LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
Data File : BF137459.D
Acq On : 01 Mar 2024 15:16
Operator : CG\JU
Sample : P1659-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

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-BF022924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137459.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	8	15	22	rVB	1210814	1601666	21.58%	4.208%
2	3.522	241	244	263	rBV	198065	439583	5.92%	1.155%
3	5.522	581	584	607	rBV	4016154	4001462	53.92%	10.513%
4	6.510	748	752	769	rBV	3950723	4059992	54.71%	10.667%
5	6.869	810	813	826	rBV	1358575	1143110	15.40%	3.003%
6	7.428	904	908	920	rBV	2663510	2496823	33.64%	6.560%
7	8.139	1026	1029	1044	rBV	1639886	1475858	19.89%	3.877%
8	8.463	1081	1084	1096	rBV	101274	152419	2.05%	0.400%
9	9.222	1209	1213	1216	rBV	4821307	4162619	56.09%	10.936%
10	9.339	1230	1233	1237	rBV	306503	270486	3.64%	0.711%
11	9.898	1324	1328	1341	rVB	1893504	1528473	20.60%	4.016%
12	10.016	1341	1348	1351	rBV	5050162	7421233	100.00%	19.497%
13	10.692	1459	1463	1479	rBV	2235555	2069794	27.89%	5.438%
14	11.392	1579	1582	1592	rBV	1469495	1277692	17.22%	3.357%
15	11.939	1671	1675	1691	rBV2	155149	248869	3.35%	0.654%
16	12.510	1767	1772	1780	rVB	81572	87707	1.18%	0.230%
17	12.992	1850	1854	1858	rBV	3375438	3123951	42.09%	8.207%
18	13.910	2006	2010	2024	rBV	132117	192326	2.59%	0.505%
19	14.051	2031	2034	2044	rBV	1120551	1144822	15.43%	3.008%
20	14.951	2183	2187	2194	rBV	200881	215007	2.90%	0.565%
21	15.586	2289	2295	2303	rBV	687202	948666	12.78%	2.492%

