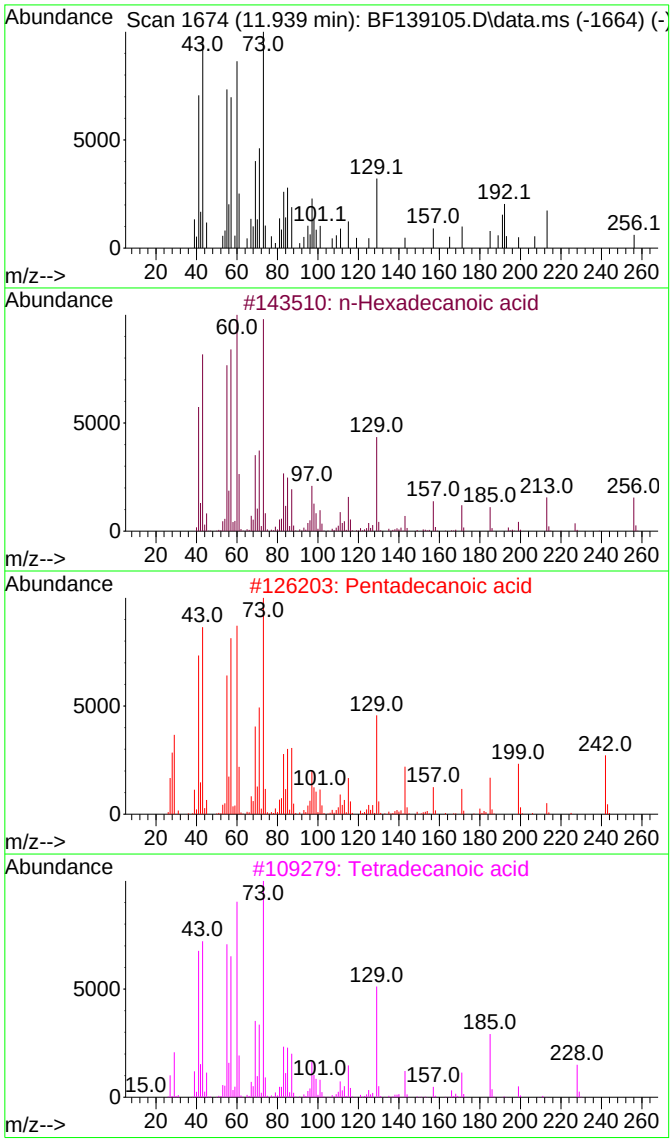
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

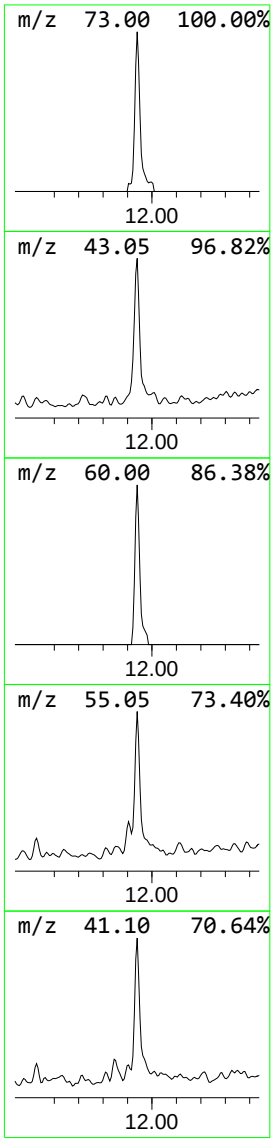
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	2.53 ng	65898	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53





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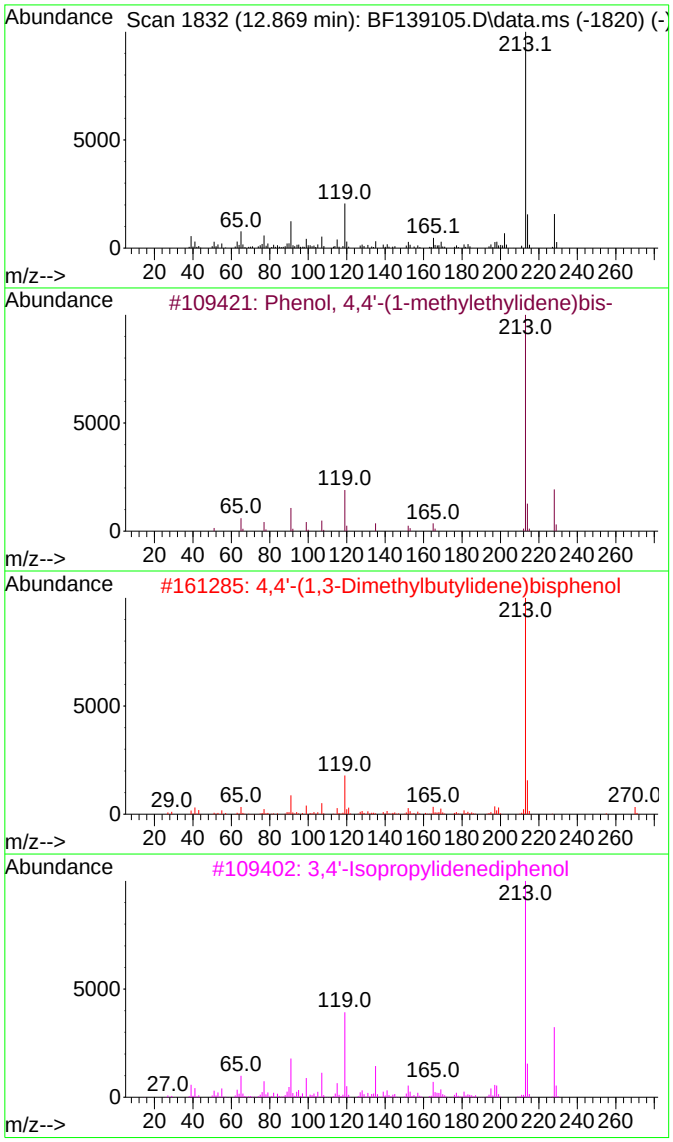
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

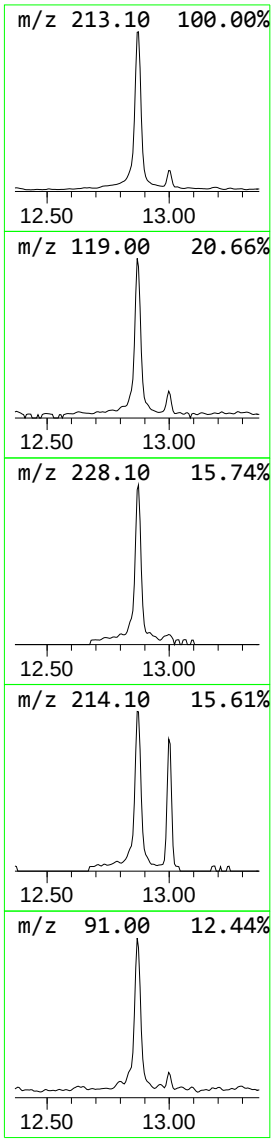
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.868	9.96 ng	265263	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	74
3	3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	70
