LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129819.D
Acq On : 16 Aug 2022 19:43
Operator : CG\JU
Sample : N4198-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GFD-TOTES

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129819.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	465	468	478	rBV	590108	628601	1.12%	0.589%
2	5.469	537	541	564	rBV	2430273	3652887	6.50%	3.422%
3	6.140	649	655	658	rBV	3817153	4319478	7.68%	4.046%
4	6.263	672	676	687	rBV2	1026368	1299055	2.31%	1.217%
5	6.487	709	714	725	rBV2	810814	2286995	4.07%	2.142%
6	6.822	767	771	774	rBV	946911	882253	1.57%	0.826%
7	7.392	862	868	871	rBV	2574233	3080306	5.48%	2.886%
8	7.628	902	908	910	rBV	546420	751844	1.34%	0.704%
9	8.104	985	989	992	rVV	1370638	1310666	2.33%	1.228%
10	8.387	1018	1037	1039	rBV	13101441	56236508	100.00%	52.681%
11	8.469	1045	1051	1053	rBV	8543811	10031722	17.84%	9.397%
12	8.487	1053	1054	1063	rVB	2718811	3154588	5.61%	2.955%
13	9.181	1166	1172	1175	rBV	5097002	4994252	8.88%	4.678%
14	9.245	1179	1183	1186	rBV	749531	824879	1.47%	0.773%
15	9.398	1205	1209	1212	rVB	1753734	1639737	2.92%	1.536%
16	9.857	1281	1287	1293	rBV2	1412312	1486923	2.64%	1.393%
17	10.657	1418	1423	1426	rBV	3469844	3152250	5.61%	2.953%
18	11.351	1537	1541	1544	rVB	1458200	1203933	2.14%	1.128%
19	12.827	1789	1792	1798	rVB	644961	658475	1.17%	0.617%
20	12.933	1806	1810	1813	rBV	4044283	3673012	6.53%	3.441%
21	13.998	1987	1991	1995	rBV	820911	713661	1.27%	0.669%
22	15.468	2236	2241	2246	rVB	621499	767437	1.36%	0.719%

Sum of corrected areas: 106749462

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
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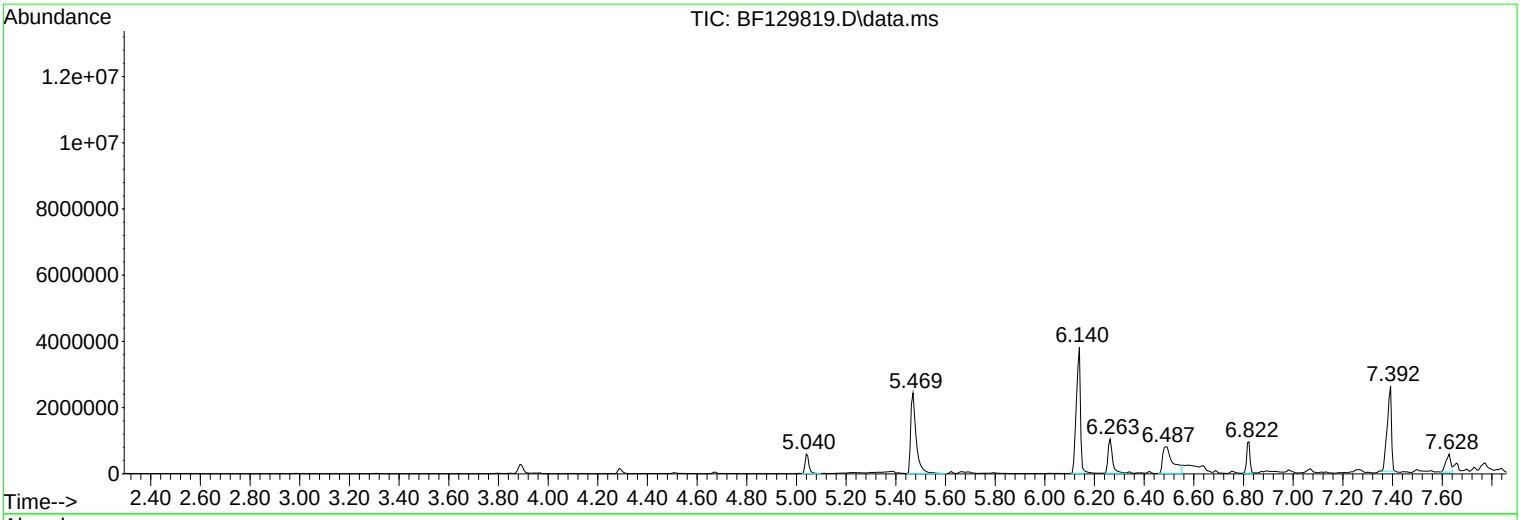
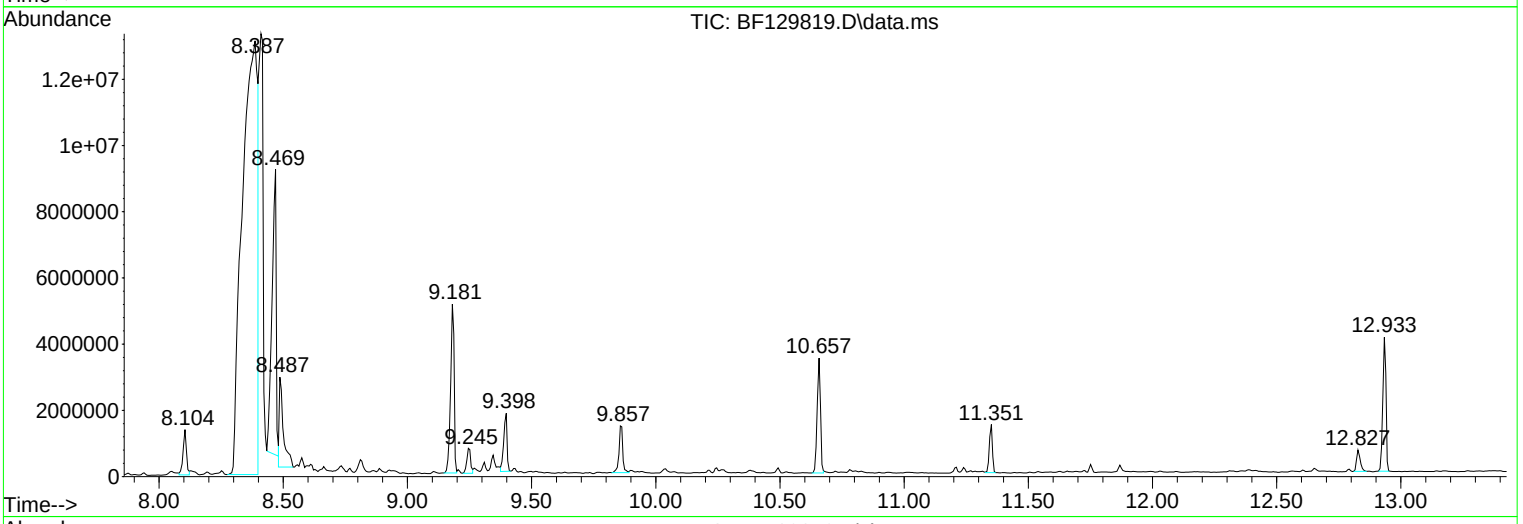
Misc :
ALS Vial : 8 Sample Multiplier: 1