Sum of corrected areas: 38062558

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ClientSampleId :
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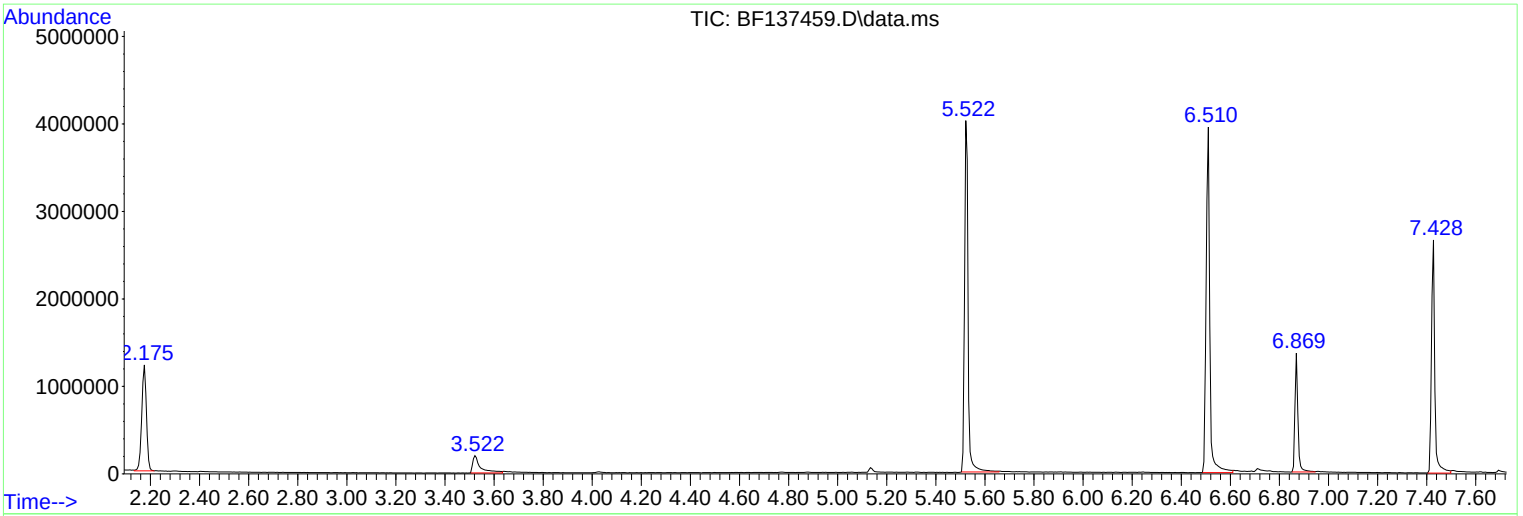
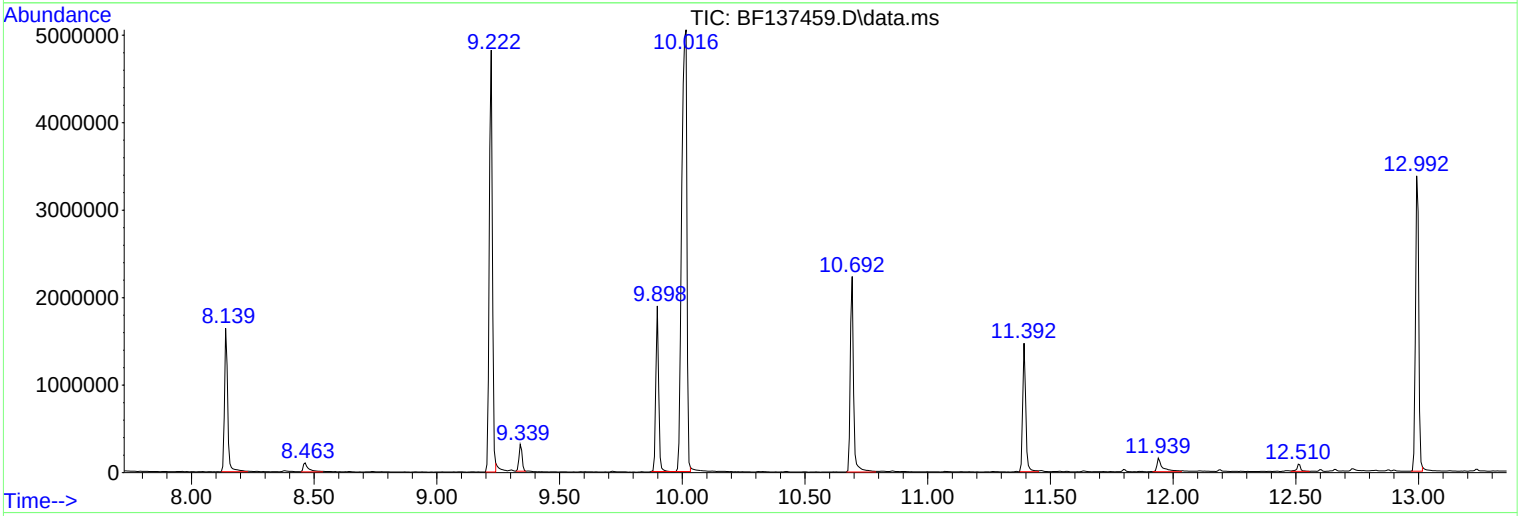
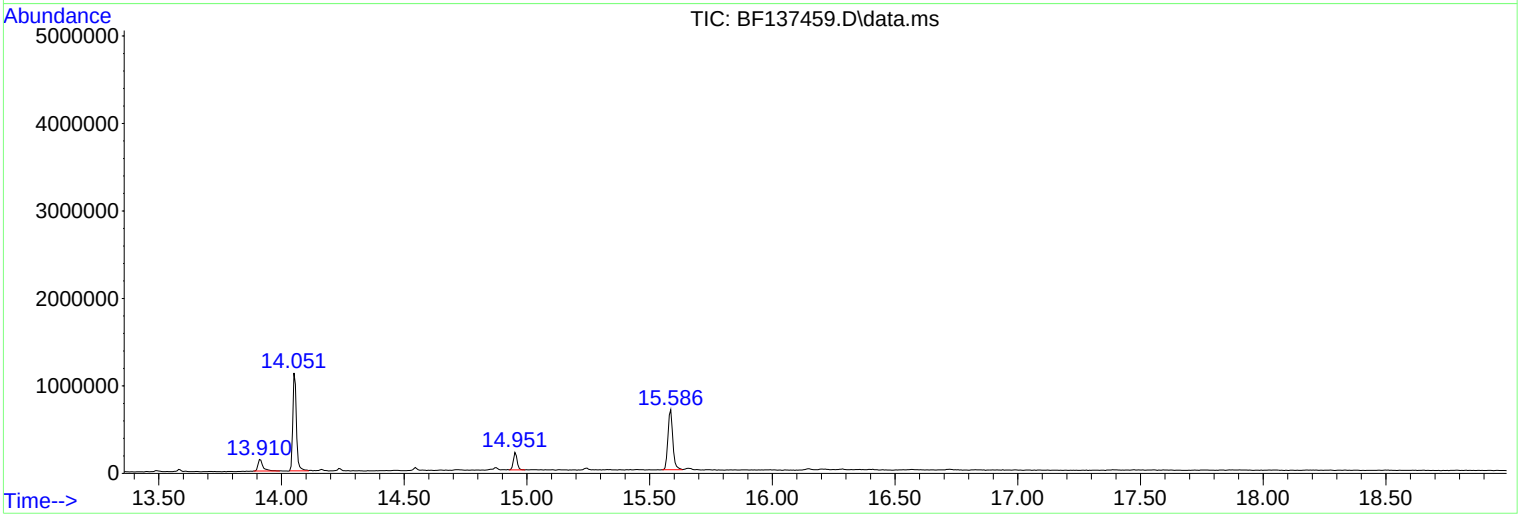
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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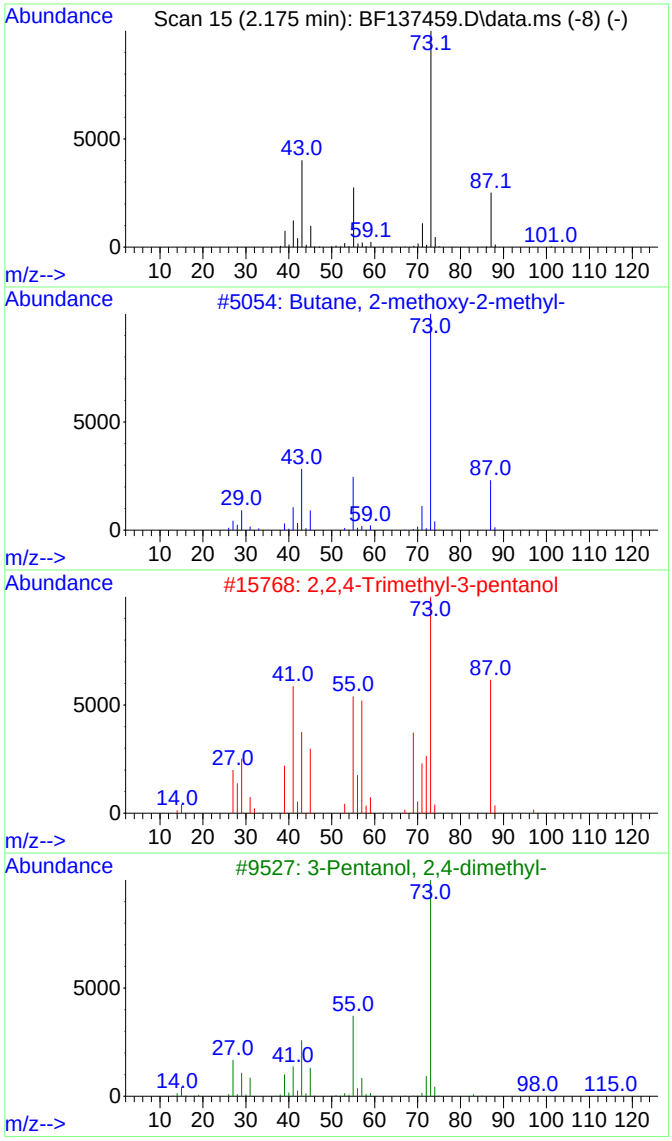
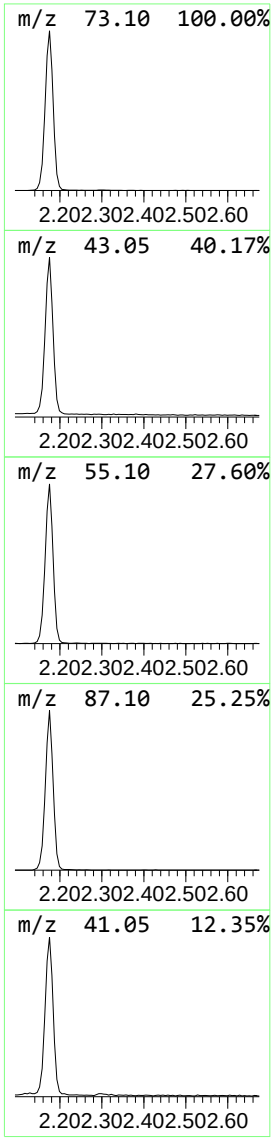
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	28.02 ng	1601670	1,4-Dichlorobenzene-d4	6.869

