LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071924\
Data File : BF138595.D
Acq On : 19 Jul 2024 18:01
Operator : RC/JU
Sample : P3294-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071724

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: BF138595.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	25	rVB	1452593	2290712	99.22%	13.213%
2	3.375	213	218	235	rBV	29637	81158	3.52%	0.468%
3	5.081	504	508	522	rVB	111901	170797	7.40%	0.985%
4	5.487	571	577	582	rBV	1544162	2078680	90.04%	11.990%
5	6.493	742	748	753	rBV	1631569	2214141	95.90%	12.771%
6	6.857	805	810	815	rBV	410175	488463	21.16%	2.817%
7	7.422	899	906	911	rBV	1065188	1411533	61.14%	8.142%
8	8.140	1022	1028	1033	rBV	515020	636733	27.58%	3.673%
9	8.451	1076	1081	1093	rBV	57176	83420	3.61%	0.481%
10	9.216	1205	1211	1216	rBV	1779651	2308738	100.00%	13.317%
11	9.892	1320	1326	1331	rBV	537173	667170	28.90%	3.848%
12	9.987	1336	1342	1348	rBV	58885	94524	4.09%	0.545%
13	10.310	1390	1397	1404	rVB3	11928	24915	1.08%	0.144%
14	10.681	1454	1460	1469	rBV	936795	1217909	52.75%	7.025%
15	10.792	1475	1479	1486	rVB	16521	27553	1.19%	0.159%
16	11.375	1573	1578	1585	rBV	460807	580800	25.16%	3.350%
17	11.898	1663	1667	1677	rBV2	99940	165255	7.16%	0.953%
18	12.457	1759	1762	1772	rVB3	20138	38179	1.65%	0.220%
19	12.686	1797	1801	1807	rBV5	16884	28701	1.24%	0.166%
20	12.957	1842	1847	1856	rVB	1280519	1685067	72.99%	9.719%
21	13.857	1995	2000	2011	rBV	85888	162797	7.05%	0.939%
22	14.010	2021	2026	2036	rBV	328064	451751	19.57%	2.606%
23	15.474	2270	2275	2286	rVB	254755	428318	18.55%	2.470%

