LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127875.D
Acq On : 25 Apr 2022 12:40
Operator : CG\JU
Sample : N2482-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-4

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-BF042222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127875.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.481	368	373	383	rVB	440927	485218	9.32%	1.539%
2	5.175	486	491	503	rBV	162124	209312	4.02%	0.664%
3	5.557	552	556	560	rBV	2147093	2062419	39.62%	6.541%
4	6.557	722	726	731	rBV	1376456	1319821	25.36%	4.186%
5	6.739	753	757	759	rBV	249912	237928	4.57%	0.755%
6	6.769	759	762	774	rVV	231289	328822	6.32%	1.043%
7	6.863	774	778	787	rVV	253361	412176	7.92%	1.307%
8	6.939	787	791	794	rVB	1122971	879136	16.89%	2.788%
9	7.504	879	887	890	rBV	2947234	2969822	57.06%	9.418%
10	7.575	895	899	902	rVV	78878	97222	1.87%	0.308%
11	7.610	902	905	918	rVB3	45916	92709	1.78%	0.294%
12	7.928	956	959	964	rBV3	48471	54365	1.04%	0.172%
13	8.175	991	1001	1005	rBV5	44106	129175	2.48%	0.410%
14	8.222	1005	1009	1016	rVB	1375827	1210108	23.25%	3.838%
15	8.445	1039	1047	1050	rBV4	31704	75589	1.45%	0.240%
16	8.551	1060	1065	1070	rBV3	109041	138814	2.67%	0.440%
17	8.628	1074	1078	1088	rVB2	65610	101772	1.96%	0.323%
18	9.216	1173	1178	1187	rBV4	89297	280041	5.38%	0.888%
19	9.298	1187	1192	1195	rBV	5123191	5102643	98.03%	16.182%
20	9.398	1205	1209	1219	rVB	1134921	1253799	24.09%	3.976%
21	9.980	1299	1308	1311	rBV	1663909	1407824	27.05%	4.465%
22	10.286	1357	1360	1363	rBV2	59248	57229	1.10%	0.181%
23	10.392	1374	1378	1381	rVB	274555	229291	4.41%	0.727%
24	10.680	1424	1427	1430	rBV	262265	211803	4.07%	0.672%
25	10.774	1438	1443	1446	rBV	3255357	3098986	59.54%	9.828%
26	10.822	1449	1451	1458	rVB2	52724	62877	1.21%	0.199%
27	11.327	1533	1537	1539	rBV	70390	60759	1.17%	0.193%
28	11.474	1558	1562	1565	rBV	1677384	1441214	27.69%	4.571%
29	11.851	1622	1626	1629	rVB	174438	134385	2.58%	0.426%
30	13.063	1827	1832	1836	rBV	4846292	5204929	100.00%	16.507%
31	14.115	2007	2011	2020	rVB	1217895	1127302	21.66%	3.575%
32	14.215	2024	2028	2034	rBV	62122	76419	1.47%	0.242%
33	15.633	2263	2269	2278	rBV	717363	978342	18.80%	3.103%