4	Diphenolic acid	286	C17H18O4	000126-00-1	56
5	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	50





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TIC Library : C:\Database\NIST20.L
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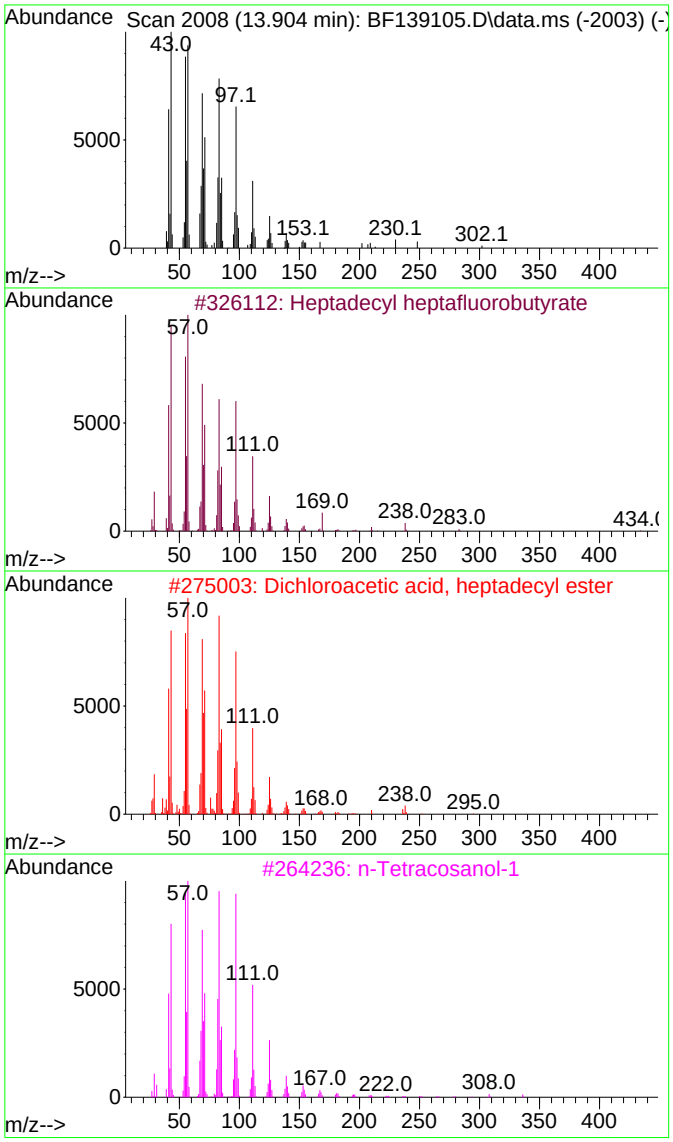
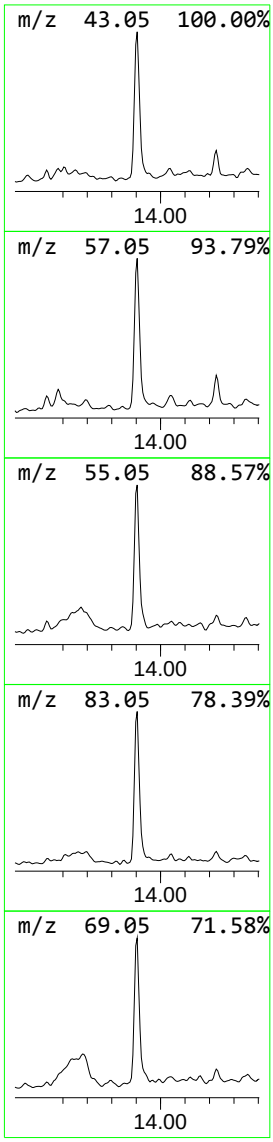
****
Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.85 ng	102493	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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TIC Library : C:\Database\NIST20.L
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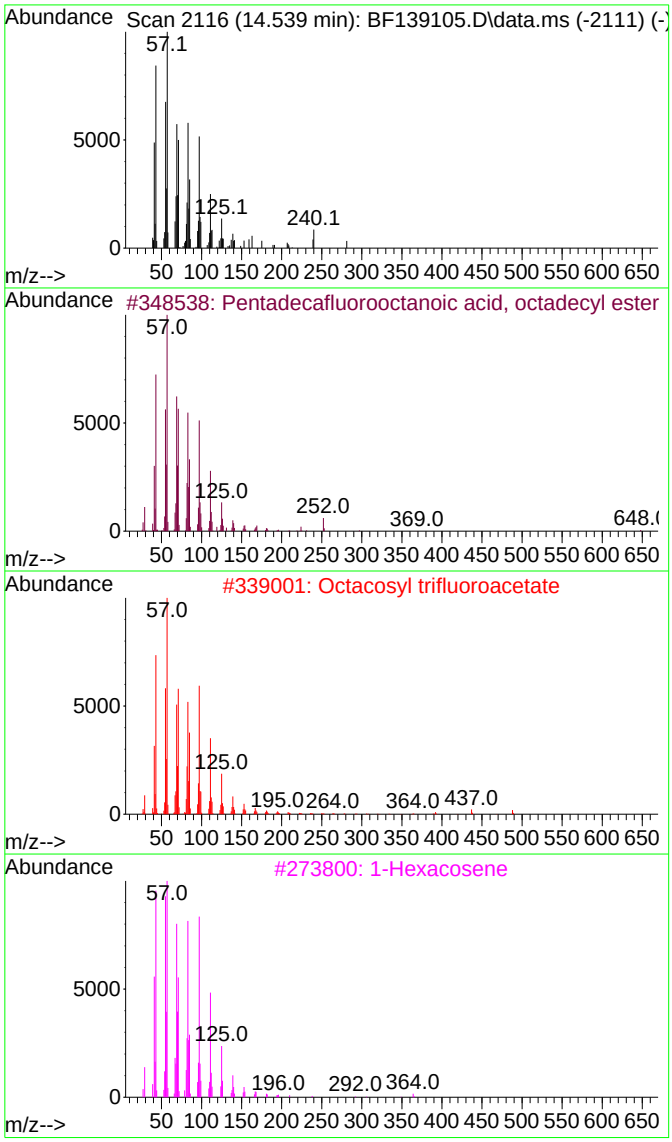
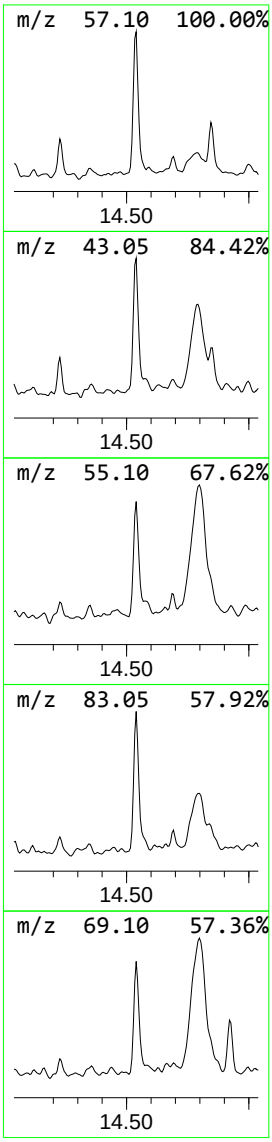
