LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022222\
Data File : BF127010.D
Acq On : 22 Feb 2022 15:55
Operator : CG\JU
Sample : N1599-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-1

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127010.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.028	292	296	302	rVB	31055	38827	1.09%	0.184%
2	4.440	362	366	374	rVB	225645	262611	7.39%	1.247%
3	5.145	482	486	494	rBV	87417	94154	2.65%	0.447%
4	5.410	527	531	535	rBV	389077	344214	9.68%	1.634%
5	5.534	545	552	555	rBV2	1718490	1782387	50.15%	8.463%
6	5.769	588	592	595	rBV	47743	40305	1.13%	0.191%
7	6.534	717	722	728	rVV	1050875	1056121	29.71%	5.014%
8	6.598	730	733	736	rVB	99698	74705	2.10%	0.355%
9	6.710	749	752	754	rBV	190745	140634	3.96%	0.668%
10	6.739	754	757	760	rVB	330869	277764	7.81%	1.319%
11	6.828	769	772	783	rBV	242975	249681	7.02%	1.185%
12	6.916	783	787	790	rBV	705942	536079	15.08%	2.545%
13	6.969	793	796	804	rBV	151536	130615	3.67%	0.620%
14	7.092	814	817	820	rVB	68973	55596	1.56%	0.264%
15	7.481	873	883	886	rBV	2003040	1896057	53.34%	9.002%
16	7.551	891	895	899	rBV	38986	45031	1.27%	0.214%
17	8.110	984	990	995	rBV2	36255	81876	2.30%	0.389%
18	8.198	1001	1005	1007	rBV	870241	731283	20.57%	3.472%
19	8.528	1055	1061	1067	rBV4	48186	61520	1.73%	0.292%
20	8.598	1070	1073	1082	rVB2	31212	40909	1.15%	0.194%
21	9.169	1163	1170	1171	rBV	32267	53995	1.52%	0.256%
22	9.275	1182	1188	1191	rBV	4063788	3548990	99.85%	16.850%
23	9.369	1201	1204	1220	rVB	819832	760203	21.39%	3.609%
24	9.951	1300	1303	1306	rVB	888951	773026	21.75%	3.670%
25	10.263	1352	1356	1359	rBV3	49735	46530	1.31%	0.221%
26	10.369	1369	1374	1378	rVB	131825	131087	3.69%	0.622%
27	10.651	1419	1422	1425	rBV	150251	133191	3.75%	0.632%
28	10.745	1433	1438	1441	rBV	2643762	2298607	64.67%	10.914%
29	11.445	1553	1557	1560	rBV	965531	806498	22.69%	3.829%
30	11.821	1618	1621	1624	rBV	146892	106942	3.01%	0.508%
31	13.033	1822	1827	1830	rBV	3995285	3554440	100.00%	16.876%
32	14.086	2002	2006	2009	rVB	530868	471755	13.27%	2.240%
33	15.580	2255	2260	2267	rBV	342056	436233	12.27%	2.071%

Sum of corrected areas: 21061866

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022222\
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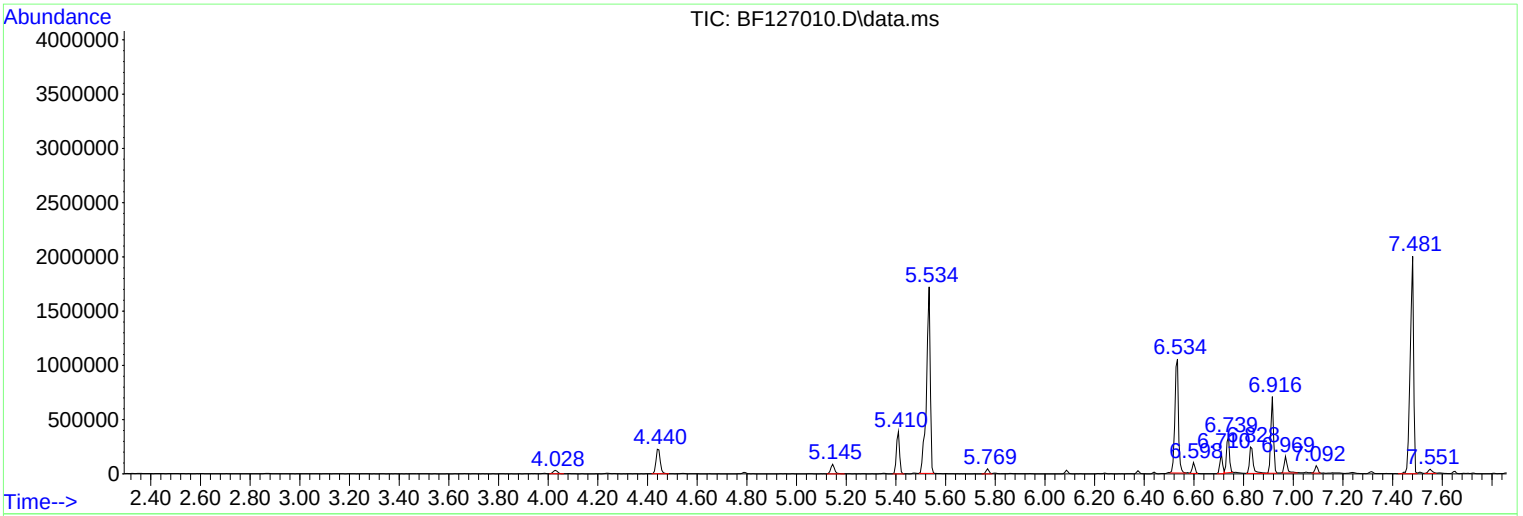
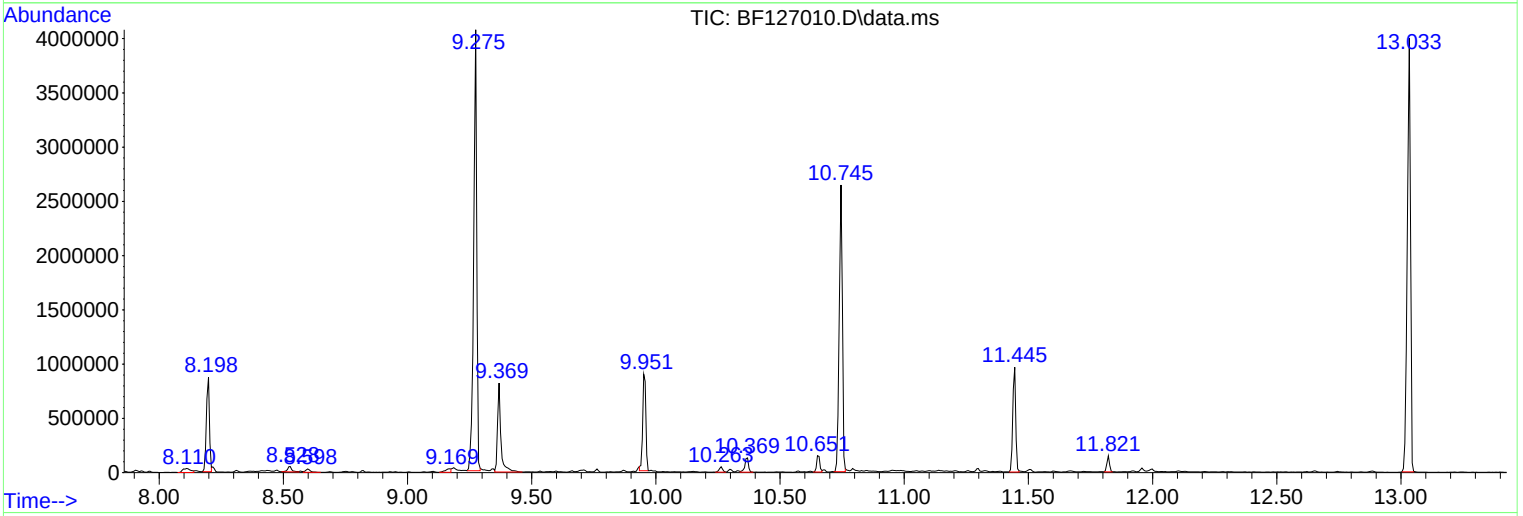
Misc :
ALS Vial : 4 Sample Multiplier: 1