Sum of corrected areas: 17337314

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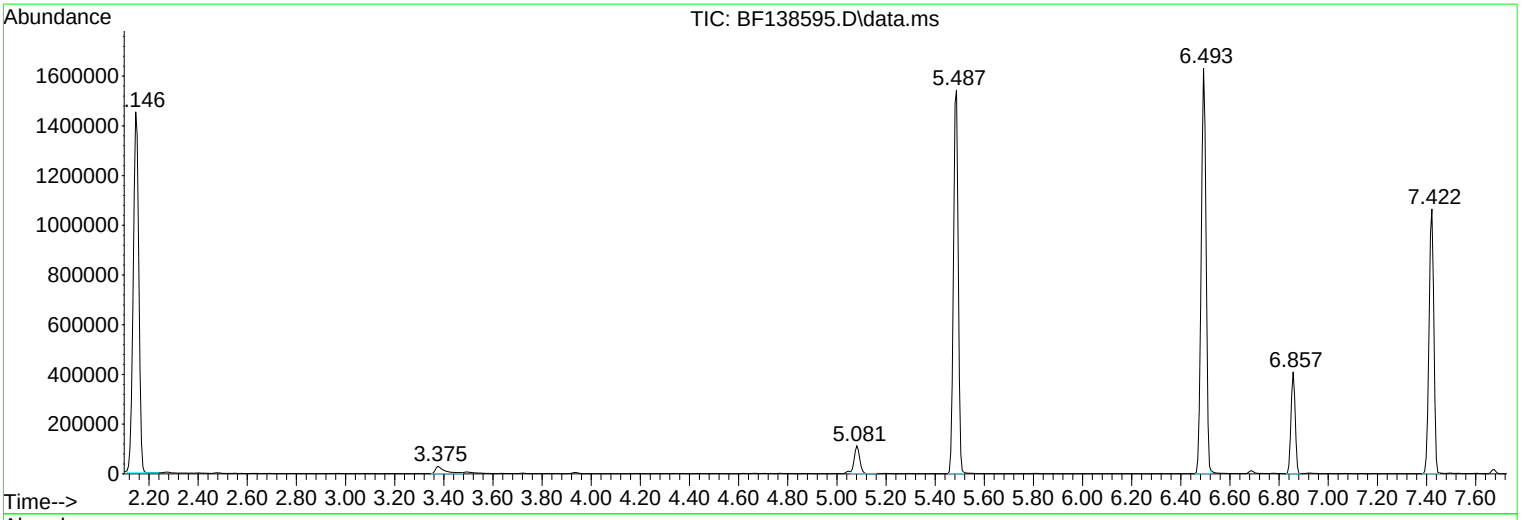
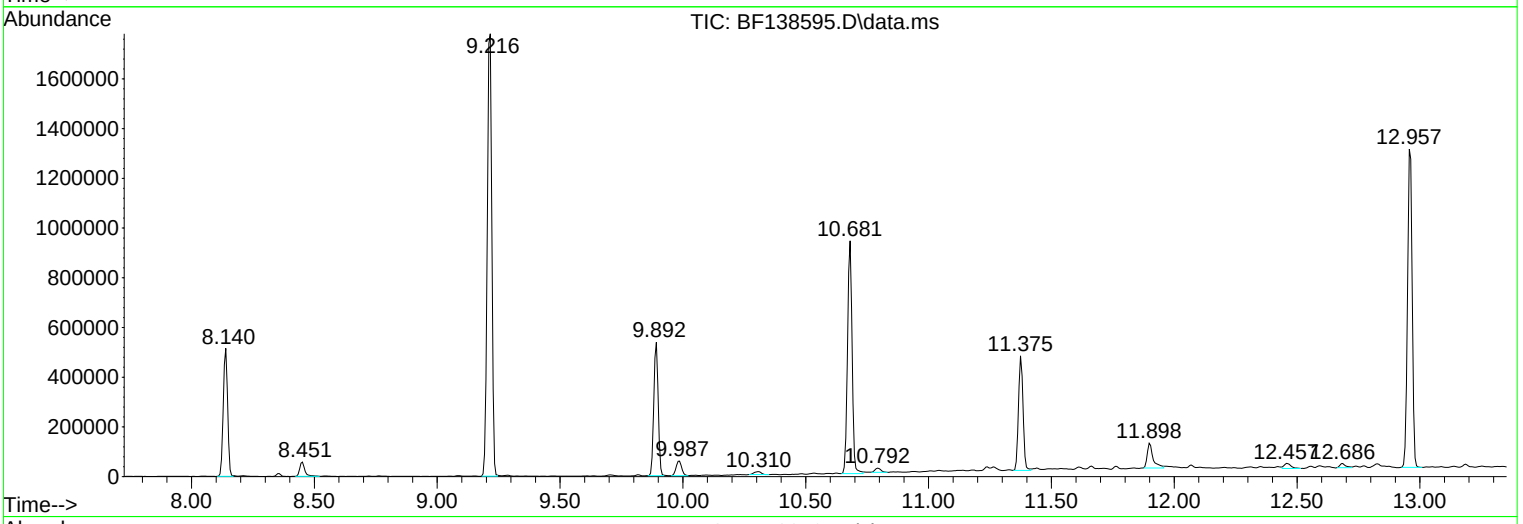
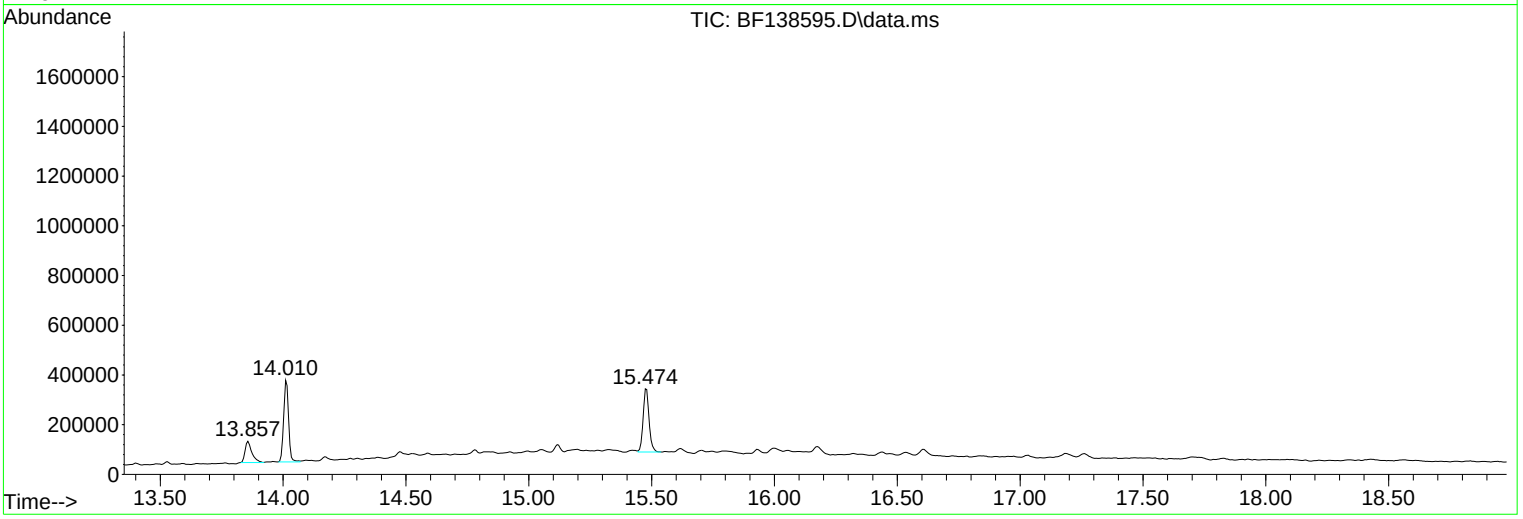
ClientSampleId :
HR-1-071724