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, 2,4-dimethyl-	116	C7H16O	000600-36-2	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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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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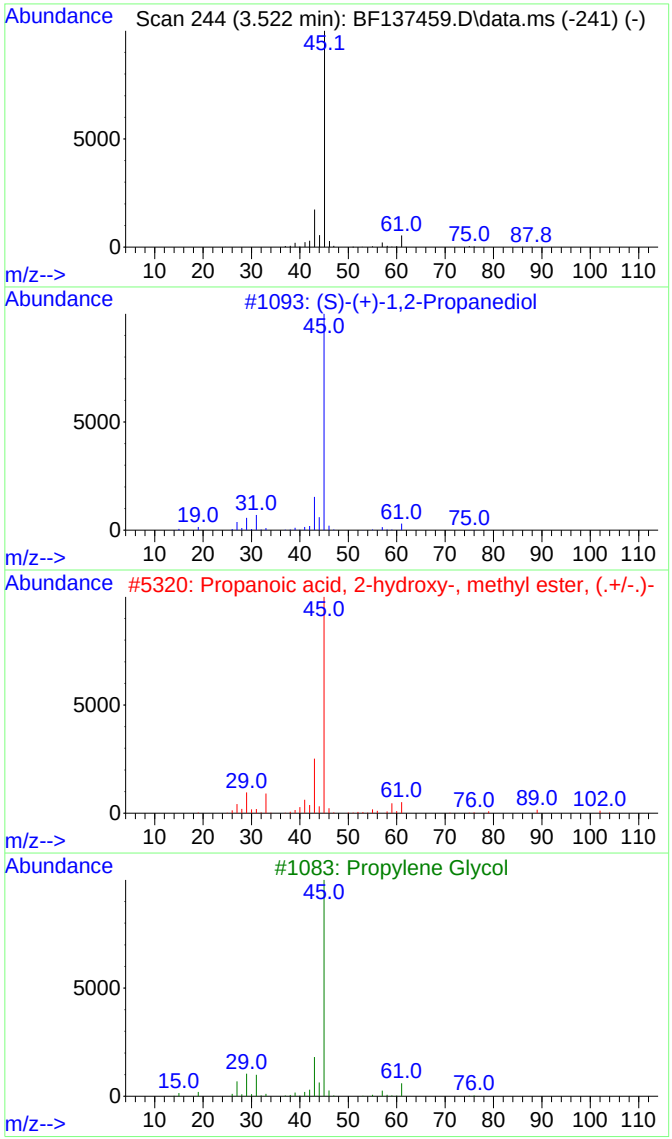
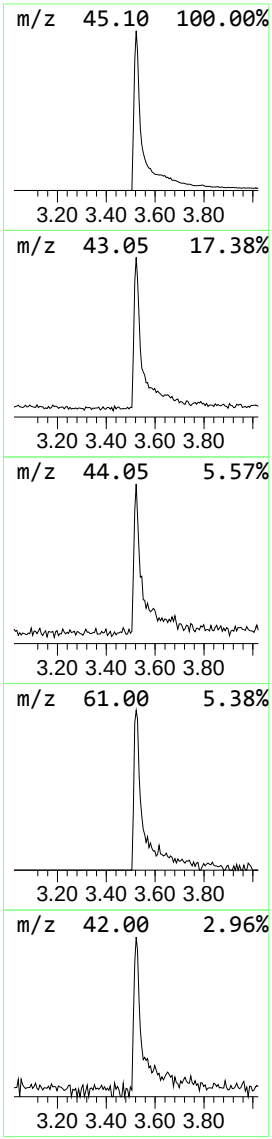
Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.522	7.69 ng	439583	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3	Propylene Glycol	76	C3H8O2	000057-55-6	37
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9