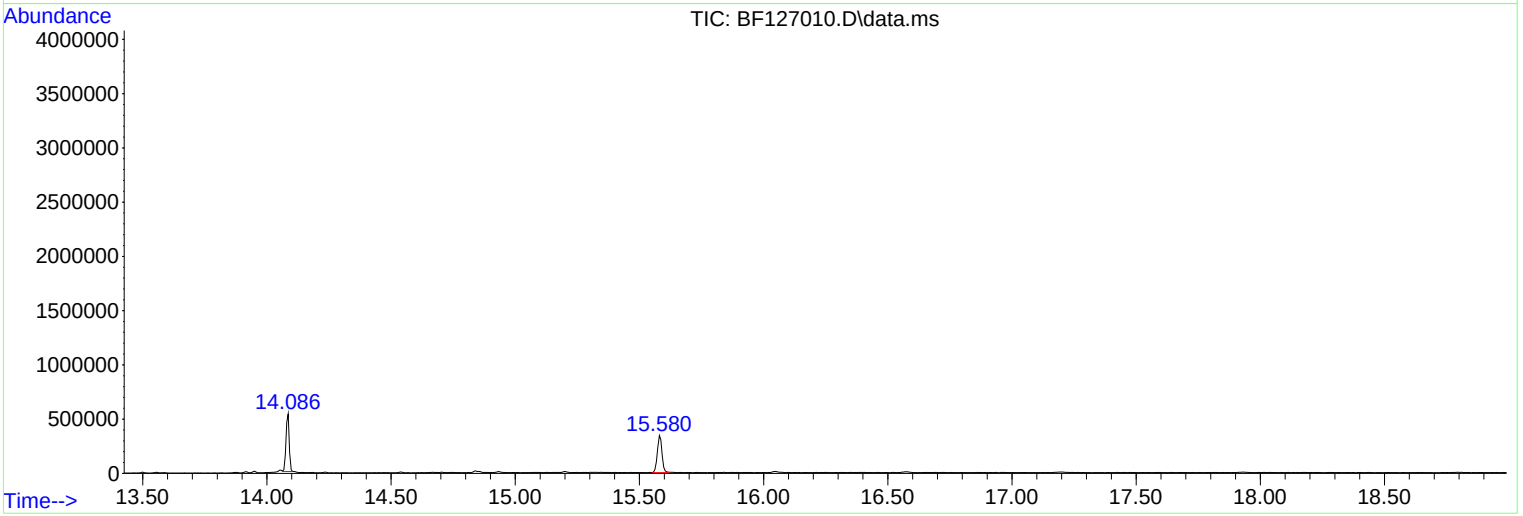
Instrument :
BNA_F
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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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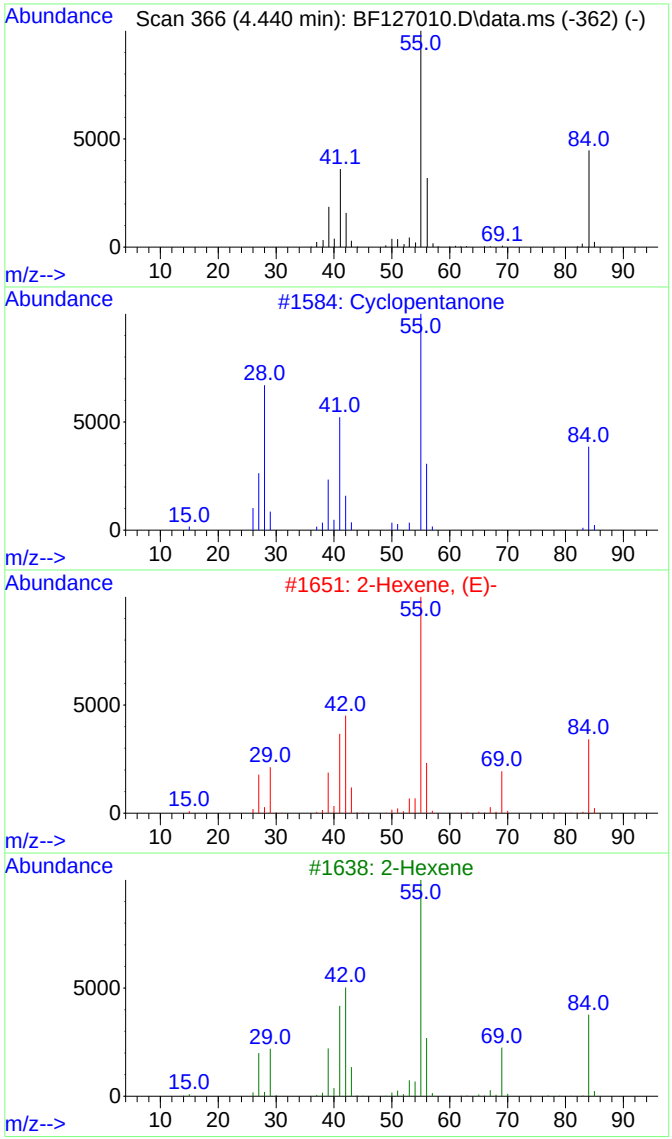
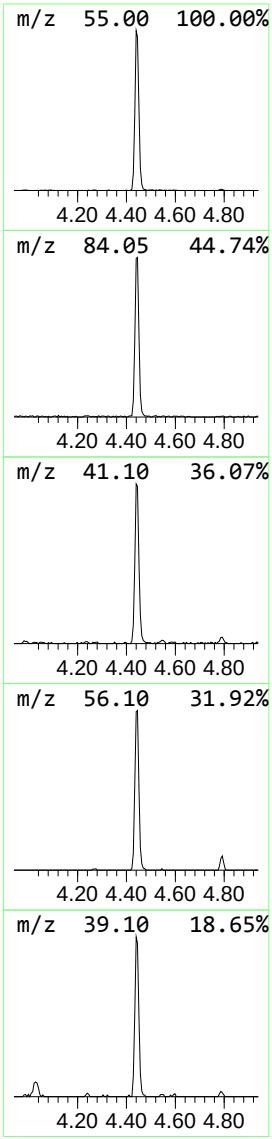
****