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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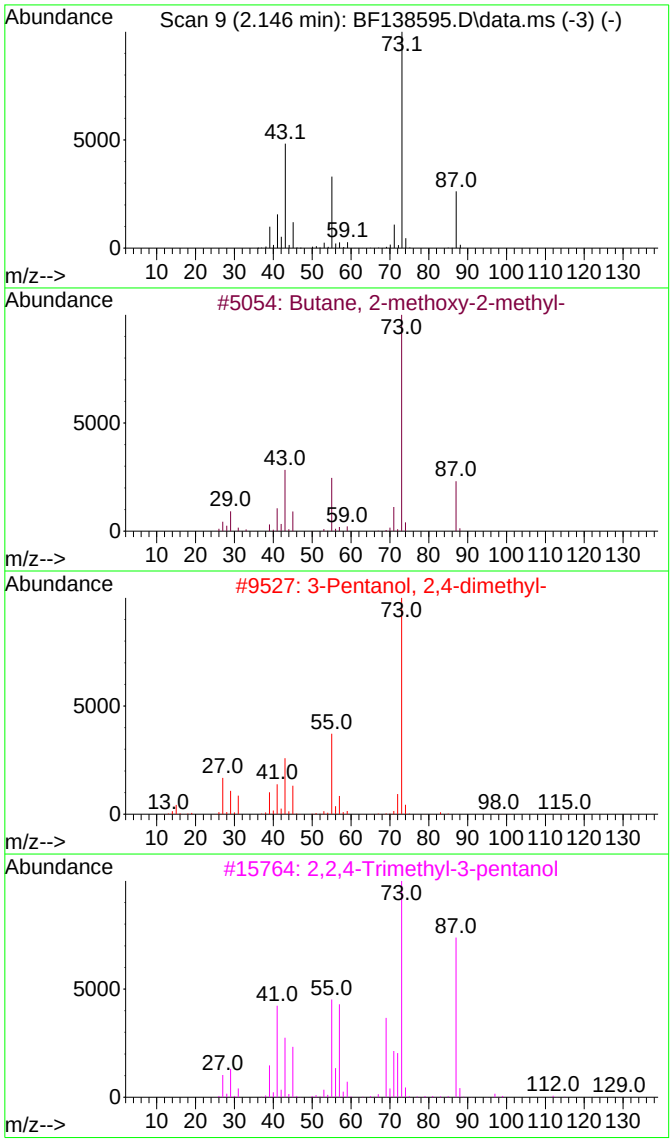
TIC Integration Parameters: LSCINT.P

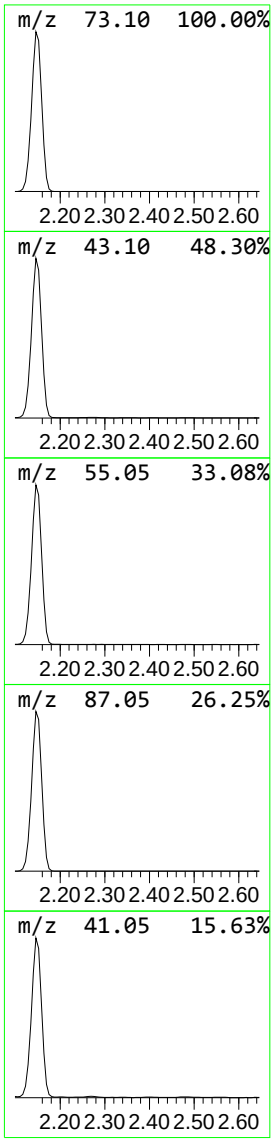
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	93.79 ng	2290710	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Sample : P3294-01
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Instrument :
BNA_F
ClientSampleId :
HR-1-071724