Sum of corrected areas: 31532251

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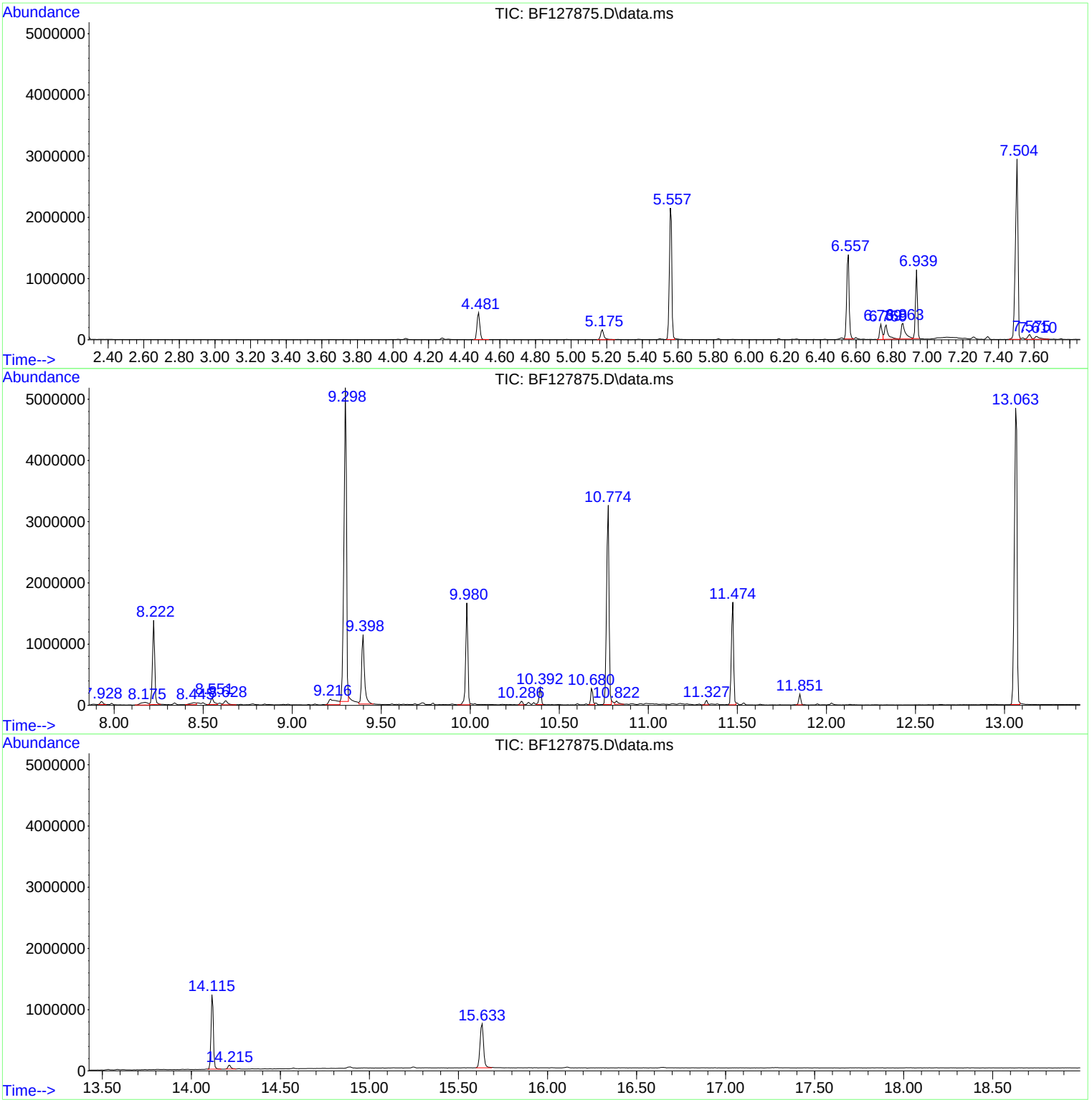
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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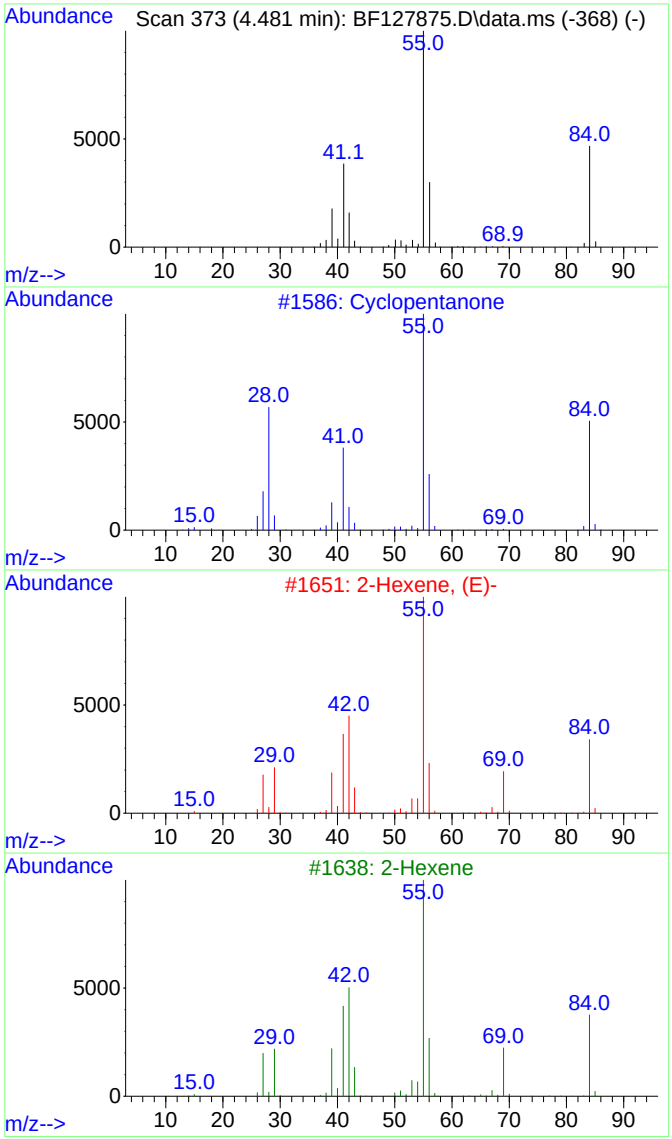
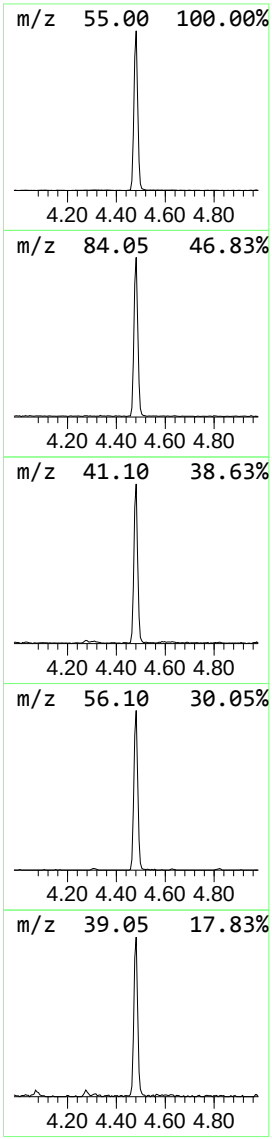
****

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	11.04 ng	485218	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene, (E)-	84	C6H12	004050-45-7	72
3	2-Hexene	84	C6H12	000592-43-8	64
4	2(5H)-Furanone	84	C4H4O2	000497-23-4	47
5	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	42