Peak Number 1 Cyclopentanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.440	9.80 ng	262611	1,4-Dichlorobenzene-d4	6.916

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	64
3	2-Hexene	84	C6H12	000592-43-8	64
4	3-Hexene, (E)-	84	C6H12	013269-52-8	59
5	3-Hexene, (Z)-	84	C6H12	007642-09-3	58





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ClientSampleId :
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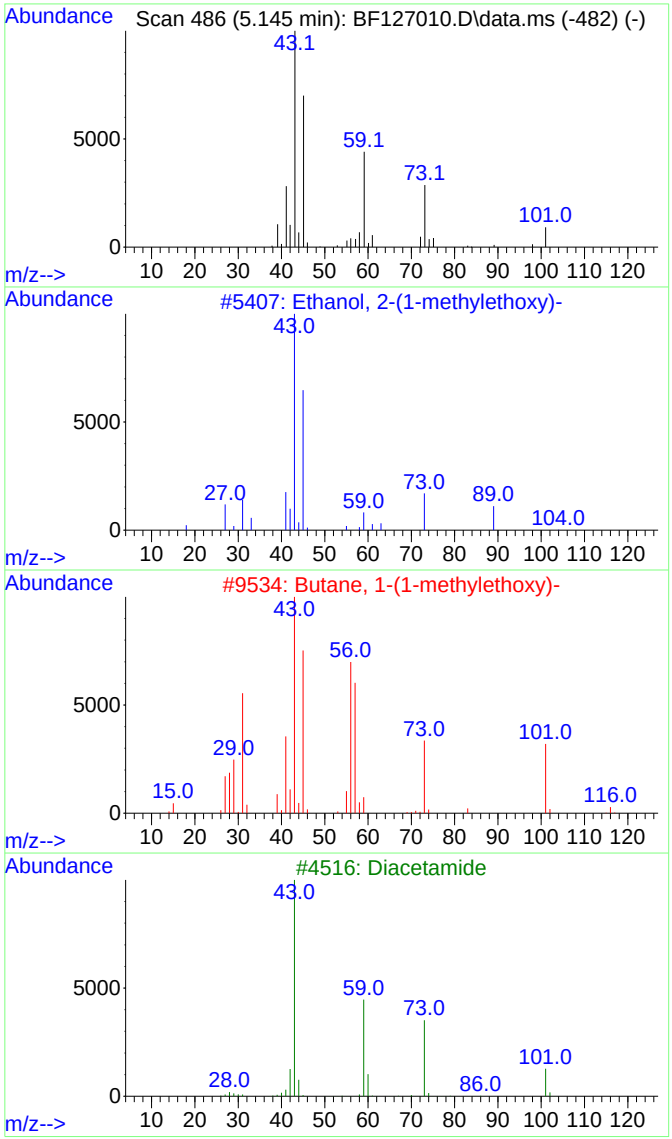
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

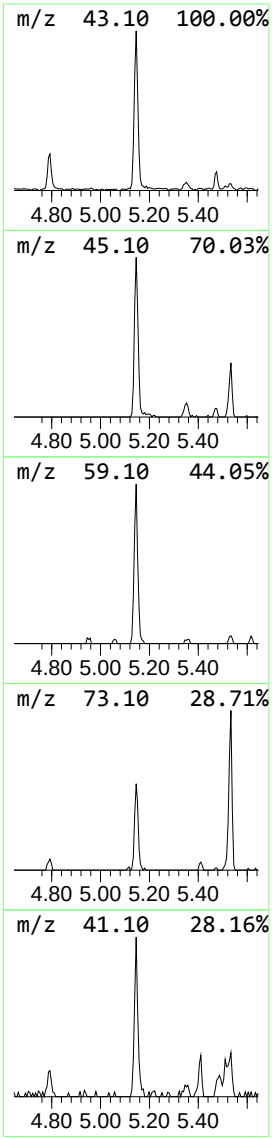
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(1-methylethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.145	3.51 ng	94154	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	53
2	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	53
3	Diacetamide	101	C4H7NO2	000625-77-4	50
4	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	47
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	42





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-1

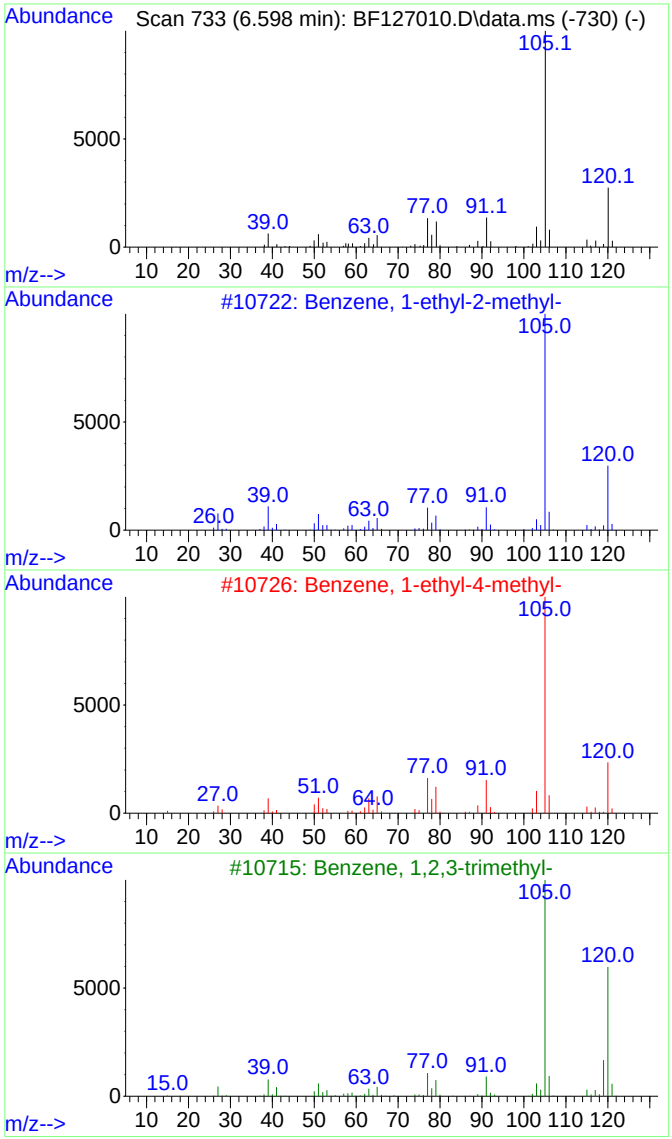
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

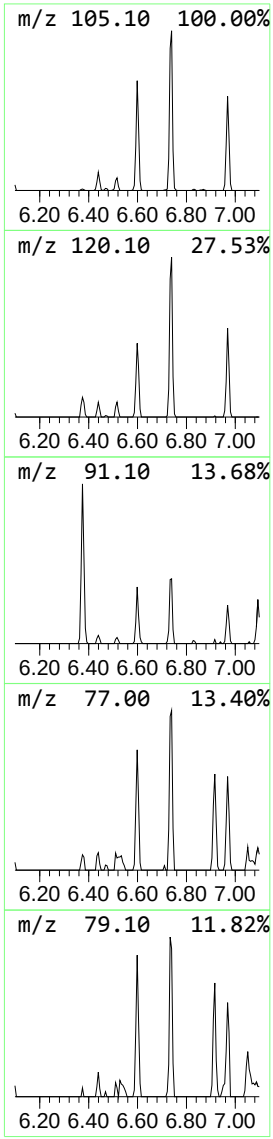
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	2.79 ng	74705	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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Acq On : 22 Feb 2022 15:55
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Sample : N1599-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