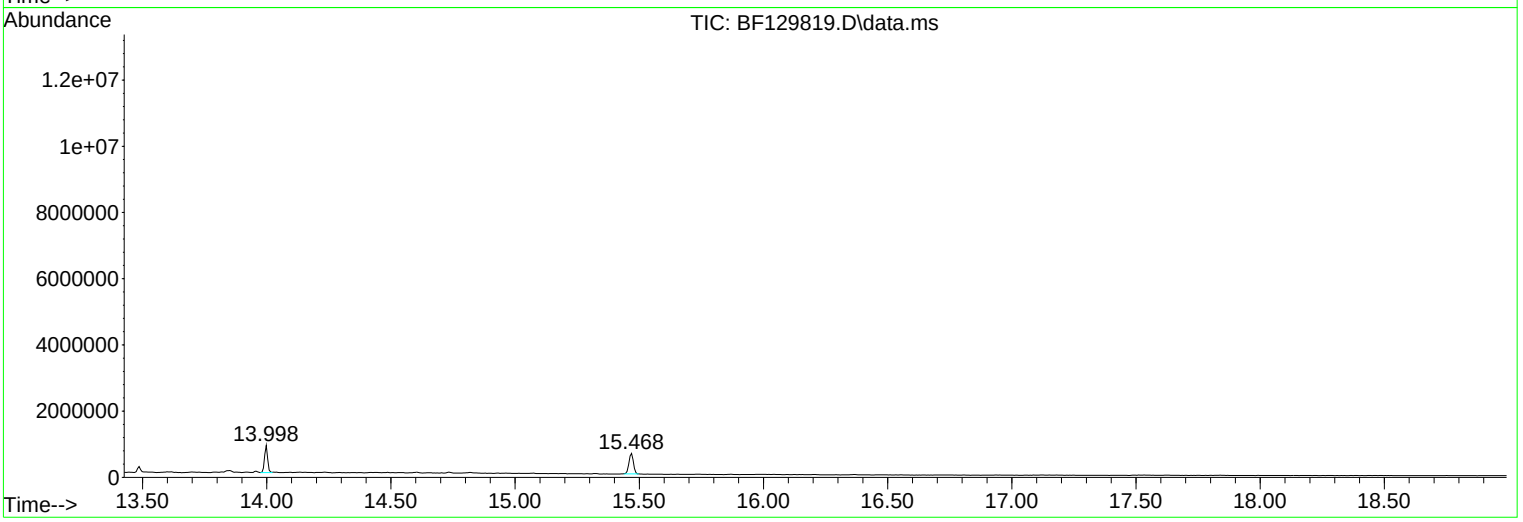
Instrument :
BNA_F
ClientSampleId :
GFD-TOTES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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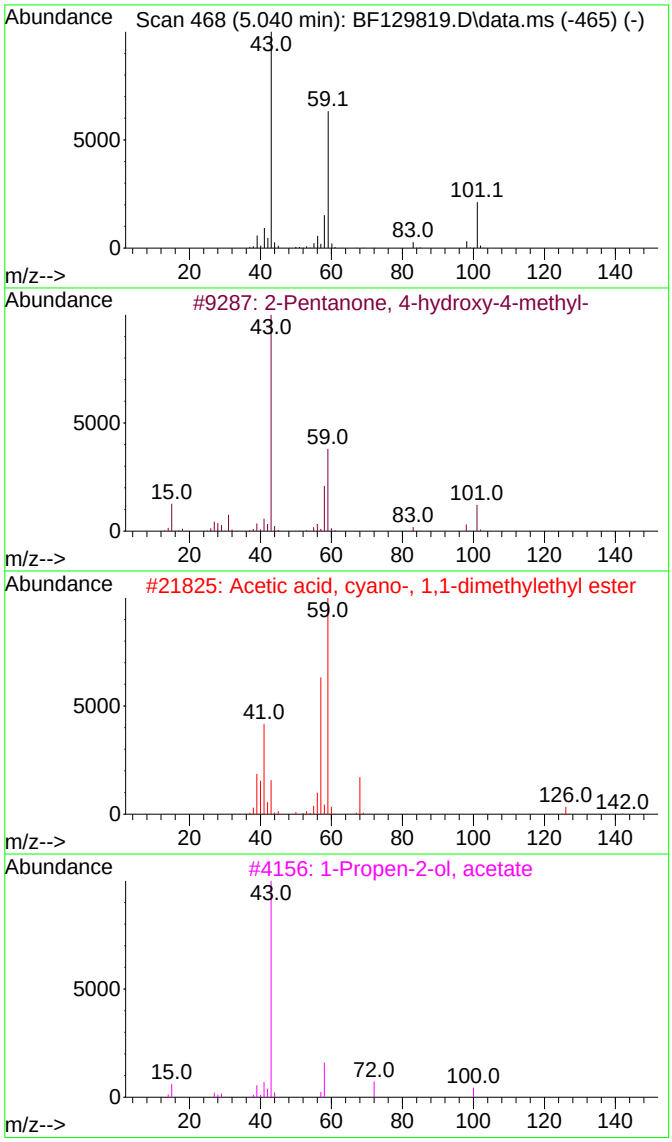
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