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Sample : P1659-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
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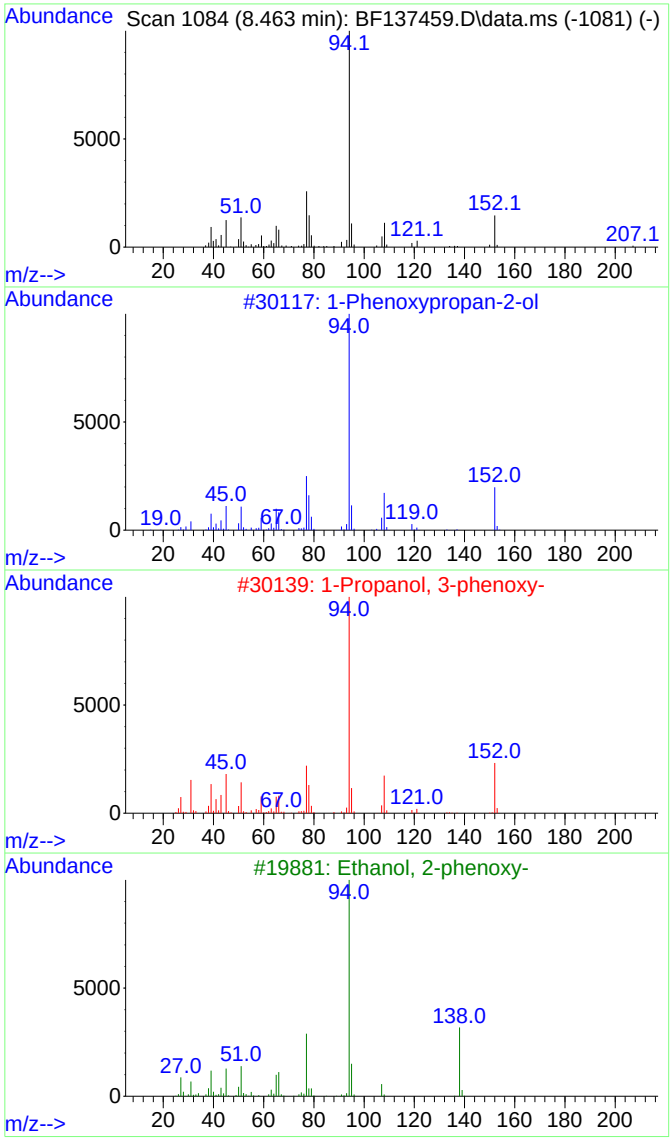
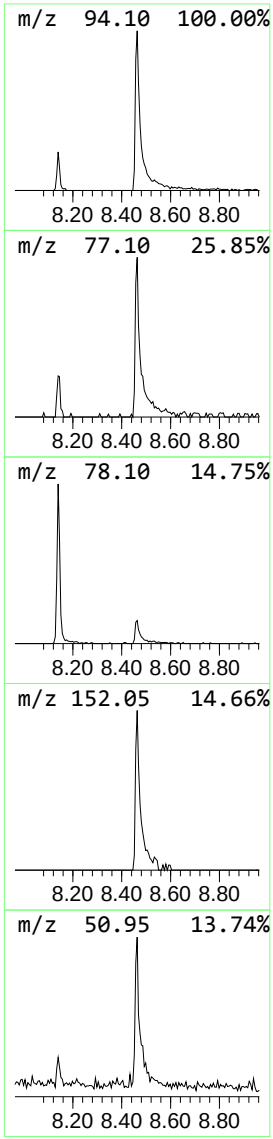
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	2.07 ng	152419	Naphthalene-d8	8.139