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Data File : BF127875.D
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
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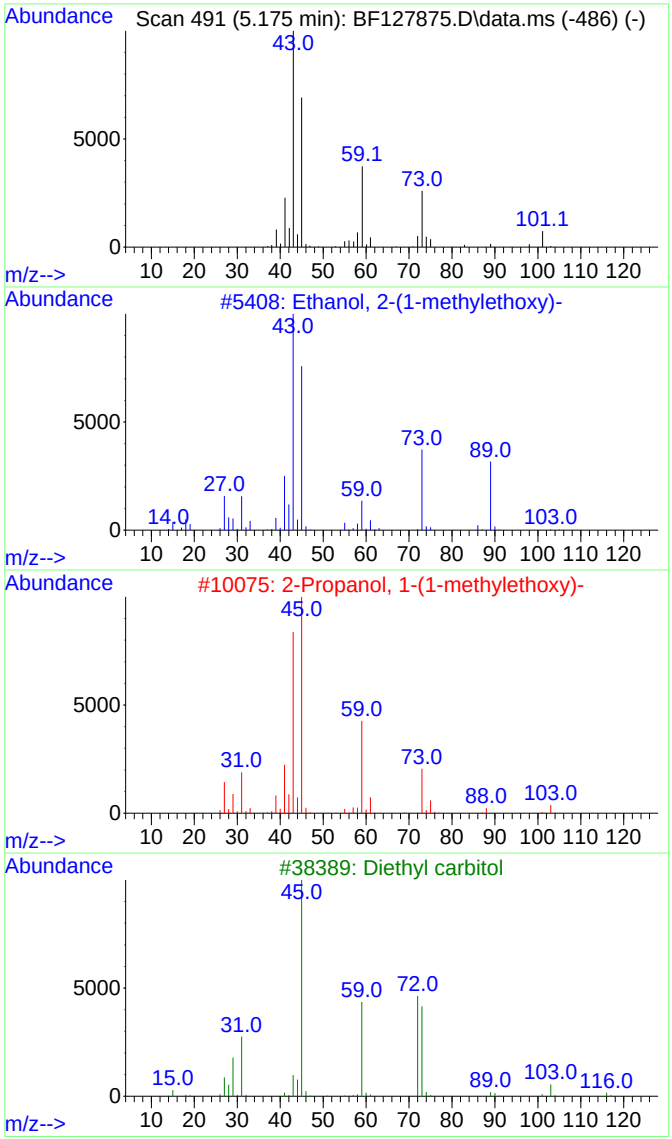
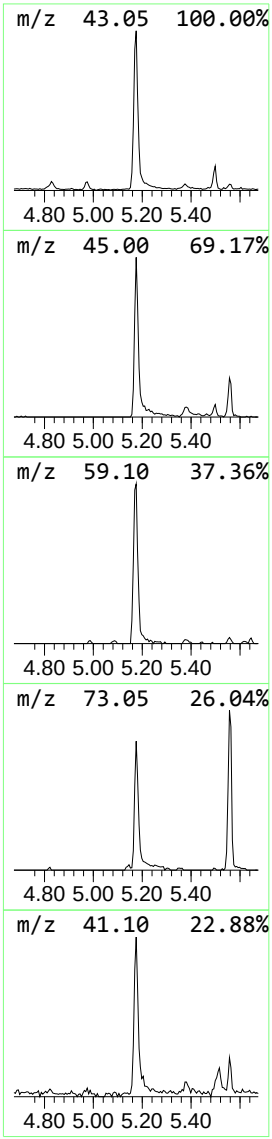
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(1-methylethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	4.76 ng	209312	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	64
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
3	Diethyl carbitol	162	C8H18O3	000112-36-7	42
4	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	42
5	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	38





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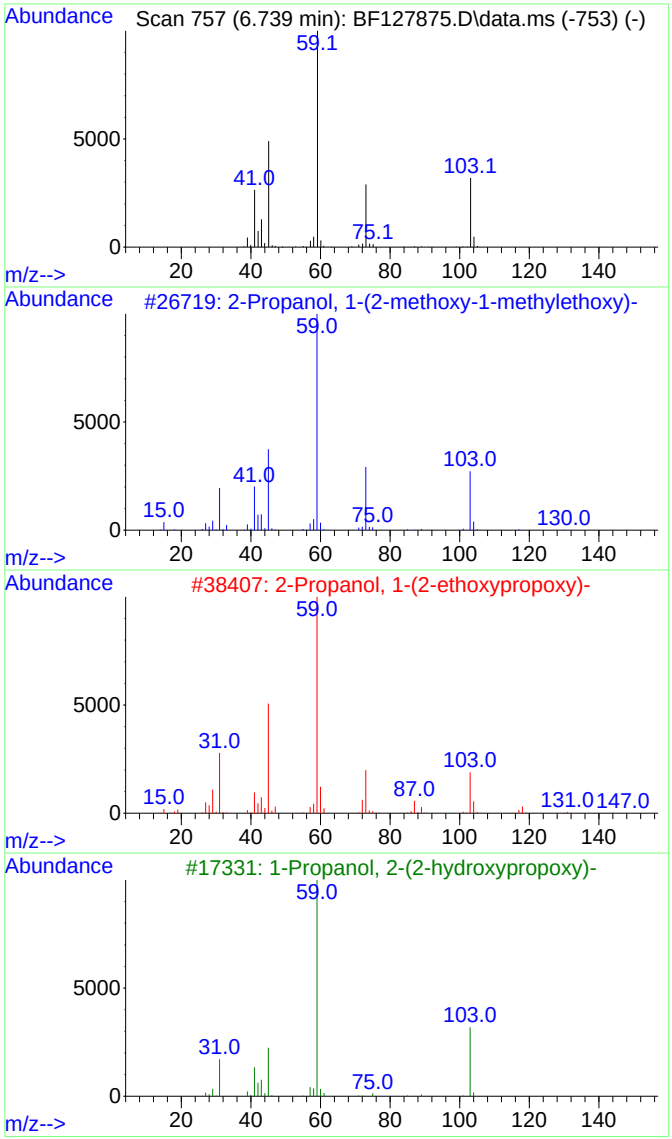
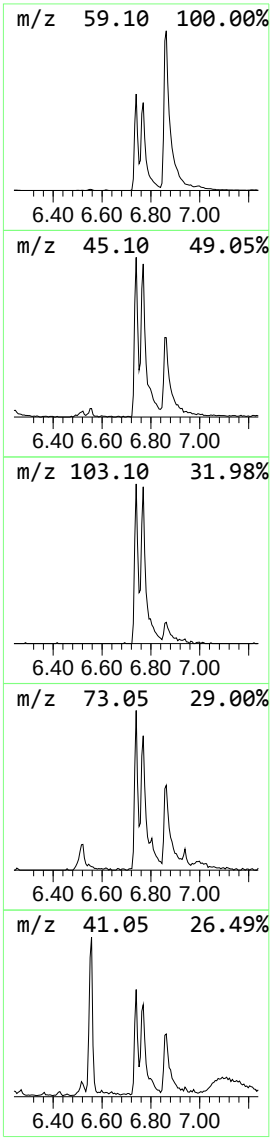
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.739	5.41 ng	237928	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	64
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	42
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	40