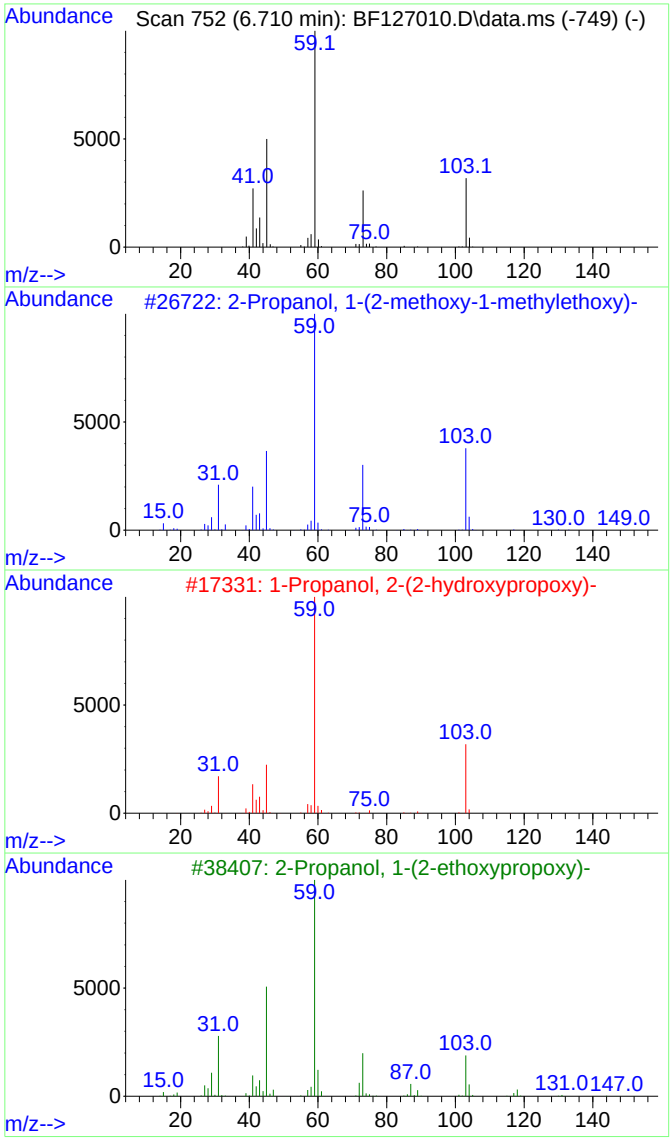
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

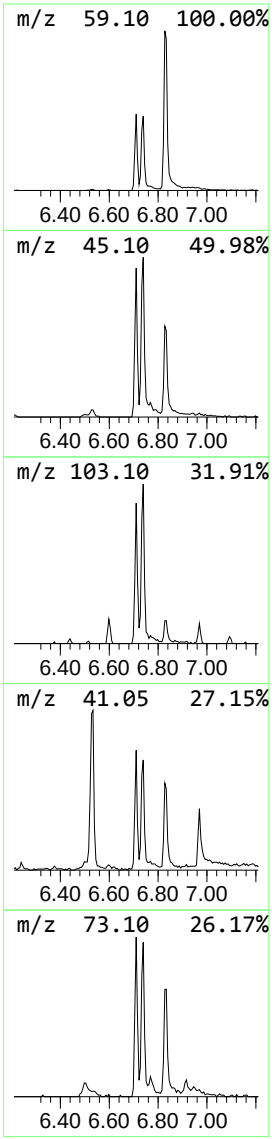
****

Peak Number 5 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.710	5.25 ng	140634	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	80
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
3	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	56
4	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	50





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Sample : N1599-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

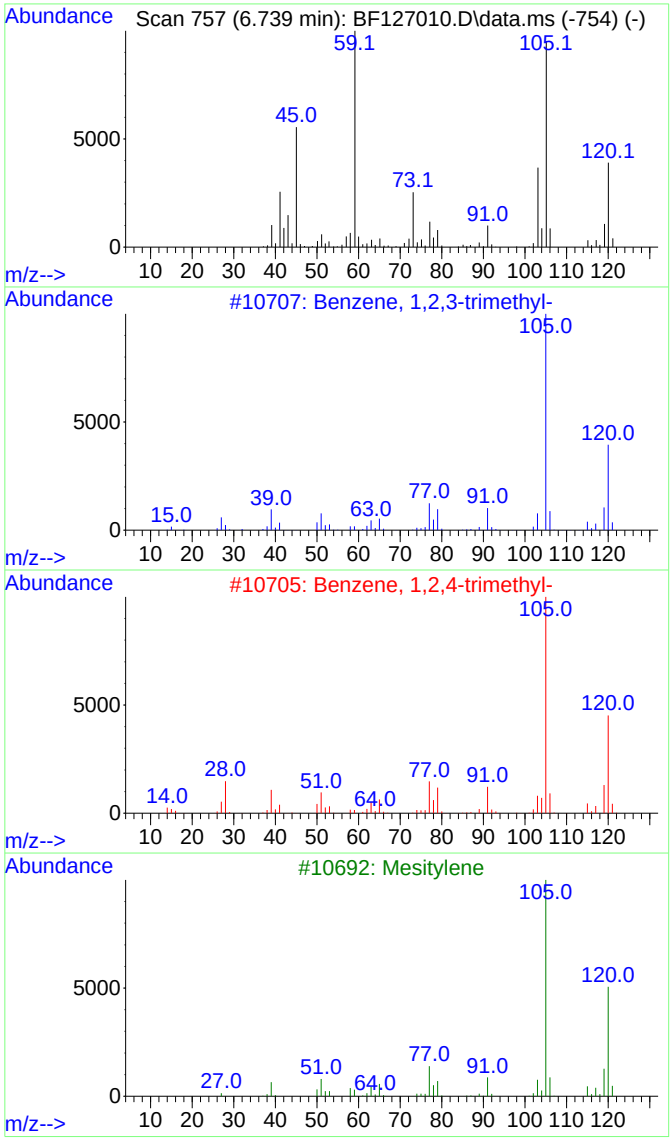
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

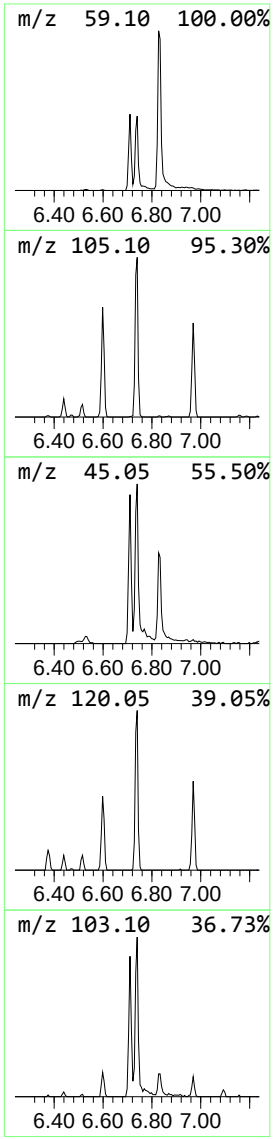
****

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.739	10.36 ng	277764	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	70
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	60
3	Mesitylene	120	C9H12	000108-67-8	38
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	35
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	35