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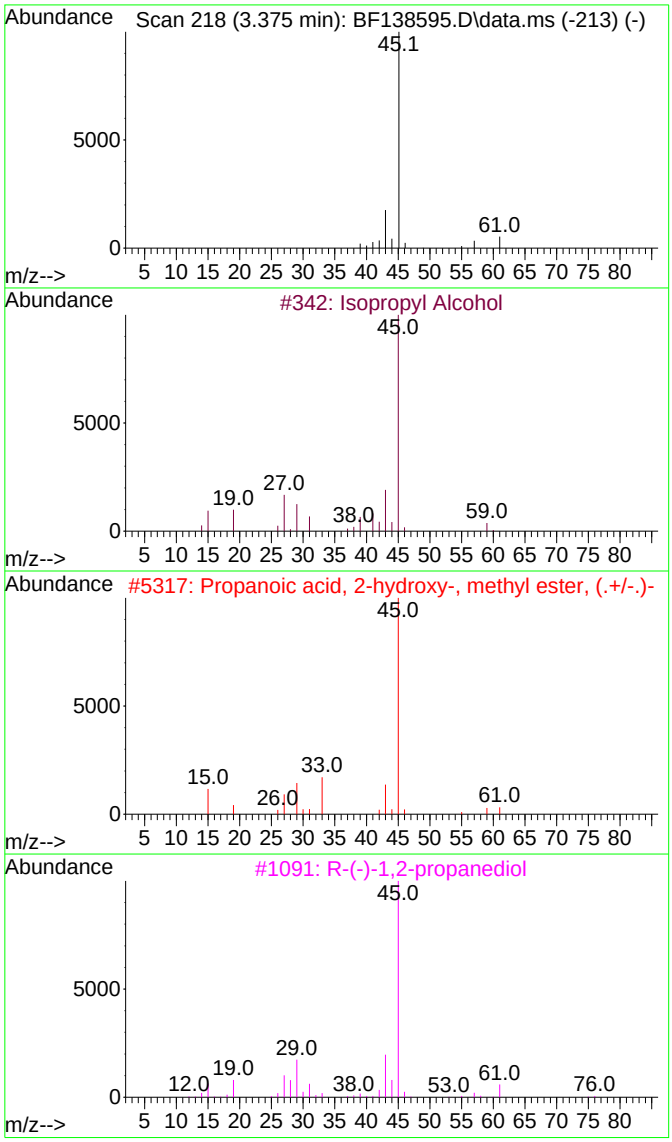
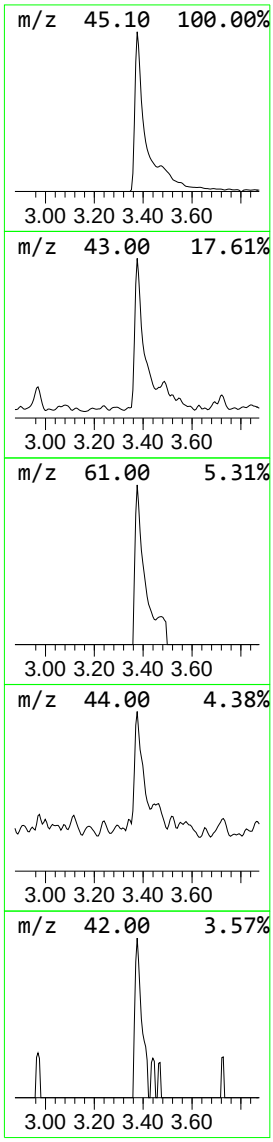
****

Peak Number 2 unknown3.375 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.375	3.32 ng	81158	1,4-Dichlorobenzene-d4	6.857

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





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Operator : RC/JU
Sample : P3294-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071724