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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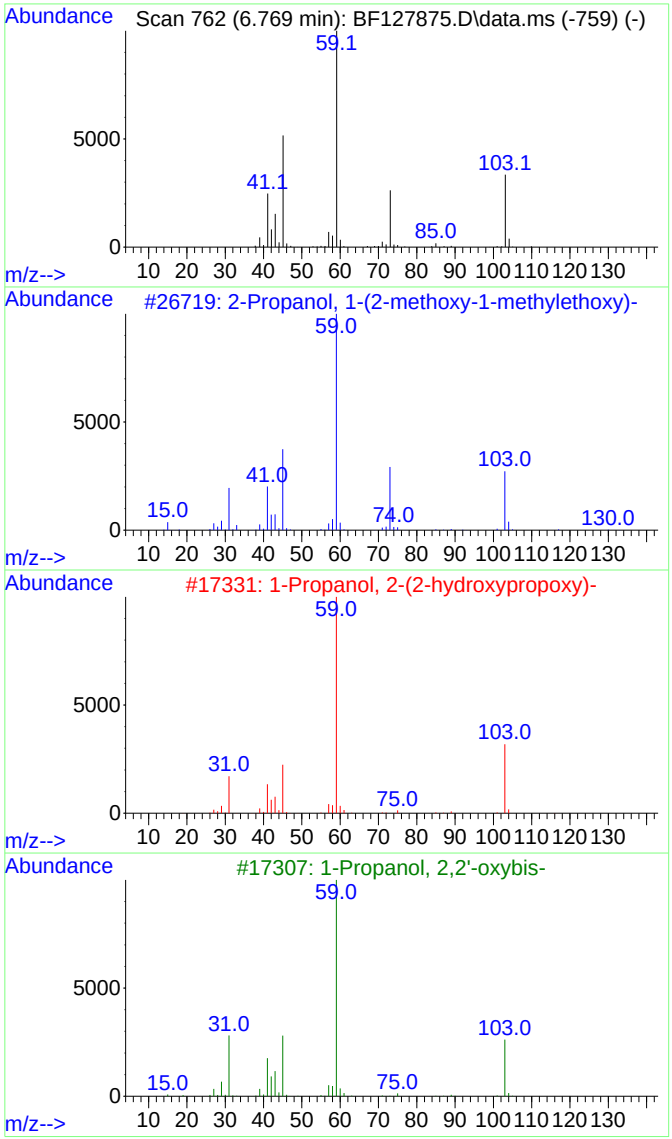
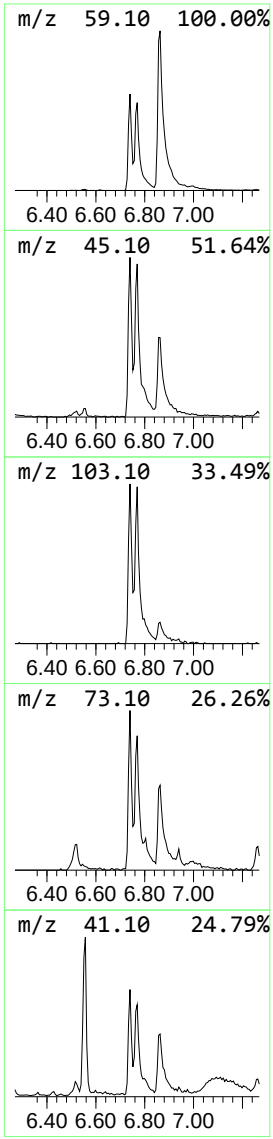
****
Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.769	7.48 ng	328822	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	56
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53
4	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	42