****
Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	2.95 ng	78527	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	94
3	1-Hexacosene	364	C26H52	018835-33-1	93
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	93
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91





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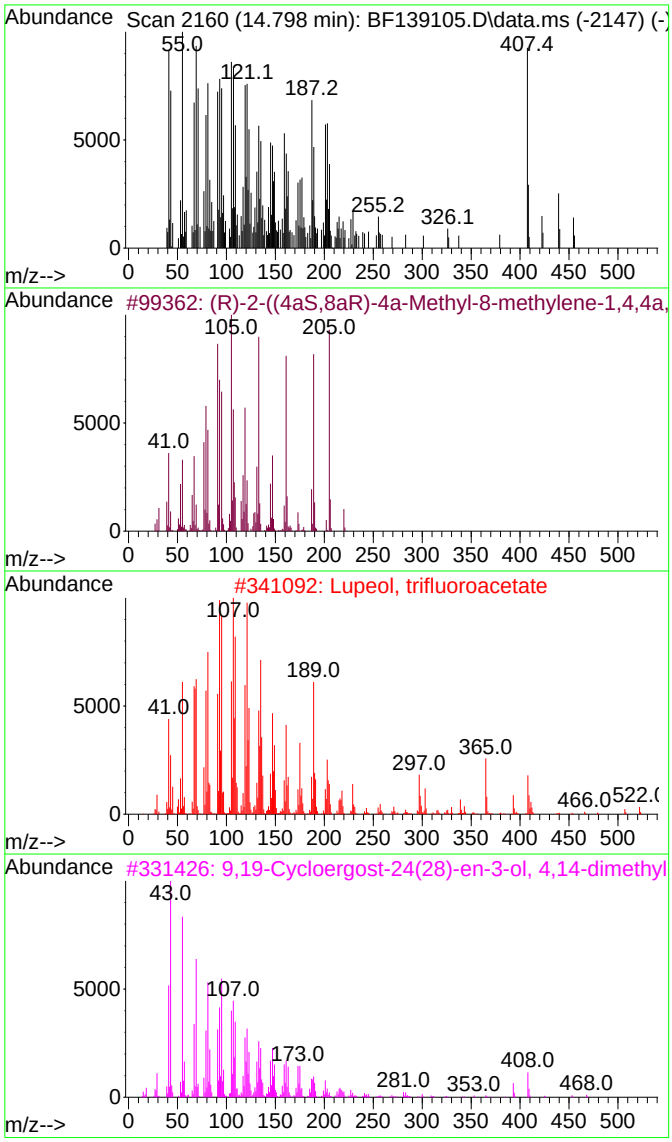
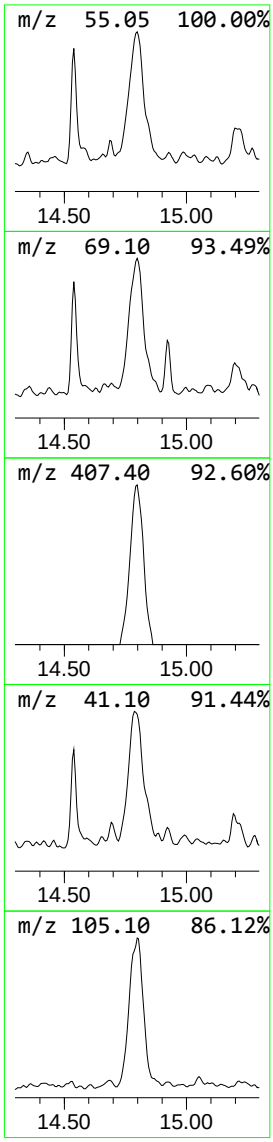
****
Peak Number 9 (R)-2-((4aS,8aR)-4a-Methyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.798	23.24 ng	496480	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-2-((4aS,8aR)-4a-Methyl-8-met...	220	C15H24O	028102-68-3	84