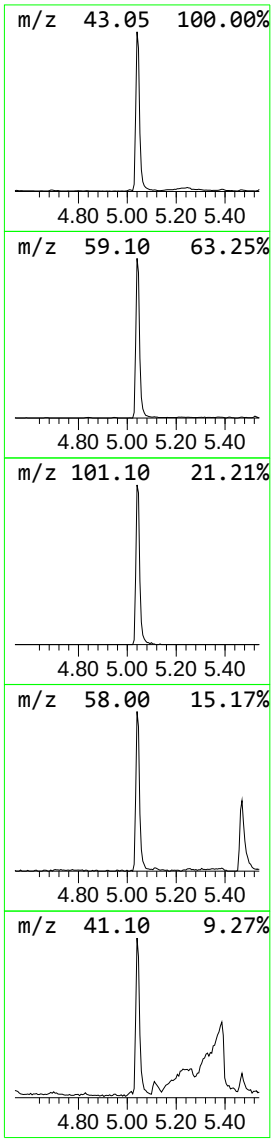
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	14.25 ng	628601	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Data File : BF129819.D
Acq On : 16 Aug 2022 19:43
Operator : CG\JU
Sample : N4198-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GFD-TOTES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

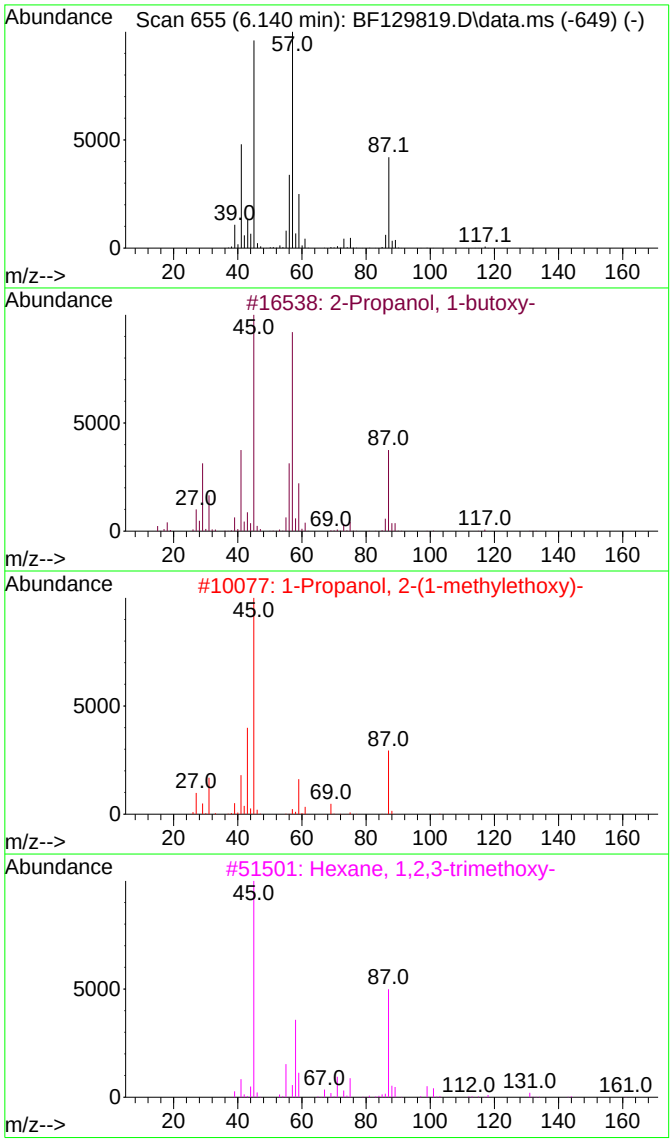
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

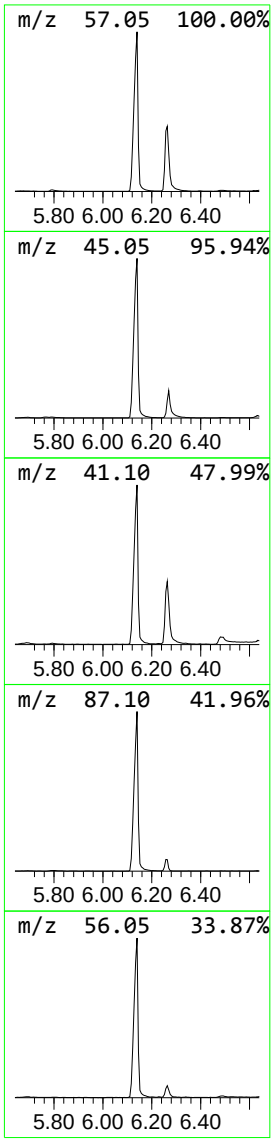
****

Peak Number 2 2-Propanol, 1-butoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.140	97.92 ng	4319480	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	59
3	Hexane, 1,2,3-trimethoxy-	176	C9H20O3	020637-29-0	50
4	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	50
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42