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	83
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5	Acetic acid, chloro-, phenyl ester	170	C8H7ClO2	000620-73-5	59





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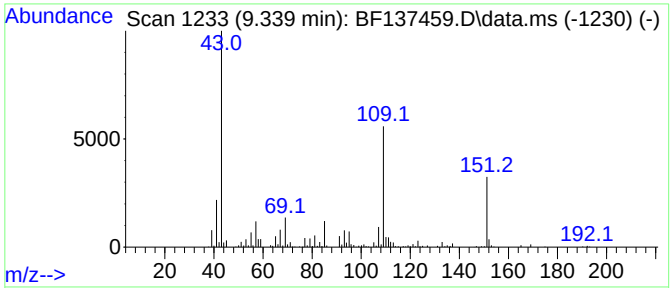
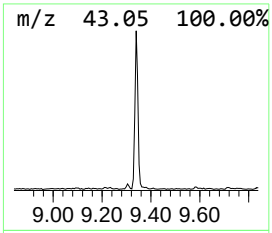
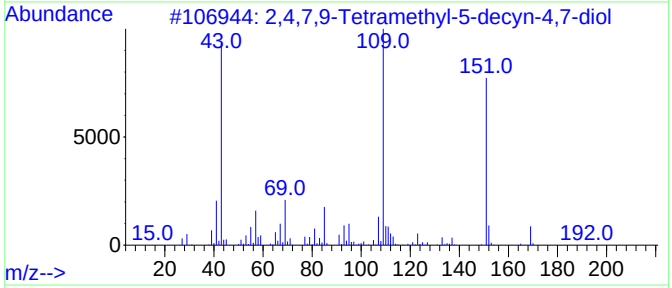
****
Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

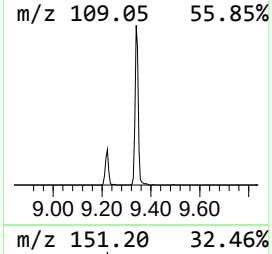
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.339	3.54 ng	270486	Acenaphthene-d10	9.898

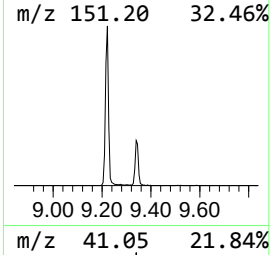
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	53
3	Metacetamol	151	C8H9NO2	000621-42-1	49
4	Acetaminophen	151	C8H9NO2	000103-90-2	47
5	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	45