2	Lupeol, trifluoroacetate	522	C32H49F3O2	1000394-56-7	46
3	9,19-Cycloergost-24(28)-en-3-ol,...	468	C32H52O2	010376-42-8	42
4	1H-Cycloprop[e]azulen-7-ol, deca...	220	C15H24O	006750-60-3	30
5	(-)-Spathulenol	220	C15H24O	077171-55-2	30





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Data File : BF139105.D
Acq On : 21 Aug 2024 16:50
Operator : RC/JU
Sample : P3660-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-901-J-0.5-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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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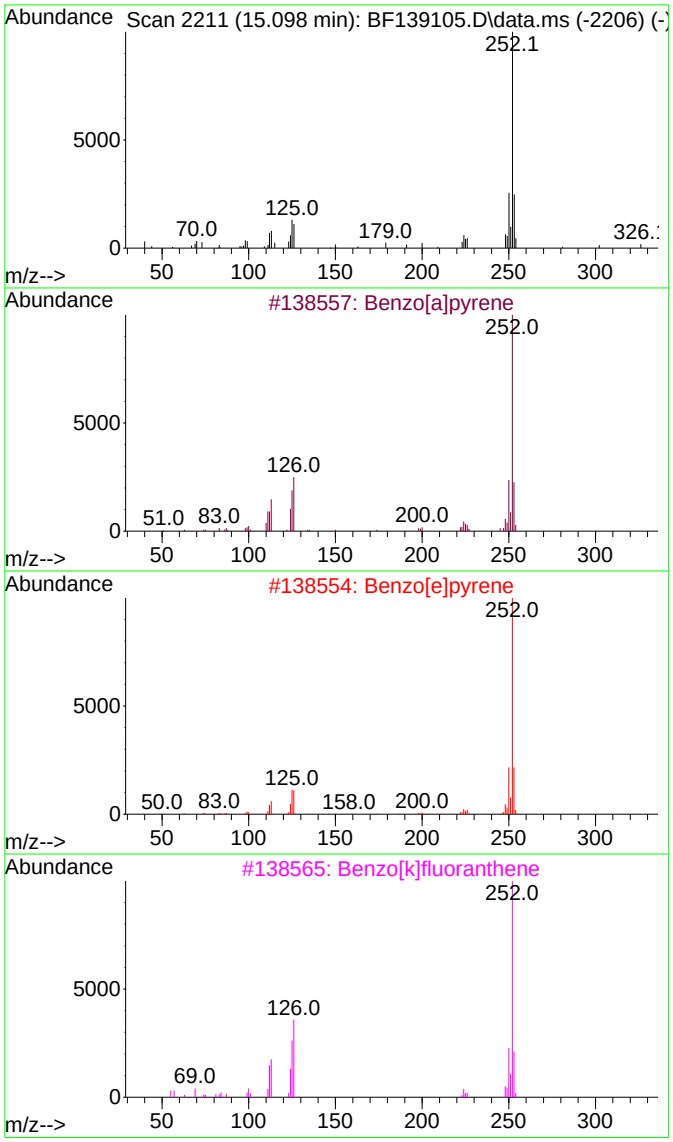
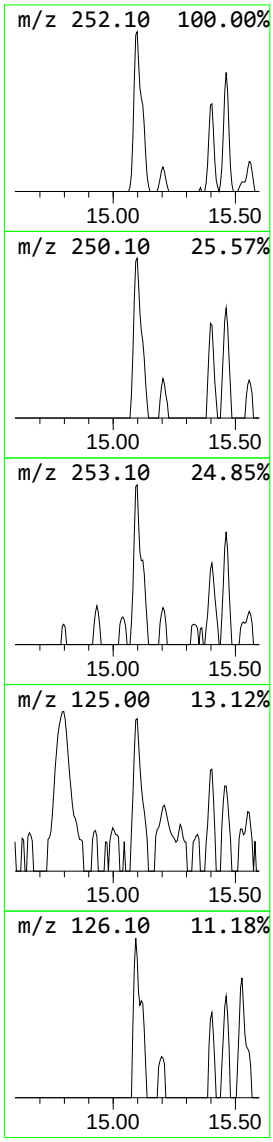