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Operator : CG\JU
Sample : N4198-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GFD-TOTES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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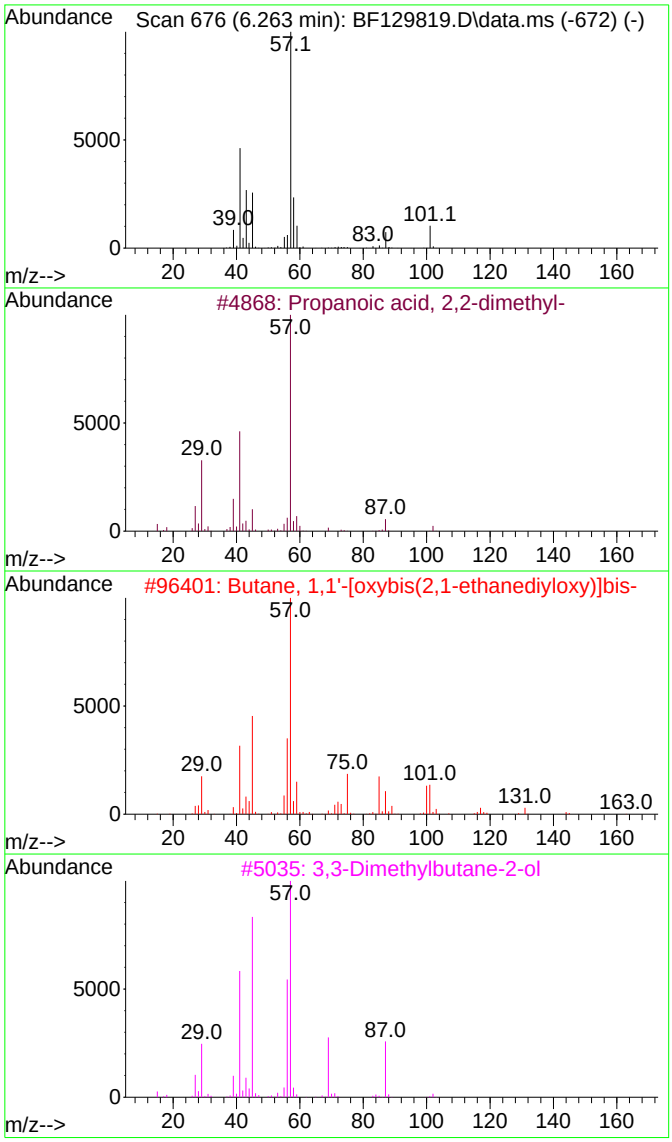
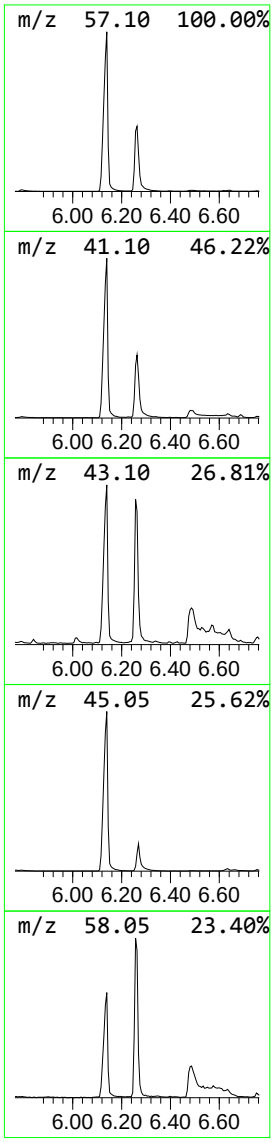
Peak Number 3 unknown6.263 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.263	29.45 ng	1299060	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	47
2	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	25
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	10
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	9
5	2-Butanone, 3,3-dimethyl-1-thioc...	157	C7H11NOS	057518-71-5	9





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GFD-TOTES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

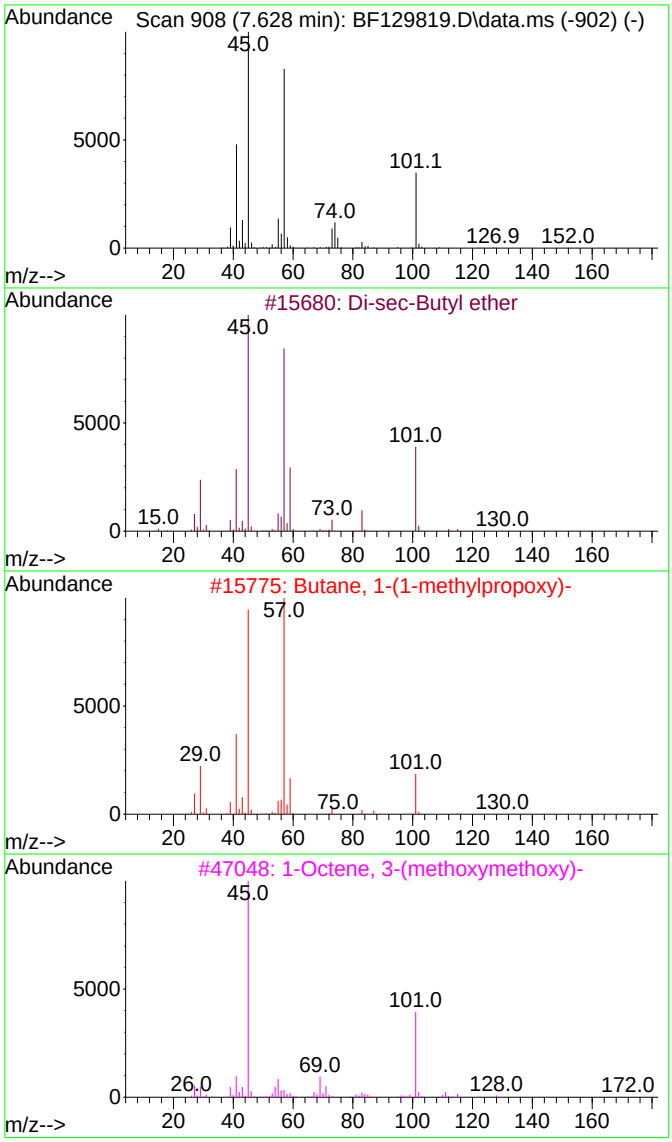
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

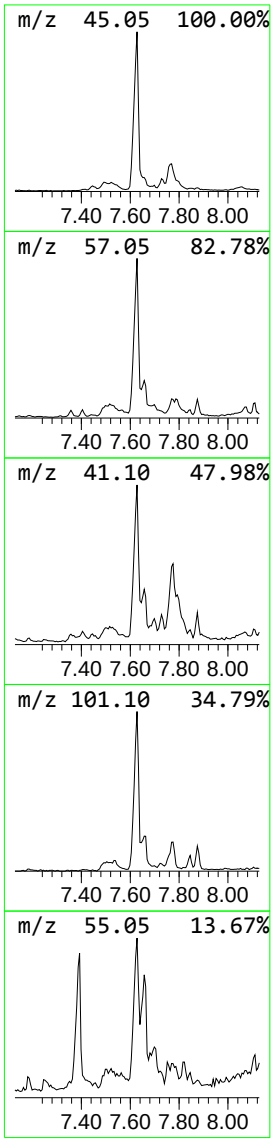
****

Peak Number 4 Di-sec-Butyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.628	11.47 ng	751844	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	72
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	72
3	1-Octene, 3-(methoxymethoxy)-	172	C10H20O2	088738-34-5	40
4	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	38
5	Methyl propyl ether	74	C4H10O	000557-17-5	38