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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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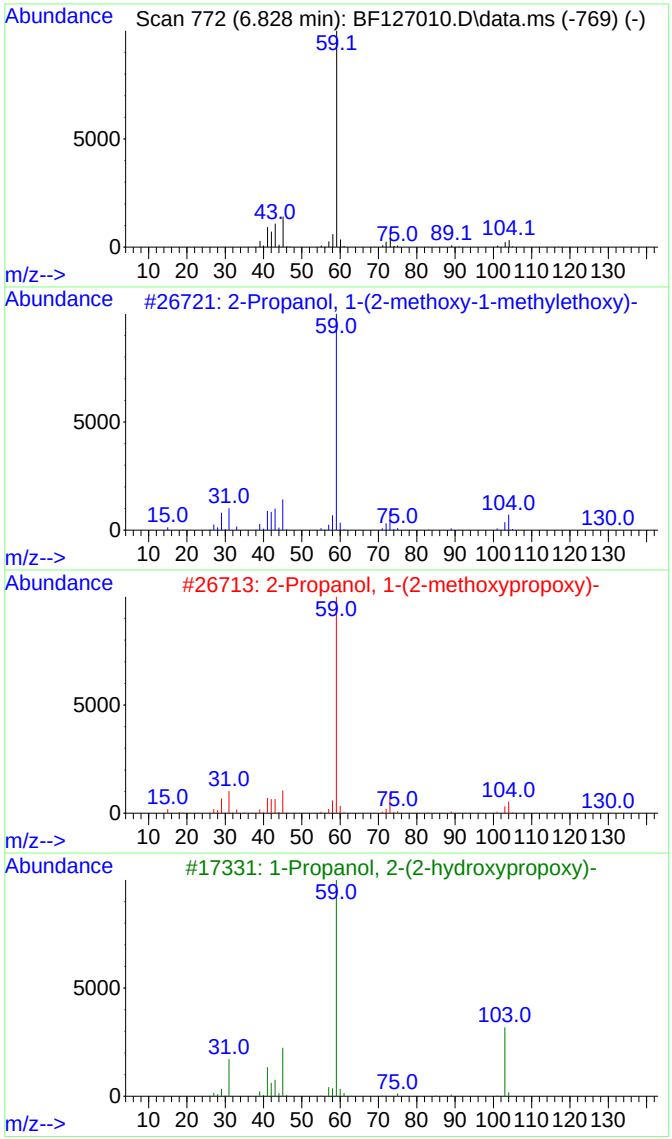
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

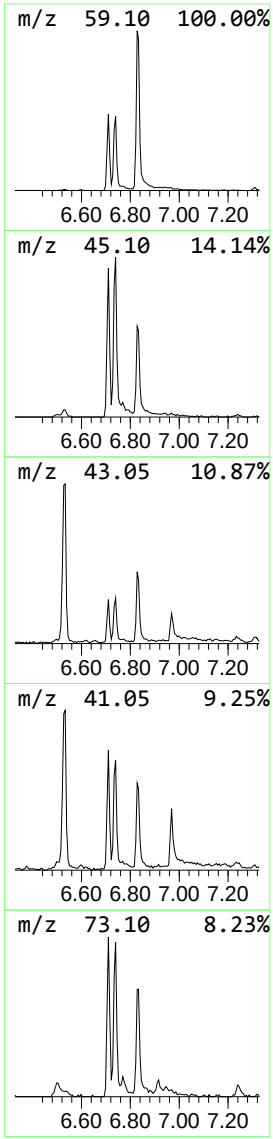
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Propanol, 1-(2-methoxypro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.828	9.32 ng	249681	1,4-Dichlorobenzene-d4	6.916

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-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	78
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	78