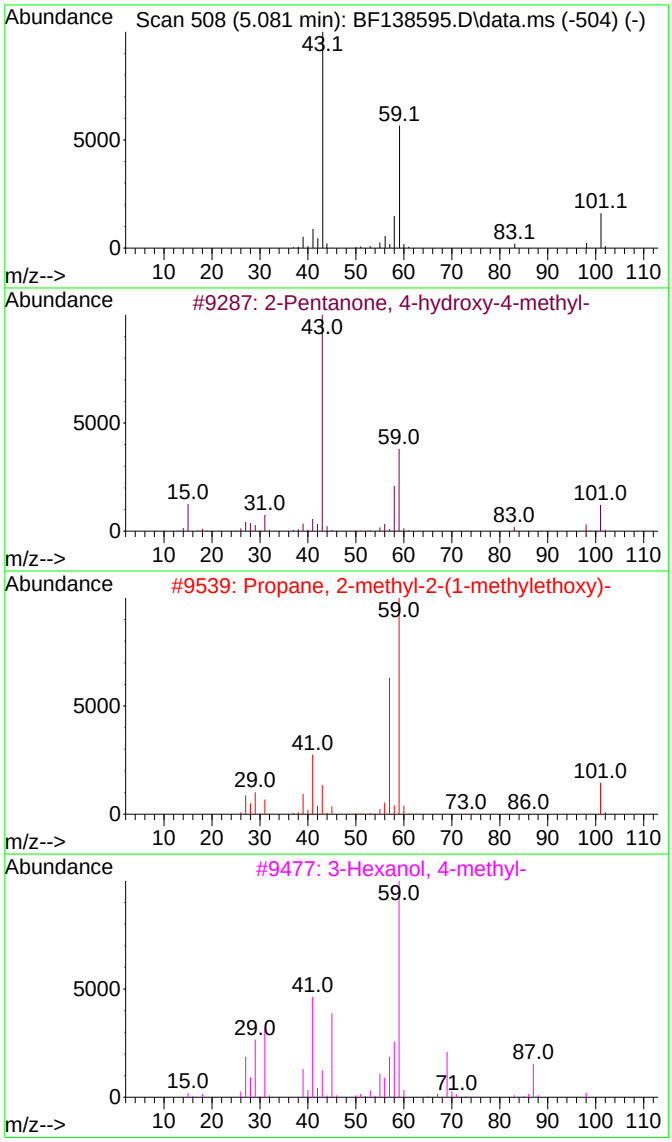
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

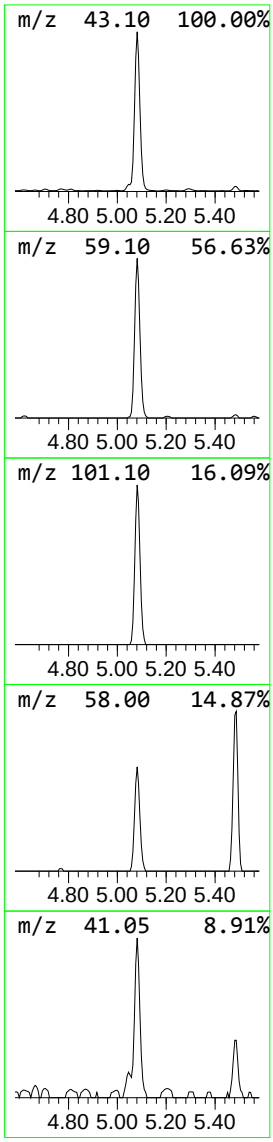
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	6.99 ng	170797	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071724

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

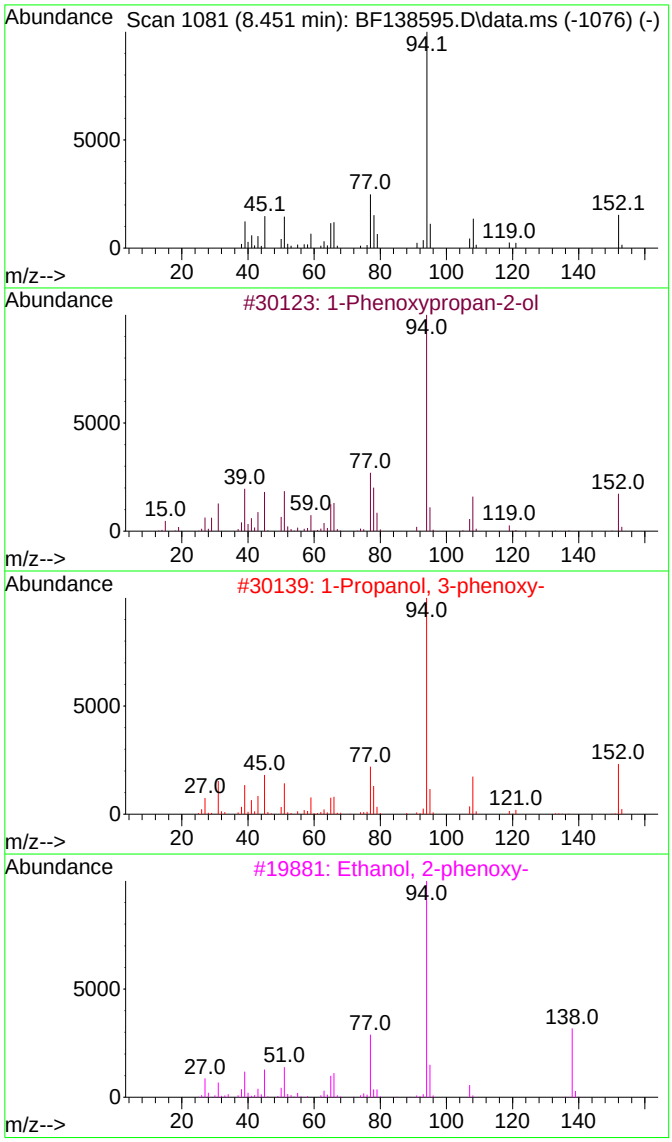
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