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Operator : CG\JU
Sample : N2482-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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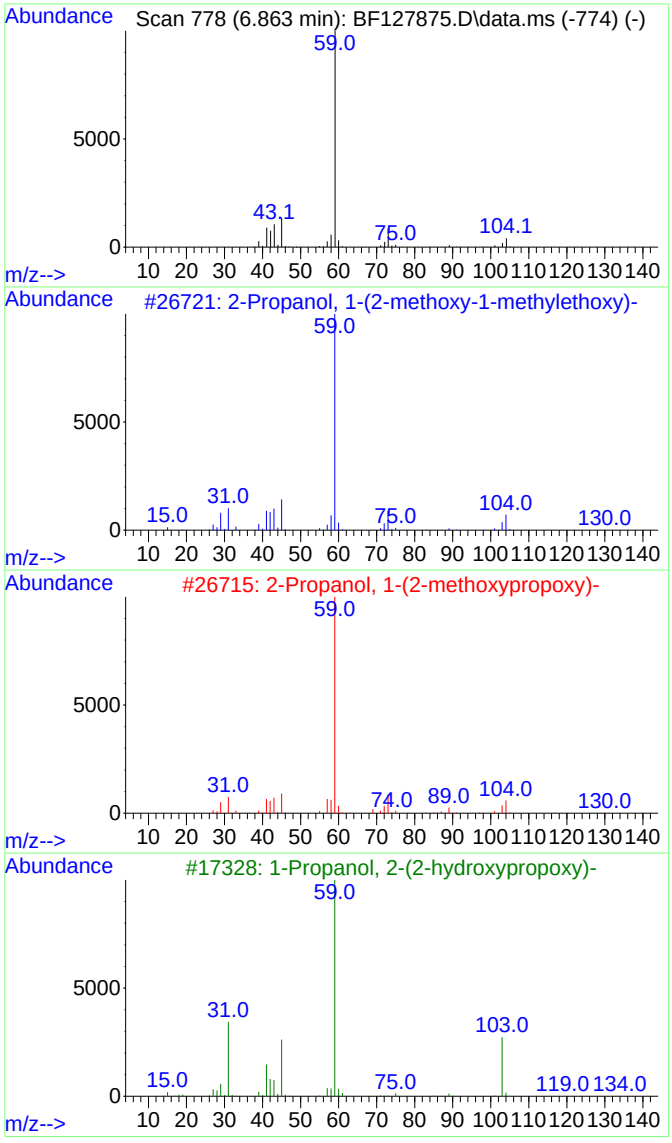
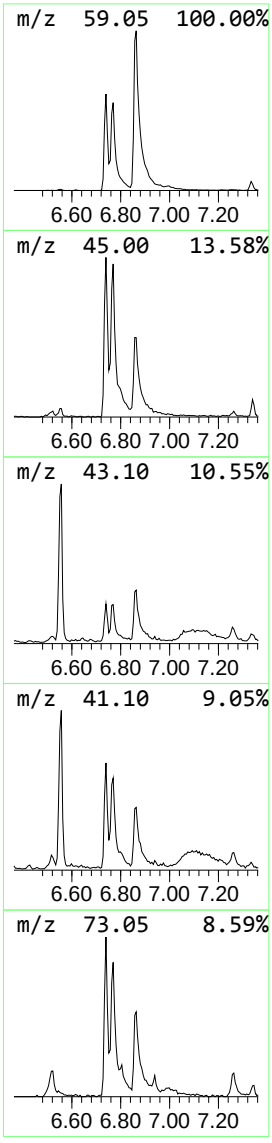
****
Peak Number 5 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.863	9.38 ng	412176	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	78
2	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	78
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
5	Tetraglyme	222	C10H22O5	000143-24-8	56





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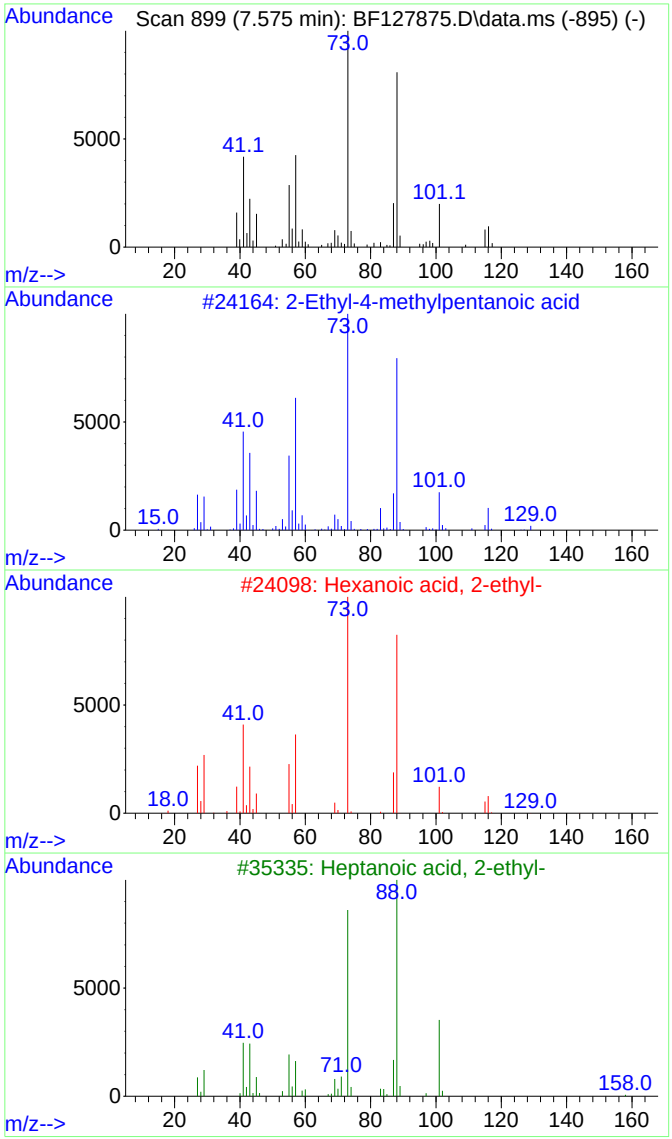
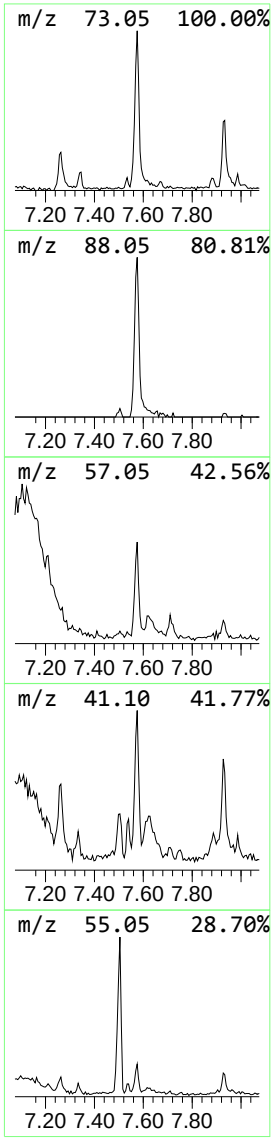
****
Peak Number 6 2-Ethyl-4-methylpentanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.575	2.21 ng	97222	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	83
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	80
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	64
4	Urea, N,N'-dimethyl-	88	C3H8N2O	000096-31-1	43
5	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	40