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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TIC Library : C:\Database\NIST20.L
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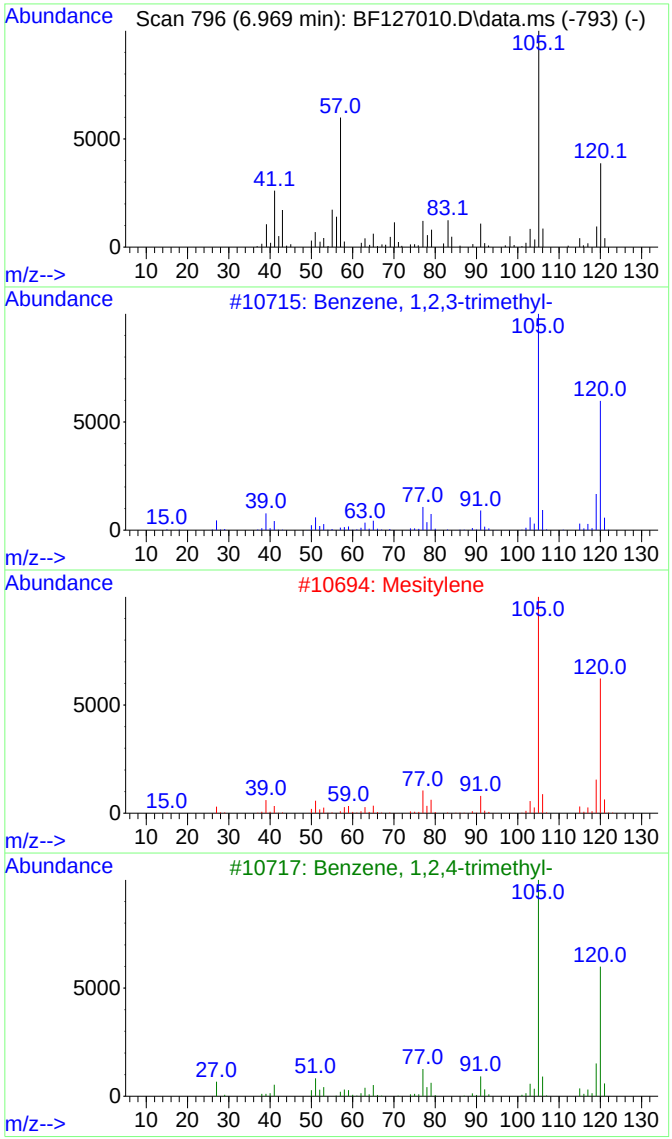
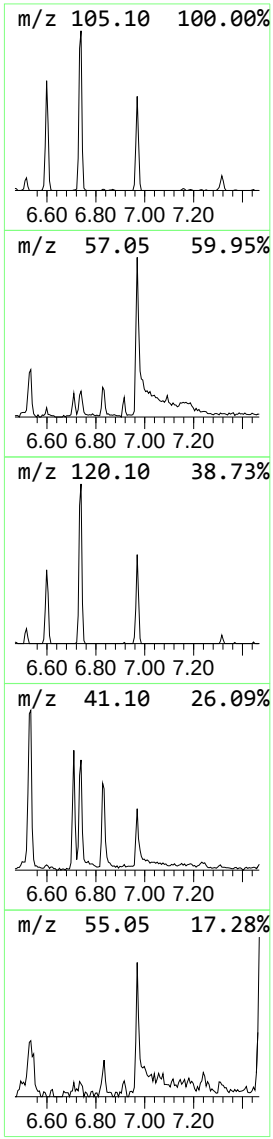
Peak Number 8 Mesitylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.969	4.87 ng	130615	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
2	Mesitylene	120	C9H12	000108-67-8	93
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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TIC Library : C:\Database\NIST20.L
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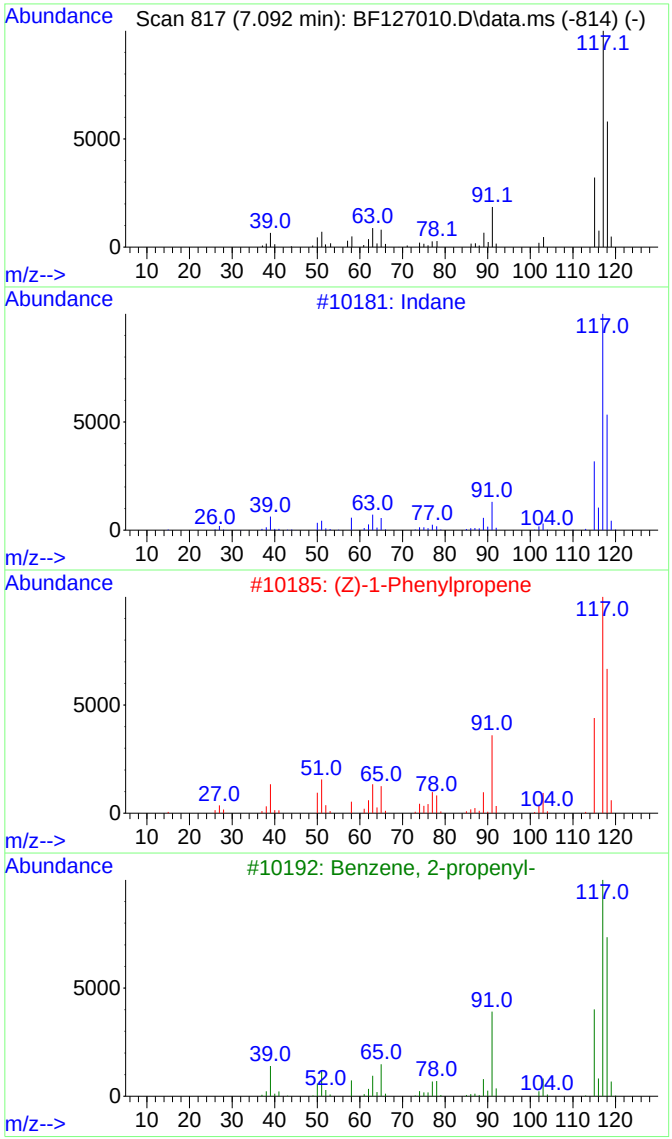
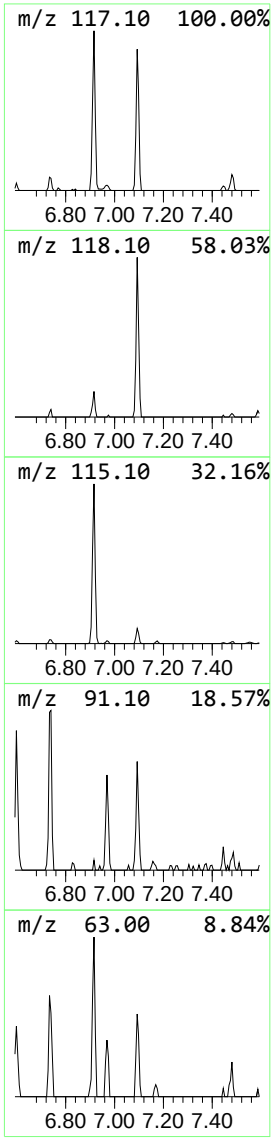
Peak Number 9 Indane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.092	2.07 ng	55596	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	87
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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TIC Library : C:\Database\NIST20.L
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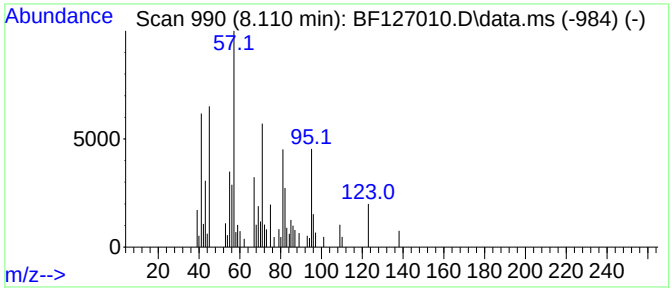
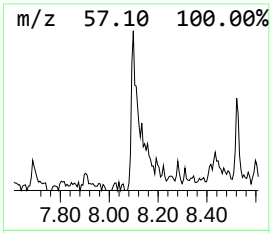
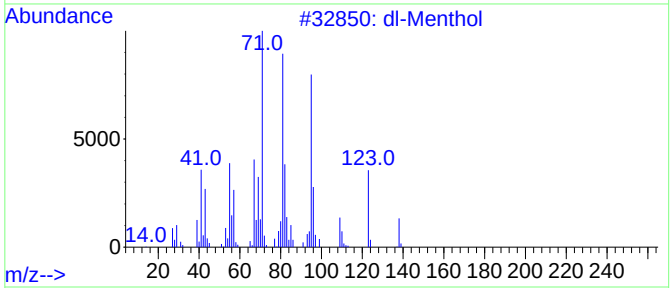
Peak Number 10 unknown8.110 Concentration Rank 12

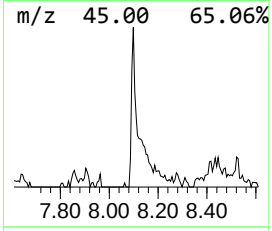
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	2.24 ng	81876	Naphthalene-d8	8.198

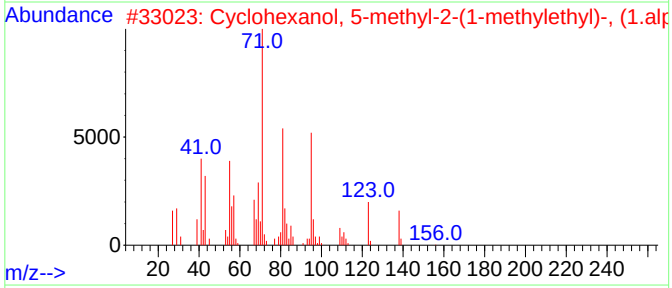
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-Menthol	156	C10H20O	000089-78-1	47
2	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	003623-52-7	38
3	Ether, 1-hexadecenyl methyl	254	C17H34O	015519-14-9	35
4	9-Decen-1-ol, methyl ether	170	C11H22O	1000352-65-1	35
5	Ethanone, 1-bicyclo[2.2.1]hept-2...	138	C9H14O	000824-58-8	22