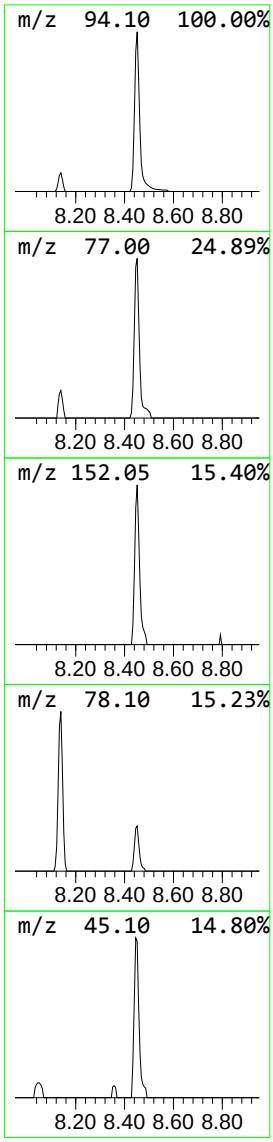
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	2.62 ng	83420	Naphthalene-d8	8.140

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	64
5	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59





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Instrument :
BNA_F
ClientSampleId :
HR-1-071724

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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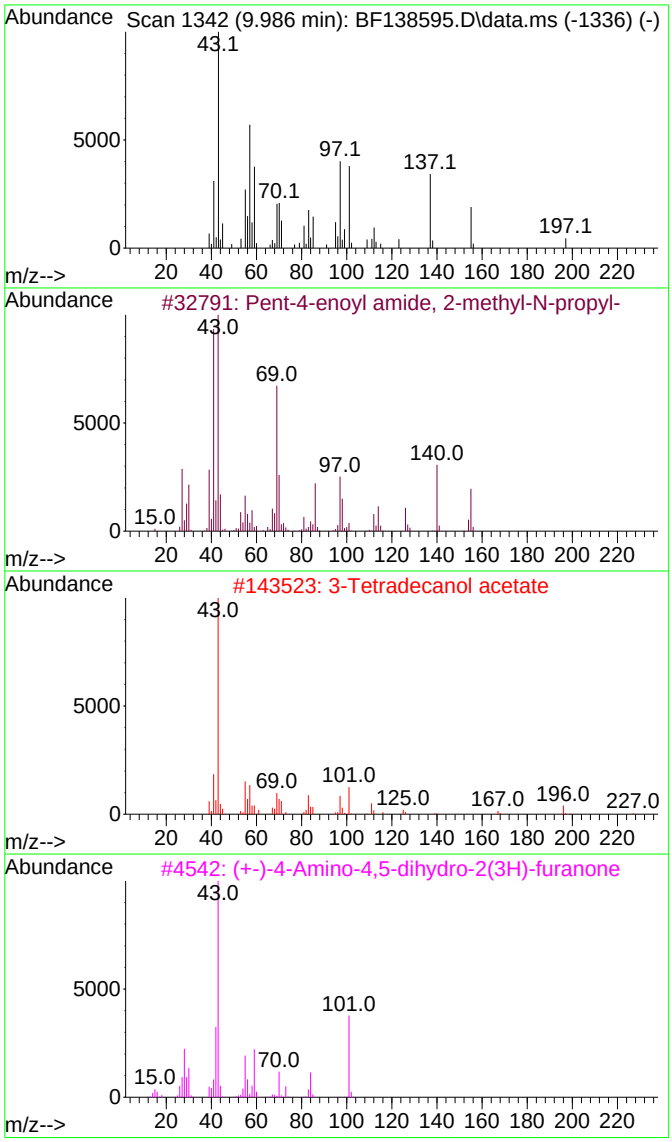
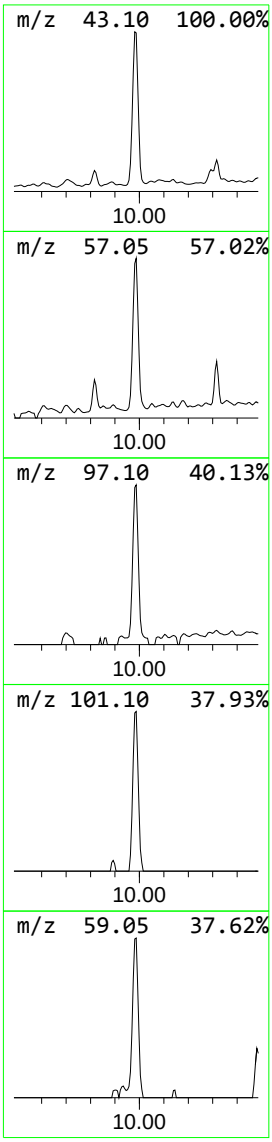
Peak Number 5 unknown9.986 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.986	2.83 ng	94524	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	27
2	3-Tetradecanol acetate	256	C16H32O2	051354-23-5	25
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	22
4	3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	22
5	5-Ethyl-3-nonanol	172	C11H24O	019780-71-3	14