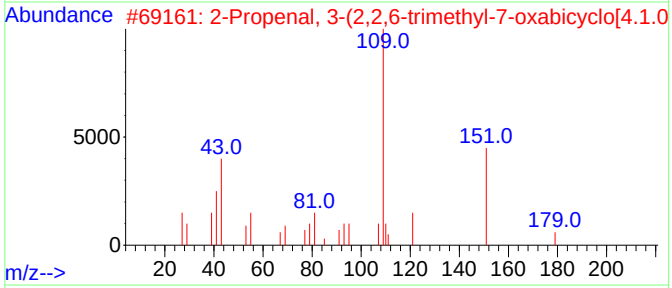


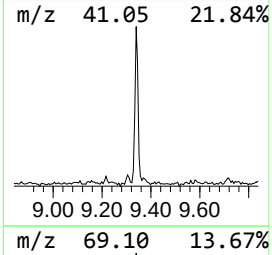


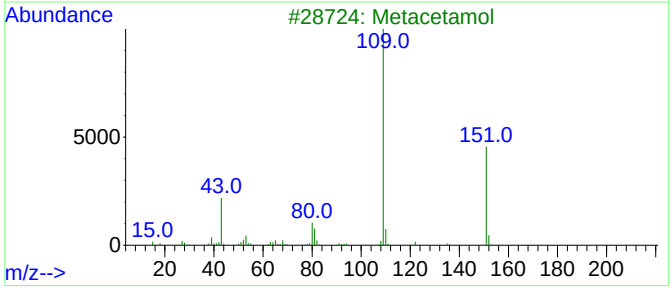


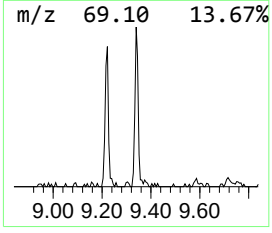












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

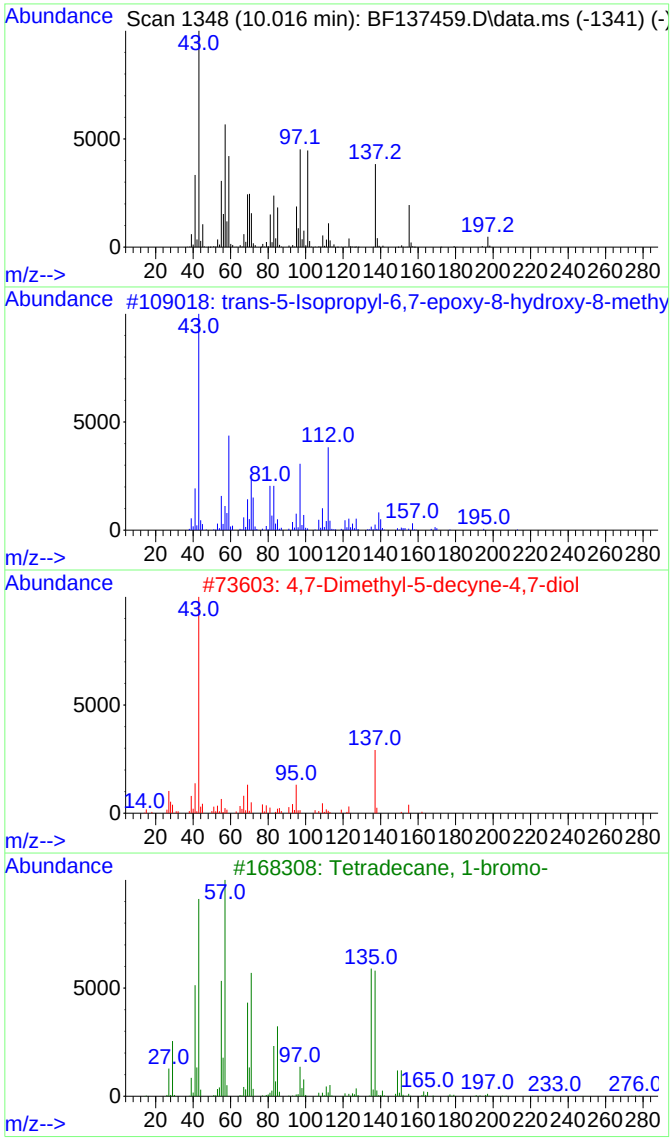
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

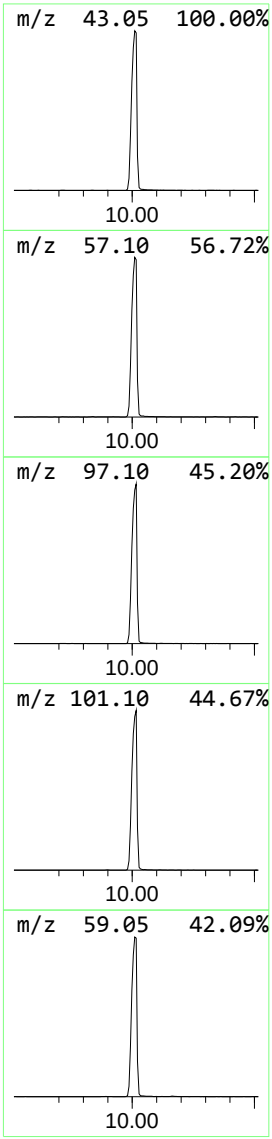
****

Peak Number 5 unknown10.016 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.016	97.11 ng	7421230	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
2	4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	10
3	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10
4	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	10
5	2,2,3,4-Tetramethylhex-5-en-3-ol	156	C10H20O	1010191-06-9	10