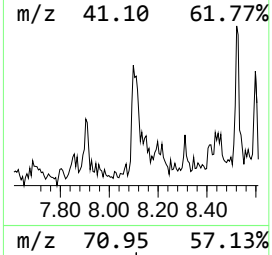


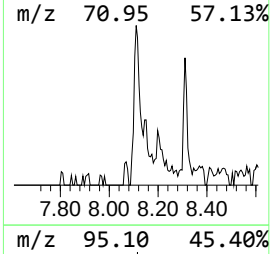


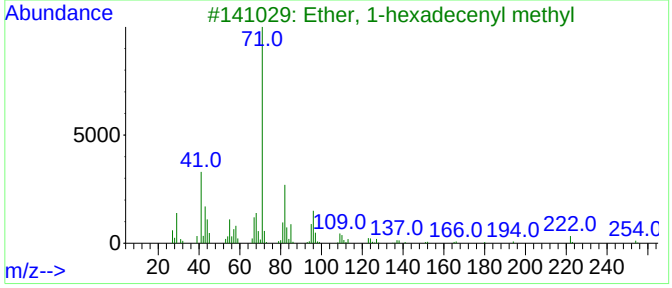


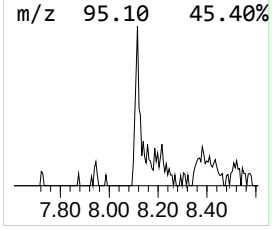












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022222\
Data File : BF127010.D
Acq On : 22 Feb 2022 15:55
Operator : CG\JU
Sample : N1599-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-1

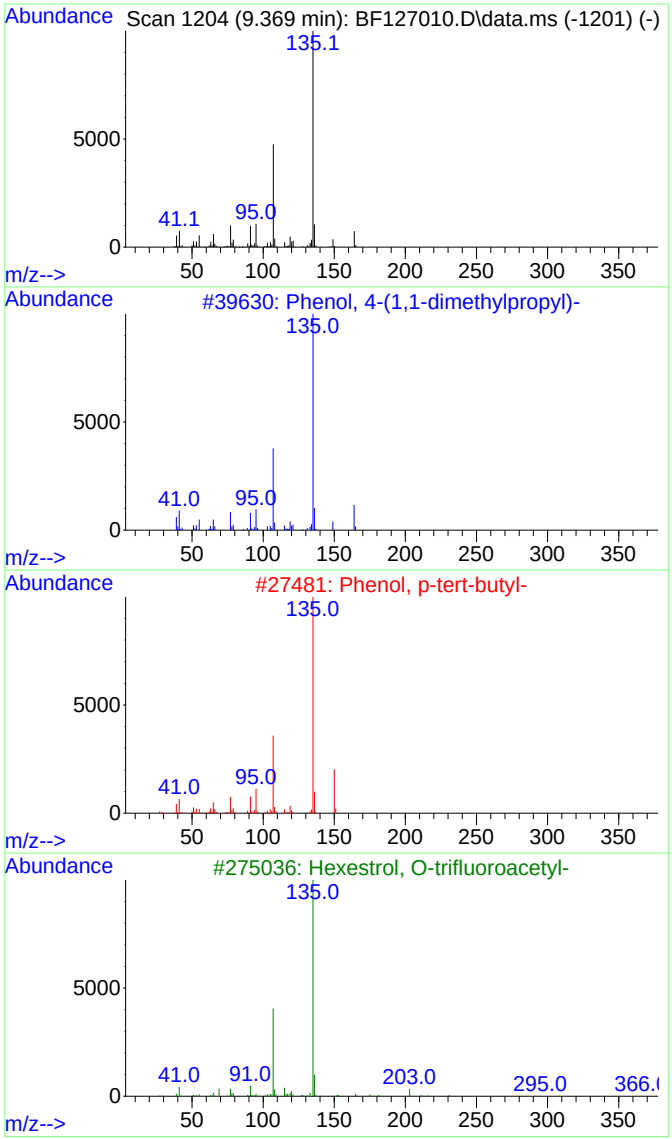
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

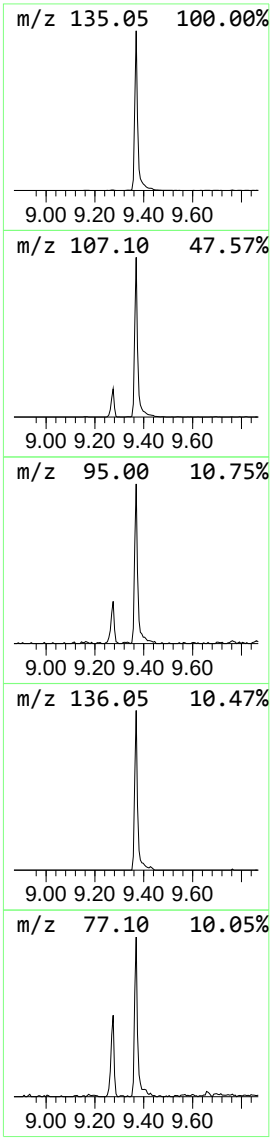
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.369	19.67 ng	760203	Acenaphthene-d10	9.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	72
4	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	72
5	Hexestrol	270	C18H22O2	000084-16-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022222\
Data File : BF127010.D
Acq On : 22 Feb 2022 15:55
Operator : CG\JU
Sample : N1599-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-1

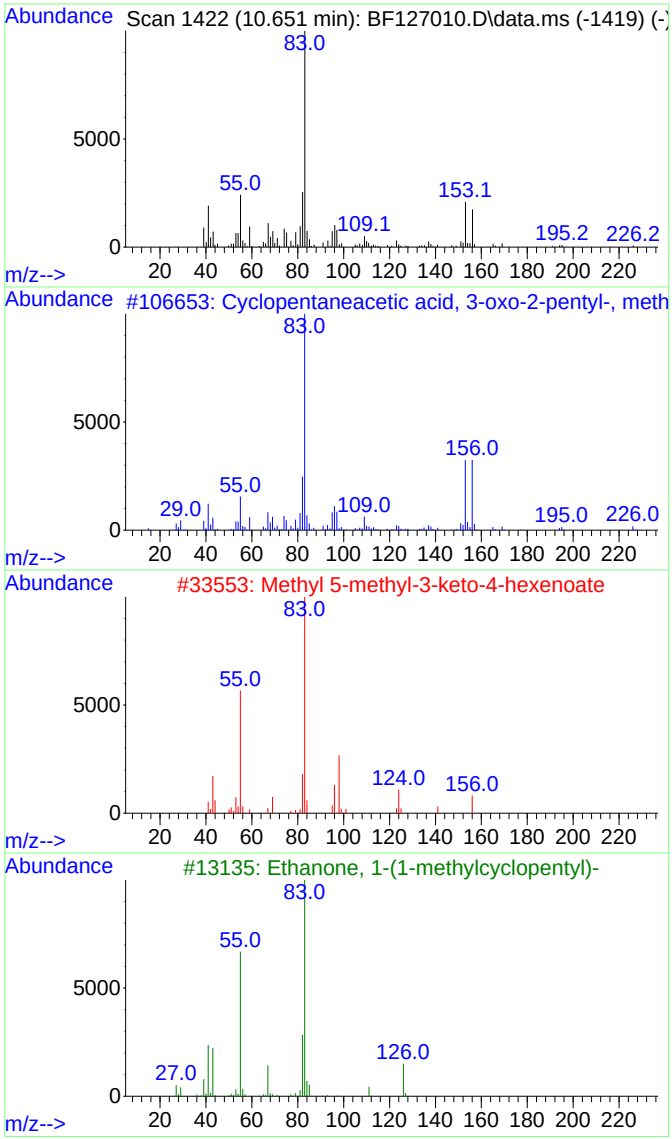
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