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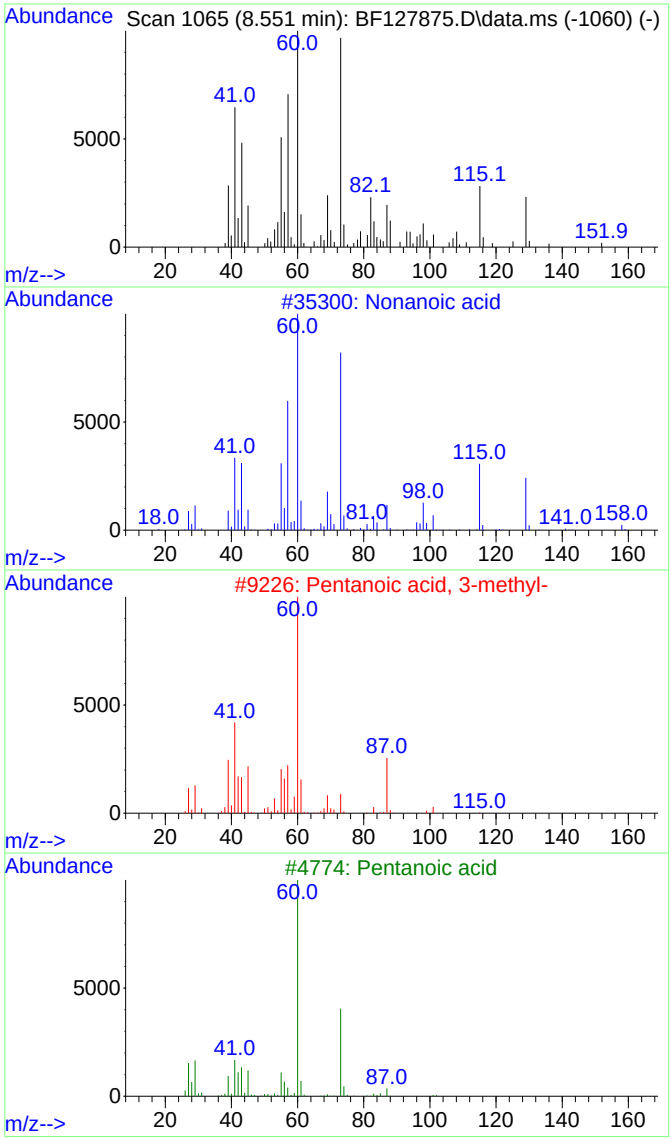
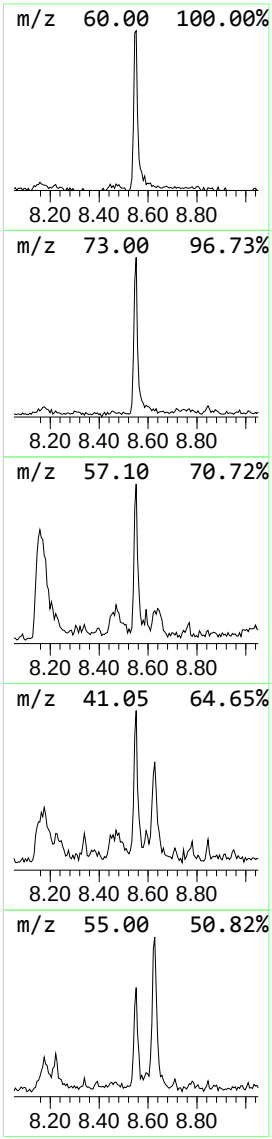
****

Peak Number 7 Nonanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	2.29 ng	138814	Naphthalene-d8	8.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	58
2	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	47
3	Pentanoic acid	102	C5H10O2	000109-52-4	43
4	Hexanoic acid	116	C6H12O2	000142-62-1	38
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	37