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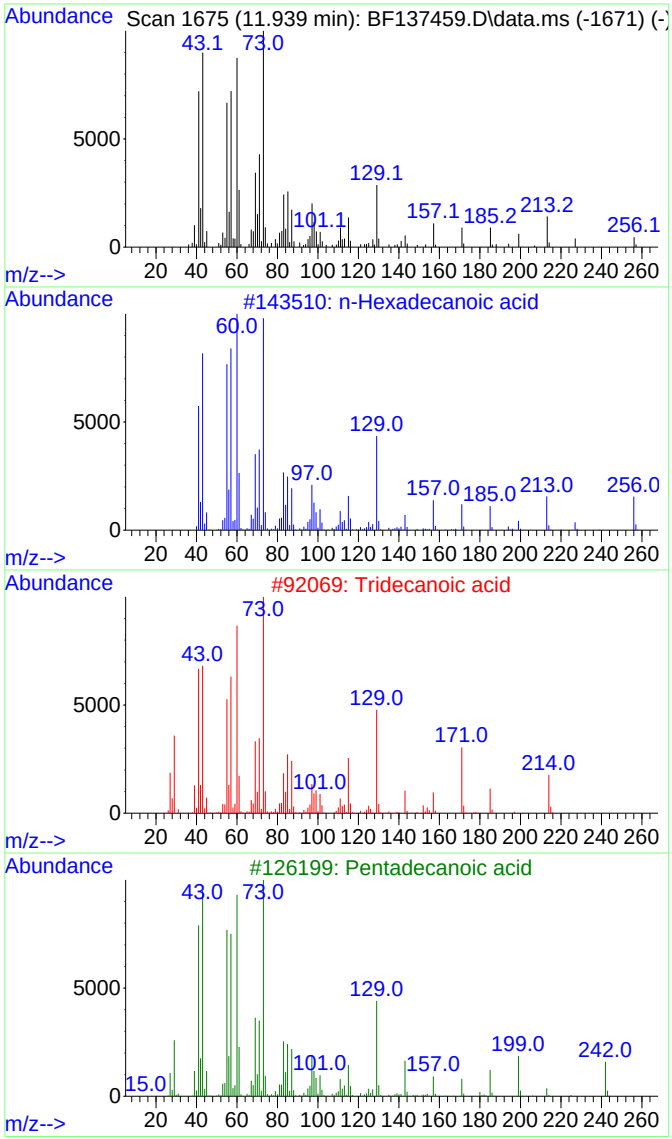
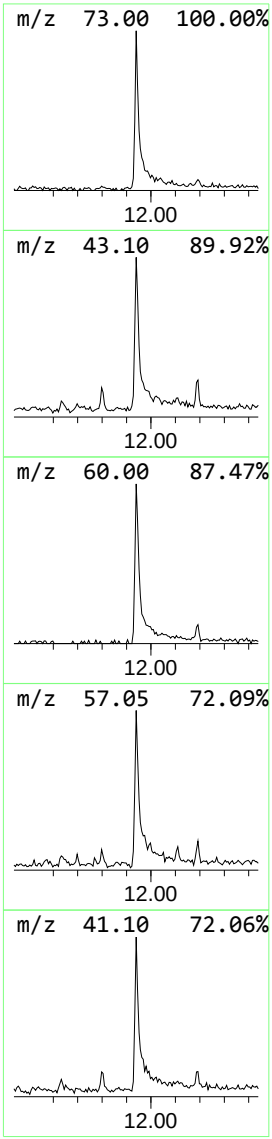
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	3.90 ng	248869	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Octanoic acid	144	C8H16O2	000124-07-2	43
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	35





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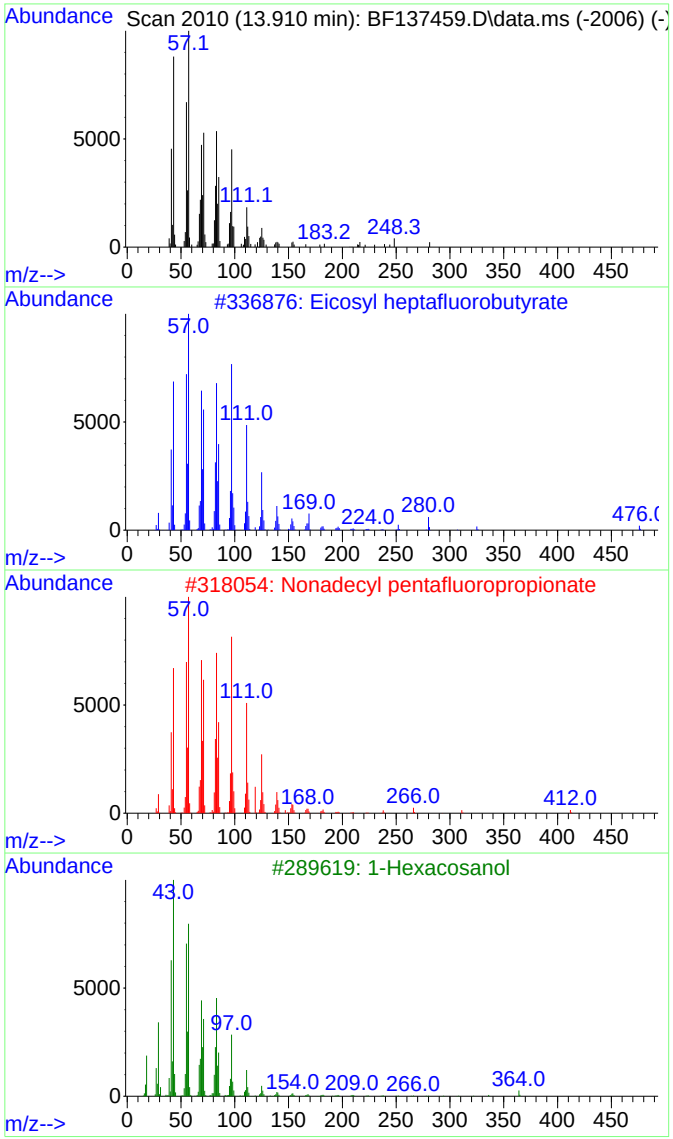
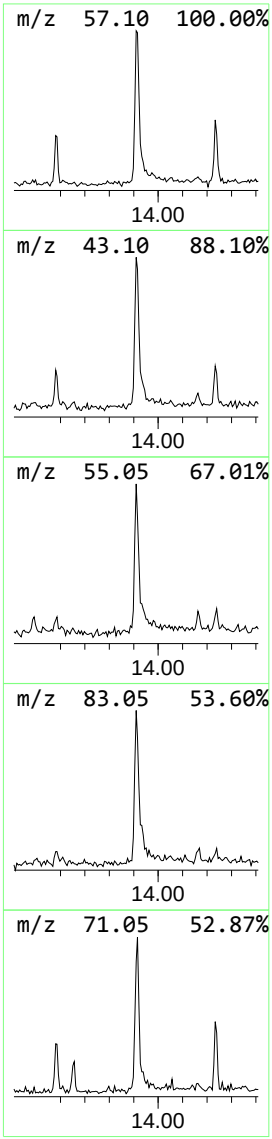
Peak Number 7 Eicosyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	3.36 ng	192326	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	1-Hexacosanol	382	C26H54O	000506-52-5	90
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	81