Peak Number 10 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	2.06 ng	44058	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	91
2	Benzo[e]pyrene	252	C20H12	000192-97-2	87
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	87
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
5	Perylene	252	C20H12	000198-55-0	81





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Data File : BF139105.D
Acq On : 21 Aug 2024 16:50
Operator : RC/JU
Sample : P3660-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-901-J-0.5-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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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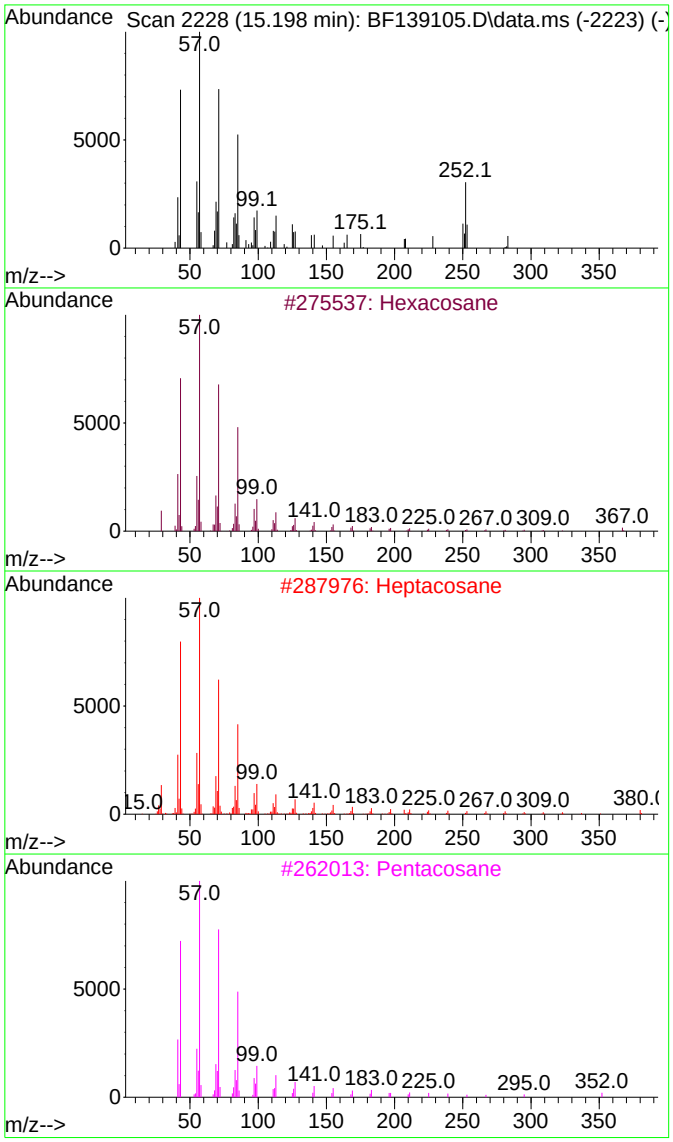