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Data File : BF129819.D
Acq On : 16 Aug 2022 19:43
Operator : CG\JU
Sample : N4198-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GFD-TOTES

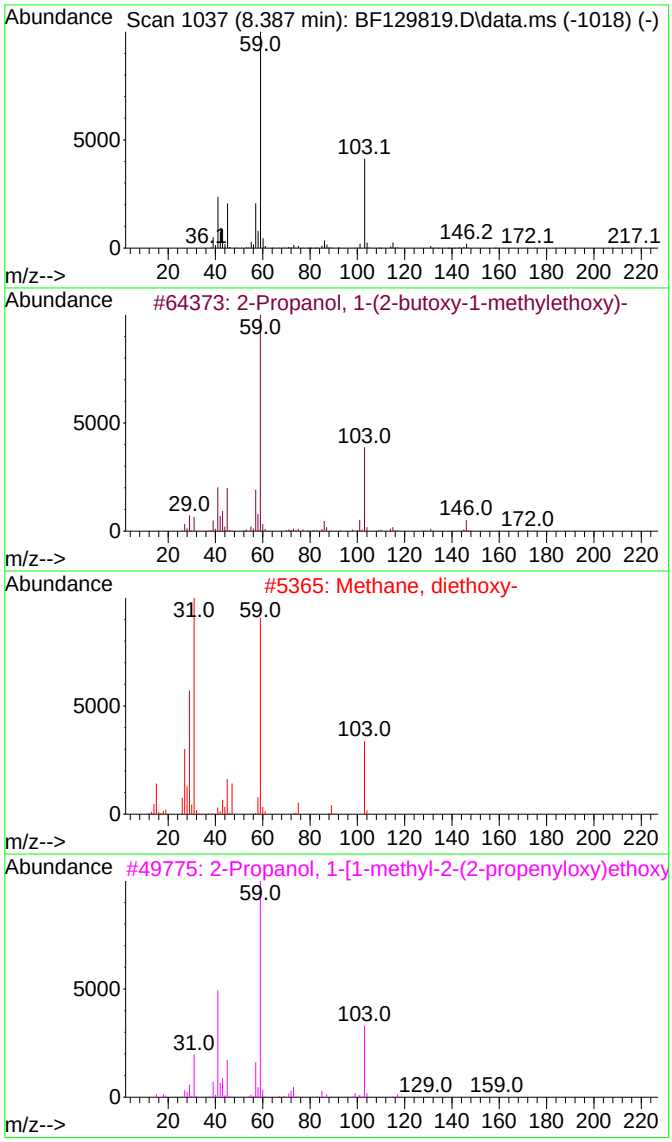
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

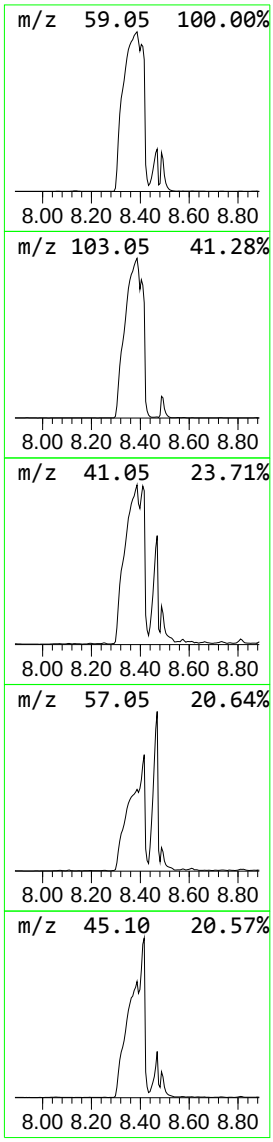
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.387	858.14 ng	56236500	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	83
2	Methane, diethoxy-	104	C5H12O2	000462-95-3	80
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
5	Propane, 1,1-diethoxy-	132	C7H16O2	004744-08-5	72





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ClientSampleId :
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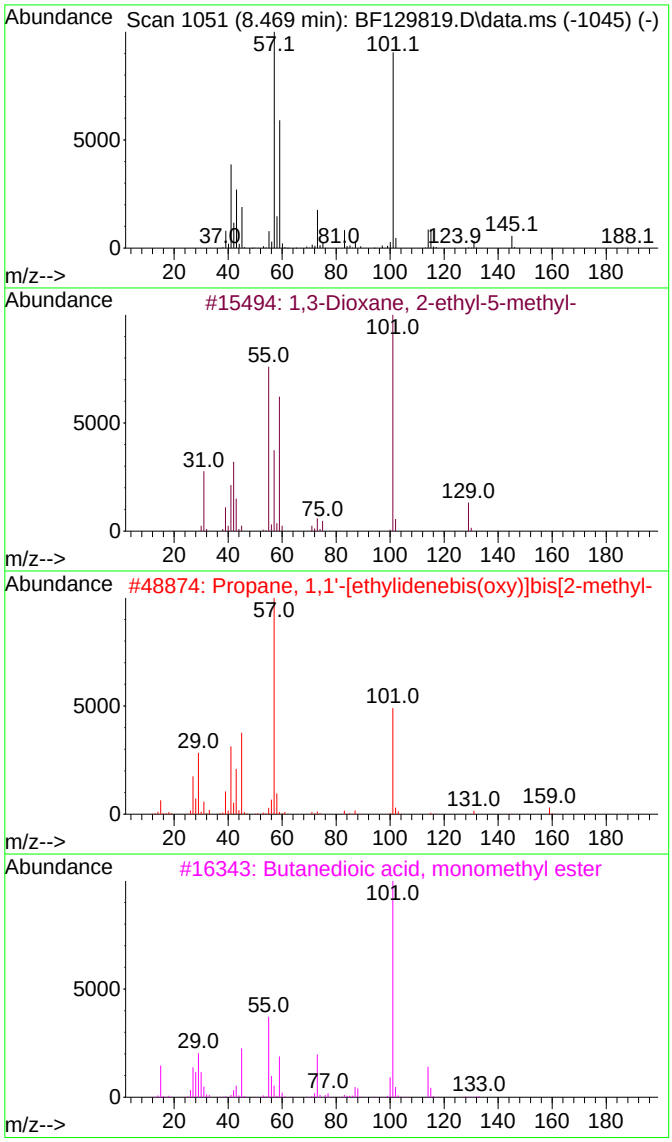
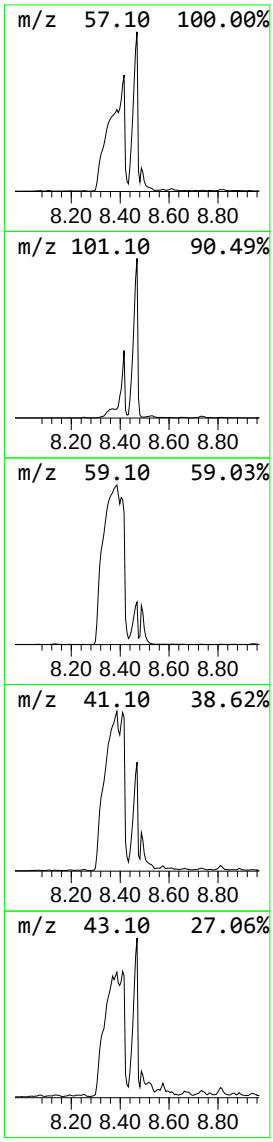
****