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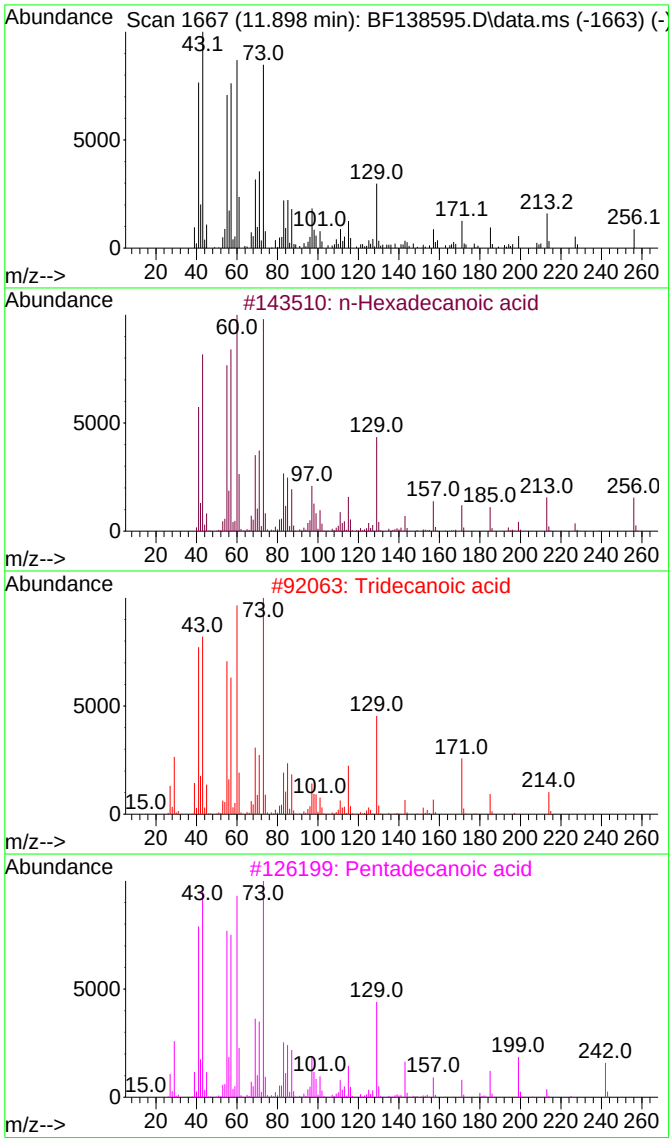
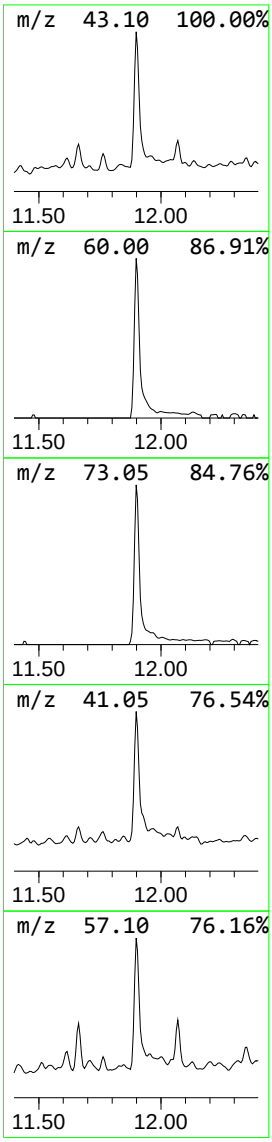
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	5.69 ng	165255	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