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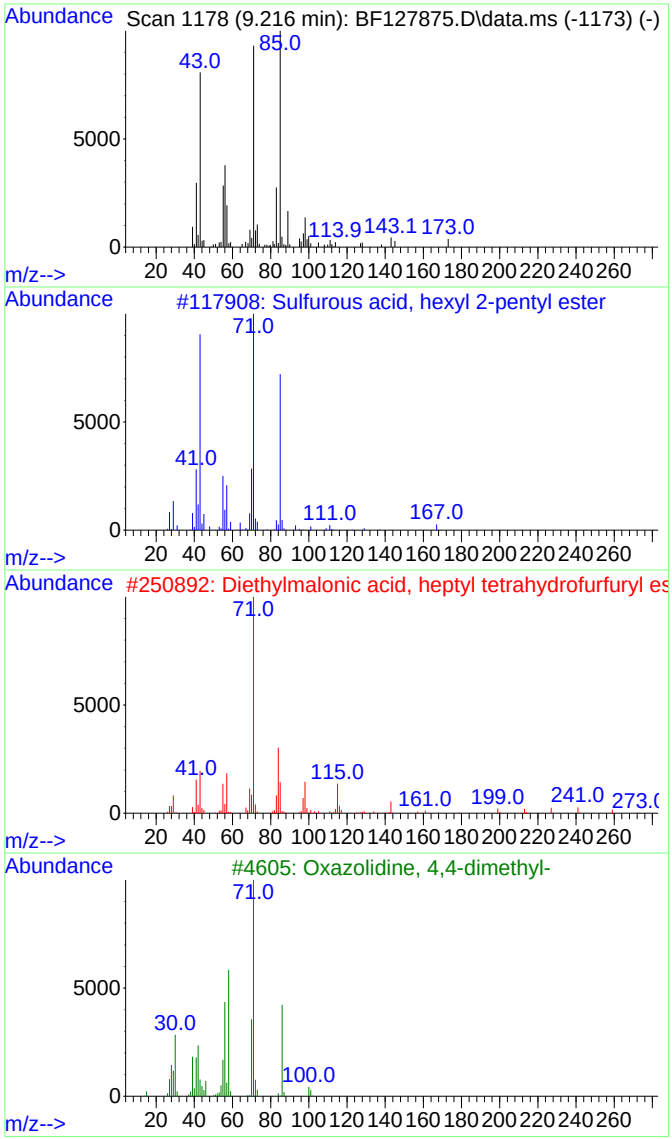
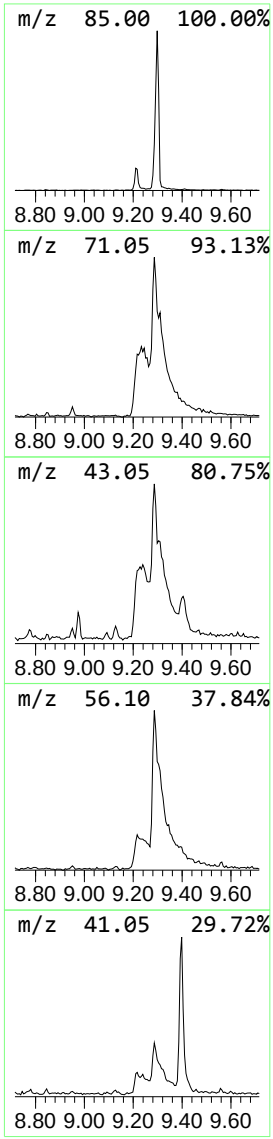
****

Peak Number 8 unknown9.216 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	3.98 ng	280041	Acenaphthene-d10	9.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	43
2	Diethylmalonic acid, heptyl tetr...	342	C19H34O5	1000370-64-2	35
3	Oxazolidine, 4,4-dimethyl-	101	C5H11NO	051200-87-4	27
4	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	27
5	Hexane, 1-(3-butenyloxy)-	156	C10H20O	107995-55-1	27





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
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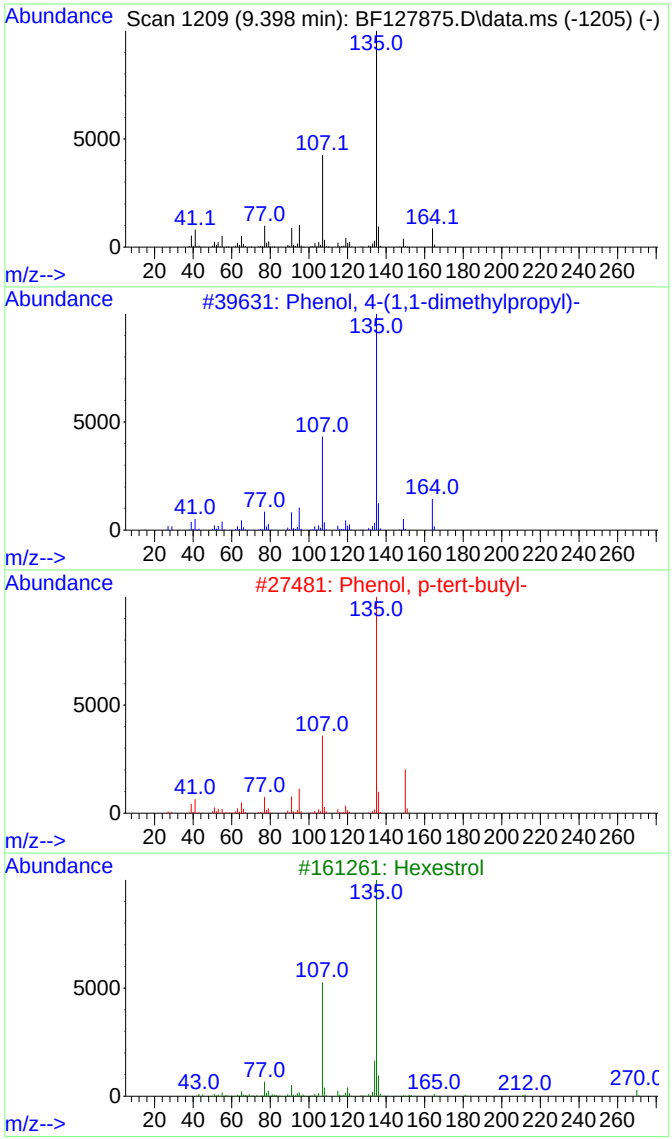
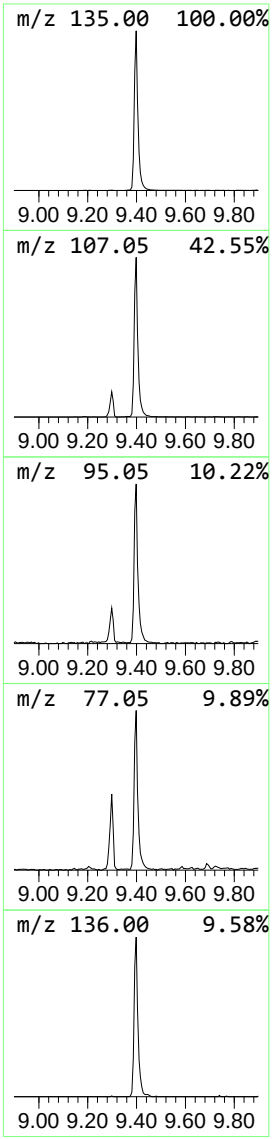
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.398	17.81 ng	1253800	Acenaphthene-d10	9.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	96
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Hexestrol	270	C18H22O2	000084-16-2	72
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127875.D
Acq On : 25 Apr 2022 12:40
Operator : CG\JU
Sample : N2482-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-4