Peak Number 6 1,3-Dioxane, 2-ethyl-5-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	153.08 ng	10031700	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-ethyl-5-methyl-	130	C7H14O2	020627-54-7	59
2	Propane, 1,1'-[ethylidenebis(oxy...	174	C10H22O2	005669-09-0	50
3	Butanedioic acid, monomethyl ester	132	C5H8O4	003878-55-5	49
4	Propanedioic acid, dimethyl ester	132	C5H8O4	000108-59-8	45
5	Adipic acid, di(4-methoxy-2-meth...	346	C18H34O6	1000324-30-7	37





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ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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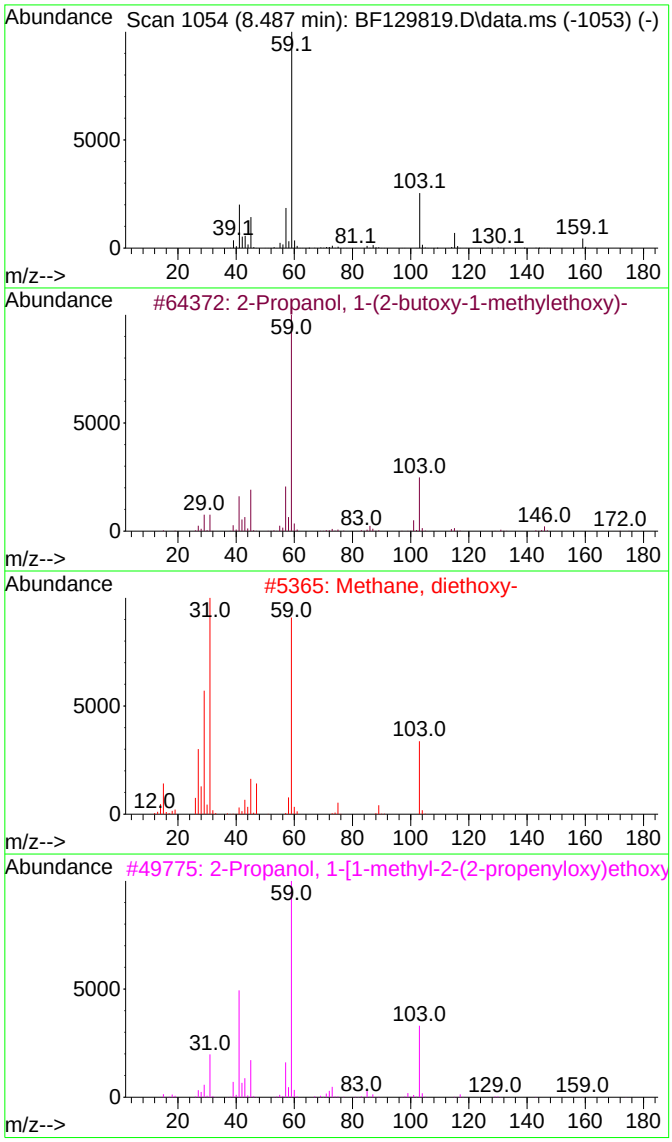
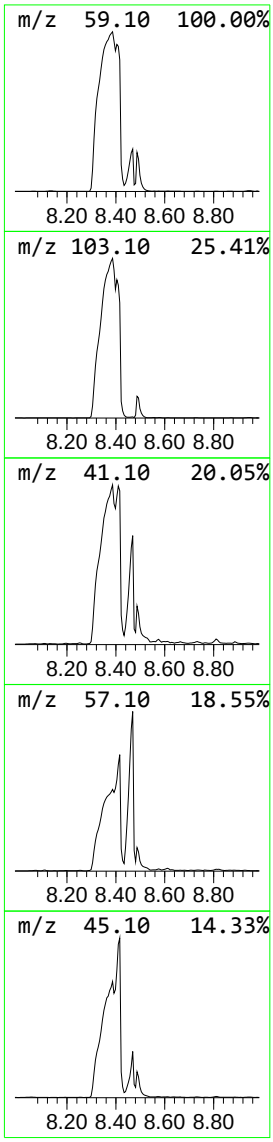
****

Peak Number 7 Methane, diethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.487	48.14 ng	3154590	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	78
2	Methane, diethoxy-	104	C5H12O2	000462-95-3	72
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
4	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1010367-13-4	59
5	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	59