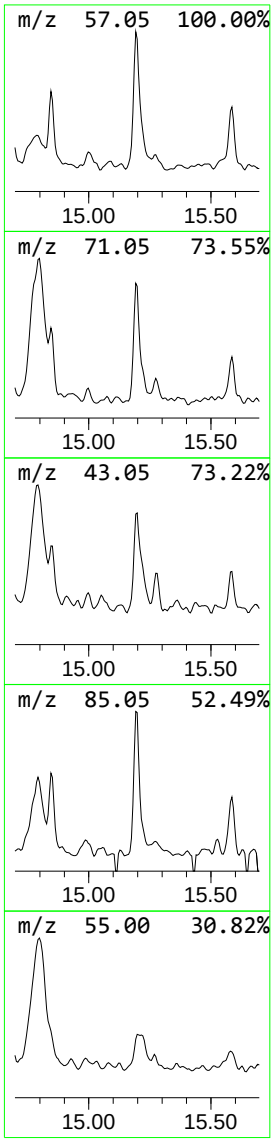
Peak Number 11 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	2.10 ng	44804	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	70
2	Heptacosane	380	C27H56	000593-49-7	70
3	Pentacosane	352	C25H52	000629-99-2	70
4	Nonadecane, 3-methyl-	282	C20H42	006418-45-7	62
5	Eicosane	282	C20H42	000112-95-8	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139105.D
Acq On : 21 Aug 2024 16:50
Operator : RC/JU
Sample : P3660-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-901-J-0.5-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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...	2.181	45.0	ng	1216850	1	6.898	540904	20.0
unknown3.381	3.381	2.4	ng	65607	1	6.898	540904	20.0
2-Pentanone, 4-...	5.104	3.6	ng	96868	1	6.898	540904	20.0
1-Phenoxypropan...	8.486	2.1	ng	68485	2	8.175	659588	20.0
n-Hexadecanoic ...	11.939	2.5	ng	65898	4	11.416	520568	20.0
Phenol, 4,4'-(1...	12.868	10.0	ng	265263	5	14.051	532563	20.0
Heptadecyl hept...	13.904	3.9	ng	102493	5	14.051	532563	20.0
Pentadecafluoro...	14.539	3.0	ng	78527	5	14.051	532563	20.0
(R)-2-((4aS,8aR...	14.798	23.2	ng	496480	6	15.527	427310	20.0
Benzo[e]pyrene	15.098	2.1	ng	44058	6	15.527	427310	20.0
Hexacosane	15.198	2.1	ng	44804	6	15.527	427310	20.0