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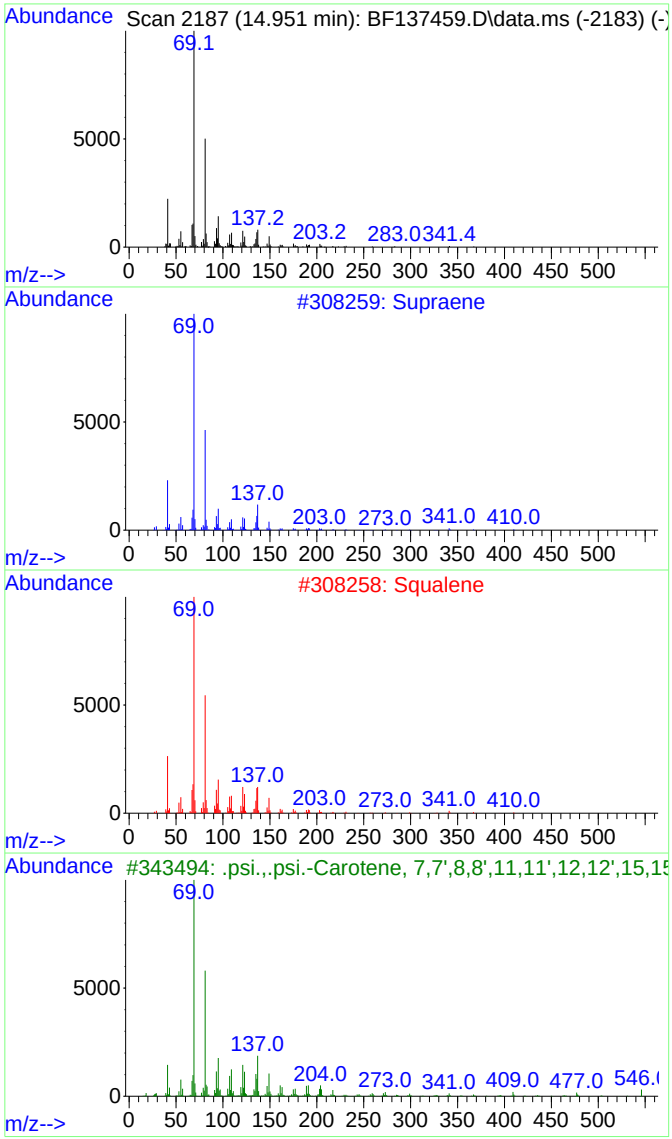
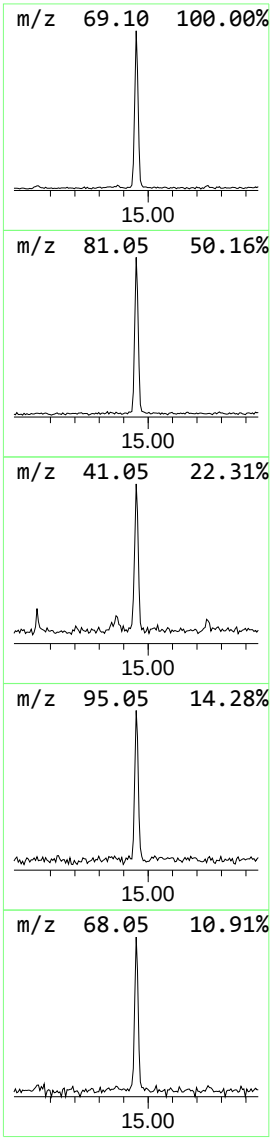
Peak Number 8 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.951	4.53 ng	215007	Perylene-d12	15.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	90
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	trans-Farnesol	222	C15H26O	000106-28-5	78
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
Data File : BF137459.D
Acq On : 01 Mar 2024 15:16
Operator : CG\JU
Sample : P1659-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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...	2.175	28.0	ng	1601670	1	6.869	1143110	20.0
(S)-(+)-1,2-Pro...	3.522	7.7	ng	439583	1	6.869	1143110	20.0
1-Phenoxypropan...	8.463	2.1	ng	152419	2	8.139	1475860	20.0
2,4,7,9-Tetrame...	9.339	3.5	ng	270486	3	9.898	1528470	20.0
unknown10.016	10.016	97.1	ng	7421230	3	9.898	1528470	20.0
n-Hexadecanoic ...	11.939	3.9	ng	248869	4	11.392	1277690	20.0
Eicosyl heptafl...	13.910	3.4	ng	192326	5	14.051	1144820	20.0
Supraene	14.951	4.5	ng	215007	6	15.586	948666	20.0