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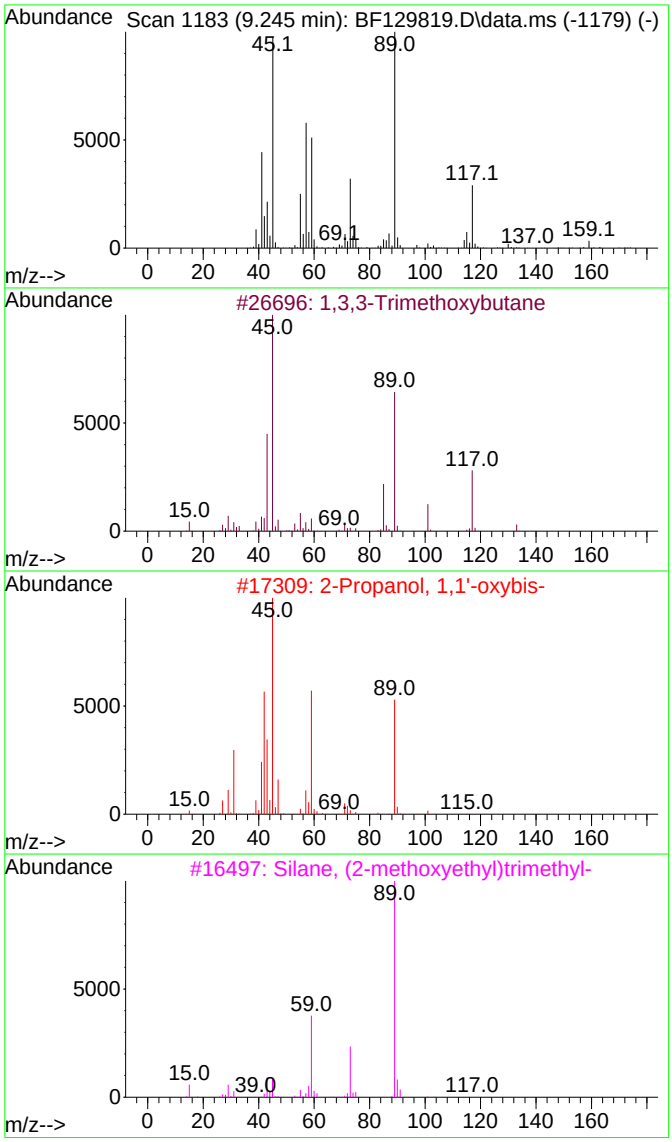
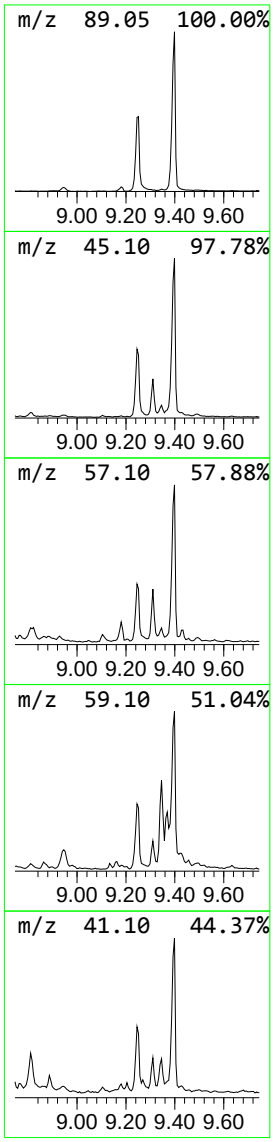
****

Peak Number 8 1,3,3-Trimethoxybutane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.245	11.10 ng	824879	Acenaphthene-d10	9.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,3-Trimethoxybutane	148	C7H16O3	006607-66-5	56
2	2-Propanol, 1,1'-oxybis-	134	C6H14O3	000110-98-5	50
3	Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	45
4	Allyl(methoxy)dimethylsilane	130	C6H14OSi	030535-30-9	45
5	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129819.D
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Operator : CG\JU
Sample : N4198-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GFD-TOTES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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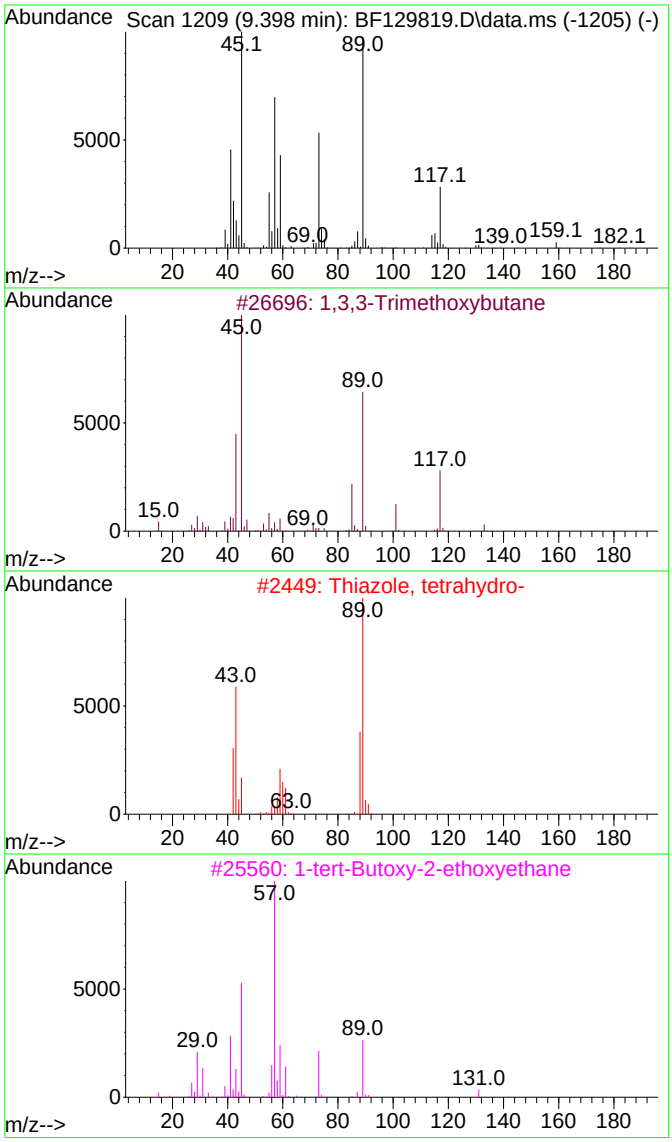
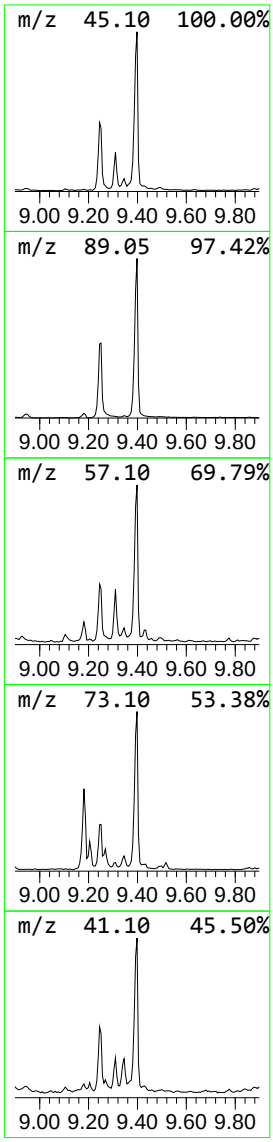
Peak Number 9 Thiazole, tetrahydro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.398	22.06 ng	1639740	Acenaphthene-d10	9.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,3-Trimethoxybutane	148	C7H16O3	006607-66-5	64
2	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	53
3	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	43
4	15-Crown-5	220	C10H20O5	033100-27-5	38
5	2-Methoxyethanol, TMS derivative	148	C6H16O2Si	018173-74-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129819.D
Acq On : 16 Aug 2022 19:43
Operator : CG\JU
Sample : N4198-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GFD-TOTES