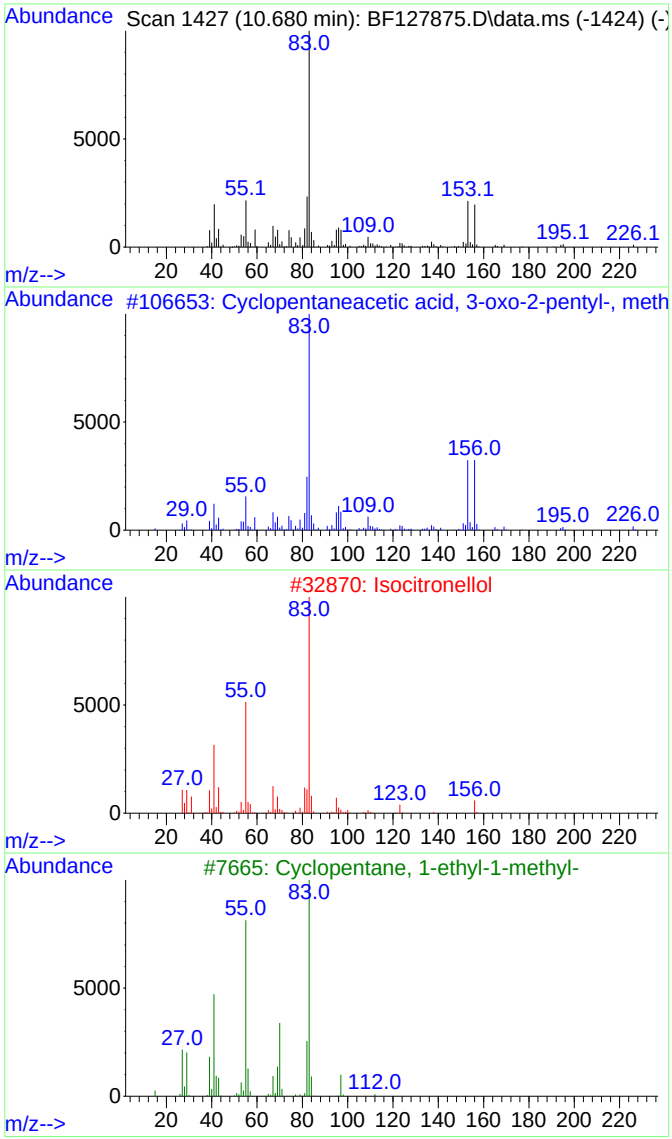
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

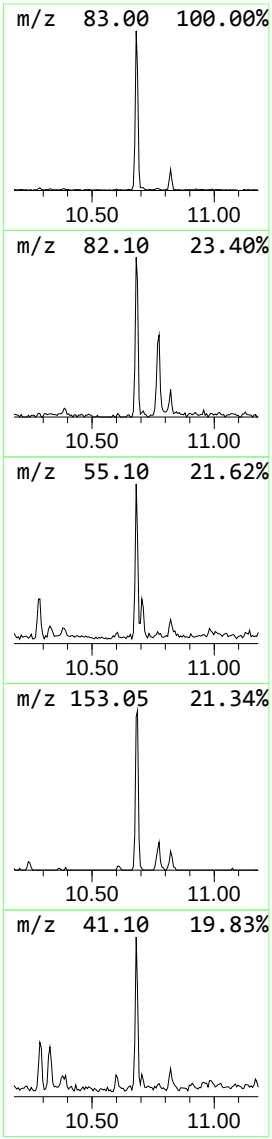
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclopentaneacetic acid, 3-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.680	3.01 ng	211803	Acenaphthene-d10	9.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	95
2	Isocitronellol	156	C10H20O	018479-52-2	53
3	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	47
4	1,5-Dicyano-2,4-dimethyl-2,4-dia...	152	C7H12N4	1010289-23-5	43
5	2-Nonen-4-one, 2-methyl-	154	C10H18O	002903-23-3	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127875.D
Acq On : 25 Apr 2022 12:40
Operator : CG\JU
Sample : N2482-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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
Cyclopentanone	4.481	11.0	ng	485218	1	6.939	879136	20.0
Ethanol, 2-(1-m...	5.175	4.8	ng	209312	1	6.939	879136	20.0
2-Propanol, 1-(...	6.739	5.4	ng	237928	1	6.939	879136	20.0
1-Propanol, 2-(...	6.769	7.5	ng	328822	1	6.939	879136	20.0
2-Propanol, 1-[...	6.863	9.4	ng	412176	1	6.939	879136	20.0
2-Ethyl-4-methy...	7.575	2.2	ng	97222	1	6.939	879136	20.0
Nonanoic acid	8.551	2.3	ng	138814	2	8.222	1210110	20.0
unknown9.216	9.216	4.0	ng	280041	3	9.980	1407820	20.0
Phenol, 4-(1,1-...	9.398	17.8	ng	1253800	3	9.980	1407820	20.0
Cyclopentaneace...	10.680	3.0	ng	211803	3	9.980	1407820	20.0