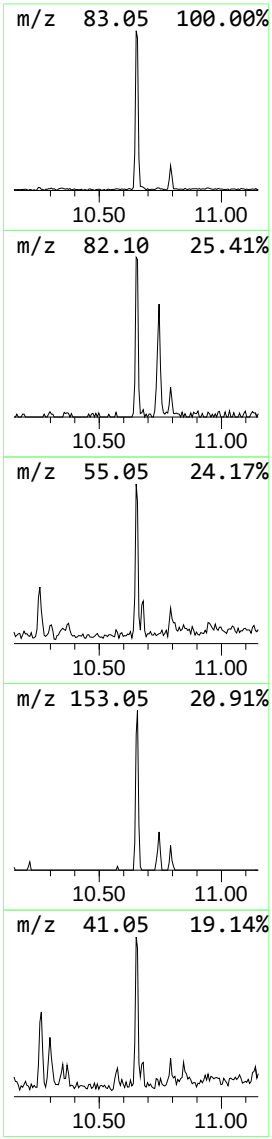
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Cyclopentaneacetic acid, 3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	3.45 ng	133191	Acenaphthene-d10	9.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	95
2	Methyl 5-methyl-3-keto-4-hexenoate	156	C8H12O3	1000427-08-8	50
3	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	47
4	Isocitronellol	156	C10H20O	018479-52-2	47
5	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022222\
Data File : BF127010.D
Acq On : 22 Feb 2022 15:55
Operator : CG\JU
Sample : N1599-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-1

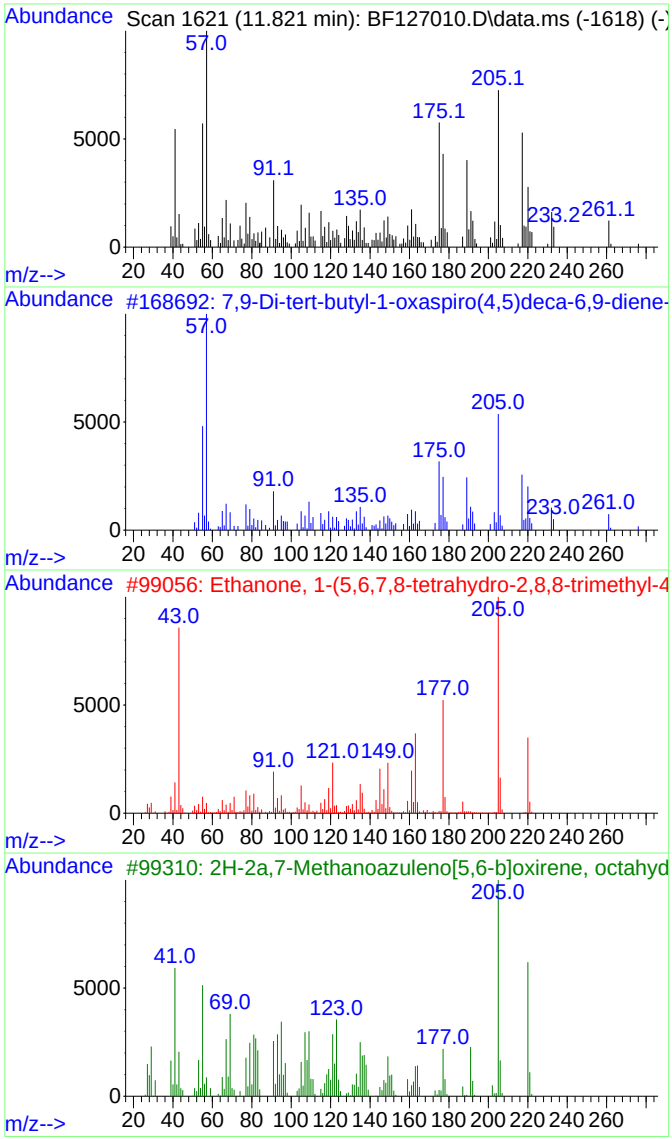
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

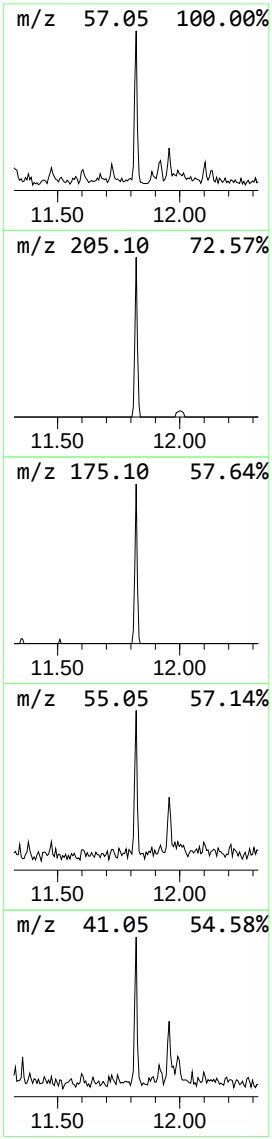
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.821	2.65 ng	106942	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50
3	2H-2a,7-Methanoazuleno[5,6-b]oxi...	220	C15H24O	029597-36-2	47
4	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	46
5	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022222\
Data File : BF127010.D
Acq On : 22 Feb 2022 15:55
Operator : CG\JU
Sample : N1599-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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	4.440	9.8	ng	262611	1	6.916	536079	20.0
Ethanol, 2-(1-m...	5.145	3.5	ng	94154	1	6.916	536079	20.0
Benzene, 1-ethy...	6.598	2.8	ng	74705	1	6.916	536079	20.0
2-Propanol, 1-(...	6.710	5.3	ng	140634	1	6.916	536079	20.0
Benzene, 1,2,3-...	6.739	10.4	ng	277764	1	6.916	536079	20.0
2-Propanol, 1-(...	6.828	9.3	ng	249681	1	6.916	536079	20.0
Mesitylene	6.969	4.9	ng	130615	1	6.916	536079	20.0
Indane	7.092	2.1	ng	55596	1	6.916	536079	20.0
unknown8.110	8.110	2.2	ng	81876	2	8.198	731283	20.0
Phenol, 4-(1,1-...	9.369	19.7	ng	760203	3	9.951	773026	20.0
Cyclopentaneace...	10.651	3.5	ng	133191	3	9.951	773026	20.0
7,9-Di-tert-but...	11.821	2.6	ng	106942	4	11.445	806498	20.0