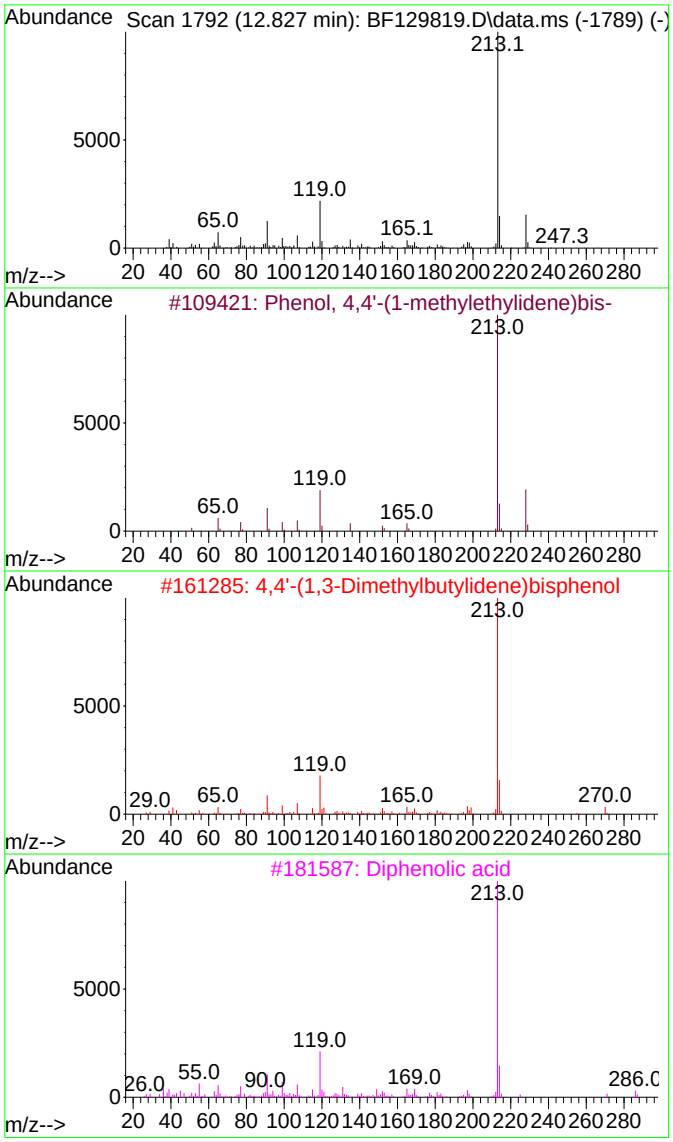
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

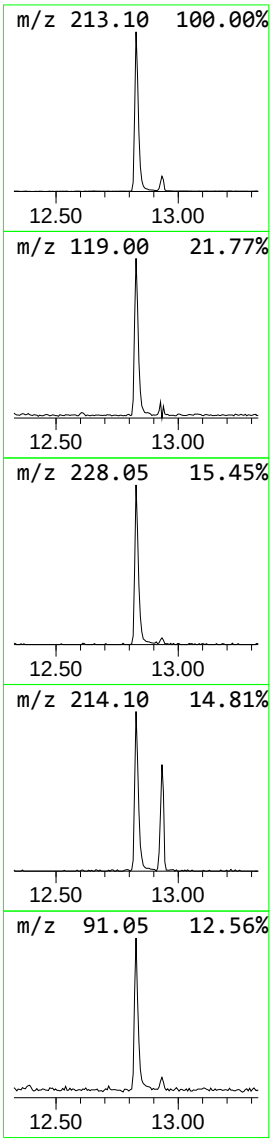
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.827	18.45 ng	658475	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	74
3	Diphenolic acid	286	C17H18O4	000126-00-1	64
4	3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	60
5	3-Cyano-4-ethyl-6-methylcoumarin	213	C13H11NO2	025937-11-5	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129819.D
Acq On : 16 Aug 2022 19:43
Operator : CG\JU
Sample : N4198-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GFD-TOTES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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
2-Pentanone, 4-...	5.040	14.3	ng	628601	1	6.822	882253	20.0
2-Propanol, 1-b...	6.140	97.9	ng	4319480	1	6.822	882253	20.0
unknown6.263	6.263	29.4	ng	1299060	1	6.822	882253	20.0
Di-sec-Butyl ether	7.628	11.5	ng	751844	2	8.104	1310670	20.0
2-Propanol, 1-(...	8.387	858.1	ng	56236500	2	8.104	1310670	20.0
1,3-Dioxane, 2-...	8.469	153.1	ng	10031700	2	8.104	1310670	20.0
Methane, diethoxy-	8.487	48.1	ng	3154590	2	8.104	1310670	20.0
1,3,3-Trimethox...	9.245	11.1	ng	824879	3	9.863	1486920	20.0
Thiazole, tetra...	9.398	22.1	ng	1639740	3	9.863	1486920	20.0
Phenol, 4,4'-(1...	12.827	18.4	ng	658475	5	13.998	713661	20.0