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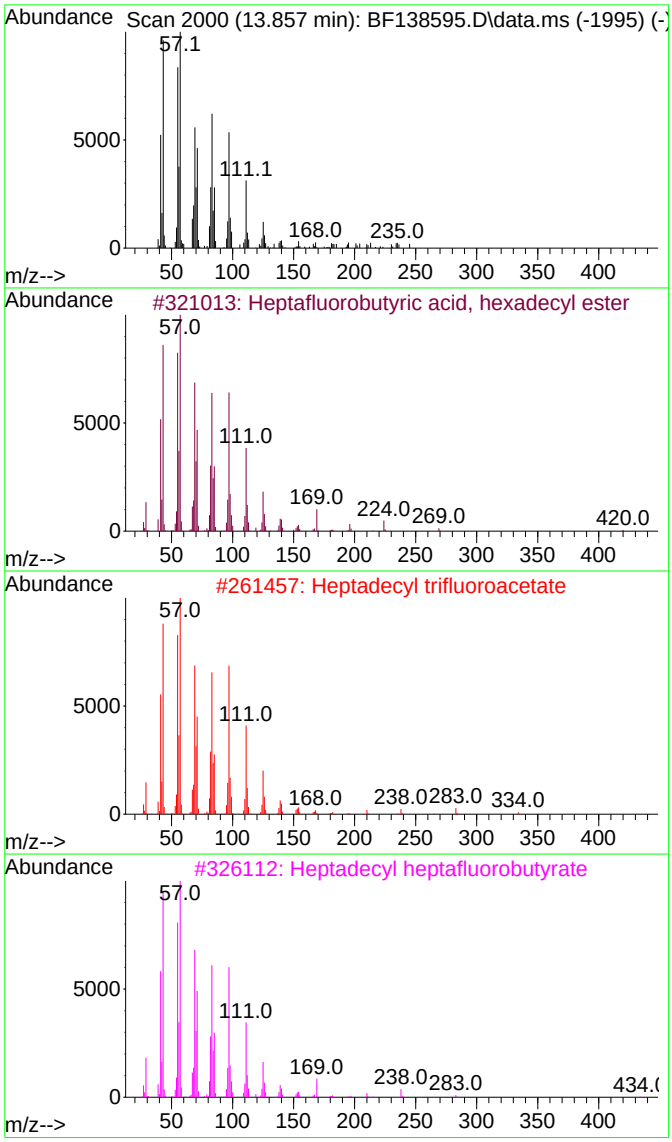
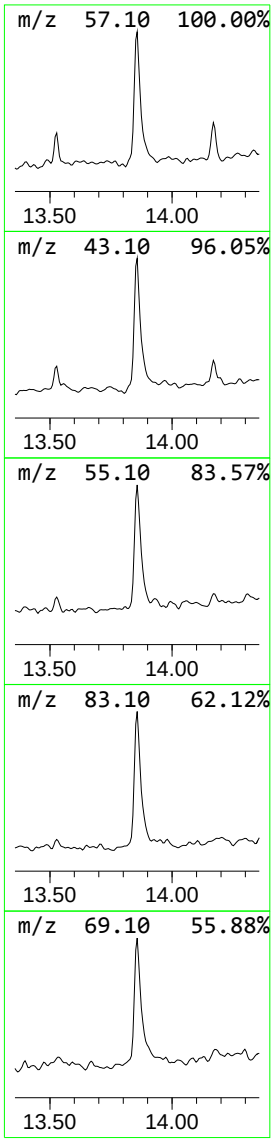
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptafluorobutyric acid, he... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	7.21 ng	162797	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Cyclopentadecane	210	C15H30	000295-48-7	92
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.146	93.8	ng	2290710	1	6.857	488463	20.0
unknown3.375	3.375	3.3	ng	81158	1	6.857	488463	20.0
2-Pentanone, 4-...	5.081	7.0	ng	170797	1	6.857	488463	20.0
1-Phenoxypropan...	8.451	2.6	ng	83420	2	8.140	636733	20.0
unknown9.986	9.986	2.8	ng	94524	3	9.892	667170	20.0
n-Hexadecanoic ...	11.898	5.7	ng	165255	4	11.375	580800	20.0
Heptafluorobuty...	13.857	7.2	ng	162797	5	14.010	451751	20.0